Lecture Notes in Quantum Mechanics

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These are the lecture notes of the quantum mechanics courses that were given by DC at Ben-Gurion University during 2005. They cover undergraduate textbook topics (e.g. as in Sakurai), and also additional advanced topics at the same level of presentation.

The topics that are covered are:

Fundamentals:

- The classical description of a particle
- Hilbert space formalism
- A particle in an N site system
- The continuum limit ($N = \infty$)
- Translations and rotations

- The fundamental postulates of the theory

- The evolution operator
- The rate of change formula
- Finding the Hamiltonian for a physical system
- The non-relativistic Hamiltonian
- The "classical" equation of motion
- Symmetries and constants of motion

- Group theory, Lie algebra
- Representations of the rotation group
- Spin 1/2, spin 1 and $Y_{\ell,m}$
- Multiplying representations
- Addition of angular momentum (*)
- The Galilei group (*)
- Transformations and invariance (*)

Quantum mechanics in practice:

- The dynamics of a two level system
- Fermions and Bosons
- Decay into the continuum
- The Aharonov-Bohm effect
- Magnetic field (Landau levels, Hall effect)
- The dynamics of a particle with spin 1/2
- Motion in a central potential
- Implications of having "spin" on the dynamics

Approximations:

- Perturbation theory for eigenstates
- Example: ring with scatterer and flux
- Beyond 1st order: Wigner Lorentzian

Dynamics and driven systems

- Systems with driving
- The interaction picture
- The transition probability formula
- Fermi golden rule
- Cross sections and Born formula

- The adiabatic equation
- The Berry phase
- Theory of adiabatic transport (*)
- Linear response theory and Kubo (*)
- The Born-Oppenheimer picture (*)

The Green function approach (*)

- The evolution operator
- Feynman path integral
- The resolvent and the Green function

- Perturbation theory for the resolvent
- Perturbation theory for the propagator
- Complex poles from perturbation theory

Scattering theory (*)

- Scattering: T matrix formalism
- Scattering: S matrix formalism
- Scattering: R matrix formalism
- Cavity with leads 'mesoscopic' geometry
- Spherical geometry, phase shifts
- Cross section, optical theorem, resonances

Special Topics (*)

- Quantization of the EM field
- Fock space formalism

- The Wigner Weyl formalism
- Theory of quantum measurements
- Theory of quantum computation

(*) Not included in the undergraduate course.

Opening remarks

These lecture notes are based on 3 courses in non-relativistic quantum mechanics that are given at BGU: "Quantum 2" (undergraduates), "Quantum 3" (graduates), and "Advanced topics in Quantum and Statistical Mechanics" (graduates). The lecture notes are self contained, and give the *road map* to quantum mechanics. However, they do not intend to come instead of the standard textbooks. In particular I recommend:

[1] L.E.Ballentine, Quantum Mechanics (library code: QC 174.12.B35).

[2] J.J. Sakurai, Modern Quantum mechanics (library code: QC 174.12.S25).

[3] Feynman Lectures Volume III.

[4] A. Messiah, Quantum Mechanics. [for the graduates]

The major attempt in this set of lectures was to give a self contained presentation of quantum mechanics, *which is not based on the historical "quantization" approach*. The main inspiration comes from Ref.[3] and Ref.[1]. The challenge was to find a compromise between the over-heuristic approach of Ref.[3] and the too formal approach of Ref.[1].

Another challenge was to give a presentation of scattering theory that goes well beyond the common undergraduate level, but still not as intimidating as in Ref.[4]. A major issue was to *avoid the over emphasis on spherical geometry*. The language that I use is much more suitable for research with "mesoscopic" orientation.

Credits

Drafts of these lecture notes were prepared and submitted by students on a weekly basis. Undergraduate students were requested to use HTML with ITEX formulas. Typically the text was written in Hebrew. Graduates were requested to use Latex. The drafts were corrected, integrated, and in many cases completely re-written by the lecturer. The English version of the "Quantum 2" sections was prepared by *Gilad Rosenberg*. He has also prepared the illustrations.

The present version is quite remote from the original drafts, but still I find it appropriate to list the names of the students who have participated: Natalia Antin, Roy Azulai, Dotan Babai, Shlomi Batsri, Ynon Ben-Haim, Avi Ben Simon, Asaf Bibi, Lior Blockstein, Lior Boker, Shay Cohen, Liora Damari, Anat Daniel, Ziv Danon, Barukh Dolgin, Anat Dolman, Lior Eligal, Yoav Etzioni, Zeev Freidin, Eyal Gal, Ilya Gurwich, David Hirshfeld, Daniel Horowitz, Eyal Hush, Liran Israel, Avi Lamzy, Roi Levi, Danny Levy, Asaf Kidron, Ilana Kogen, Roy Liraz, Arik Maman, Rottem Manor, Nitzan Mayorkas, Vadim Milavsky, Igor Mishkin, Dudi Morbachik, Ariel Naos, Yonatan Natan, Idan Oren, David Papish, Smadar Reick Goldschmidt, Alex Rozenberg, Chen Sarig, Adi Shay, Dan Shenkar, Idan Shilon, Asaf Shimoni, Raya Shindmas, Ramy Shneiderman, Elad Shtilerman, Eli S. Shutorov, Ziv Sobol, Jenny Sokolevsky, Alon Soloshenski, Tomer Tal, Oren Tal, Amir Tzvieli, Dima Vingurt, Tal Yard, Uzi Zecharia, Dany Zemsky, Stanislav Zlatopolsky.

Warning

This is the first version. It may contain typos.

Contents

Fundamentals (part I)

[1] Introduction

[1.1] The Building Blocks of the Universe

The world we live in consists of a variety of particles which are described by the "standard model". The known particles are divided into two groups:

- Quarks: constituents of the proton and the neutron, which form the ~ 100 nuclei known to us.
- Leptons: include the electrons, muons, taus, and the neutrinos.

In addition, the interaction between the particles is by way of fields (direct interaction between particles is contrary to the principles of the special theory of relativity). These interactions are responsible for the way material is "organized". The gravity field has yet to be incorporated into quantum theory. We will be concerned mostly with the electromagnetic interaction. The electromagnetic field is described by the Maxwell equations.

[1.2] What Happens to a Particle in an Electromagnetic Field?

Within the framework of classical electromagnetism, the electromagnetic field is described by the scalar potential $V(x)$ and the vector potential $\vec{A}(x)$. In addition one defines:

$$\begin{aligned} \mathcal{B} &= \nabla \times \frac{1}{c}\vec{A} \\ \mathcal{E} &= -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \nabla V \end{aligned} \tag{1}$$

We will not be working with natural units in this course, but form now on we are going to absorb the constants c and e in the definition of the scalar and vector potentials:

$$\begin{aligned} \frac{e}{c}A &\rightarrow A, & eV &\rightarrow V \\ \frac{e}{c}\mathcal{B} &\rightarrow \mathcal{B}, & e\mathcal{E} &\rightarrow \mathcal{E} \end{aligned} \tag{2}$$

In classical mechanics, the effect of the electromagnetic field is described by Newton's second law with the Lorentz force. Using the above units convention we write:

$$\ddot{x} = \frac{1}{\mathsf{m}}\left(\mathcal{E} - \mathcal{B} \times v\right) \tag{3}$$

The Lorentz force dependents on the velocity of the particle. This seems arbitrary and counter intuitive, but we shall see in the future how it can be derived from general and fairly simple considerations.

In analytical mechanics it is customary to derive the above equation from a Lagrangian. Alternatively, one can use a Legendre transform and derive the equations of motion from a Hamiltonian:

$$\begin{aligned} \dot{x} &= \frac{\partial \mathcal{H}}{\partial p} \\ \dot{p} &= -\frac{\partial \mathcal{H}}{\partial x} \end{aligned} \tag{4}$$

Where the Hamiltonian is:

$$\mathcal{H}(x,p) = \frac{1}{2\mathsf{m}}(p - A(x))^2 + V(x) \tag{5}$$

[1.3] Canonical Quantization

The historical method of deriving the quantum description of a system is canonical quantization. In this method we assume that the particle is described by a "wave function" that fulfills the equation:

$$\frac{\partial \Psi(x)}{\partial t} = -\frac{i}{\hbar}\mathcal{H}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x) \tag{6}$$

This seems arbitrary and counter-intuitive. In this course we will not use this historical approach. Rather, we will construct quantum mechanics in a natural way using only simple considerations. Later we will see that classical mechanics can be obtained as a special limit of the quantum theory.

[1.4] Second Quantization

The method for quantizing the electromagnetic field is to write the Hamiltonian as a sum of harmonic oscillators (normal modes) and then to quantize the oscillators. It is exactly the same as finding the normal modes of spheres connected with springs. Every normal mode has a characteristic frequency. The ground state of the field (all the oscillators are in the ground state) is called the "vacuum state". If a specific oscillator is excited to level n, we say that there are n photons with frequency ω in the system.

A similar formalism is used to describe a many particle system. A vacuum state and occupation states are defined. This formalism is called "second quantization". A better name would be "formalism of quantum field theory".

In the first part of this course we will not talk about "second quantization": The electromagnetic field will be described in a classic way using the potentials $V(x), A(x)$, while the distinction between fermions and bosons will be done using the (somewhat unnatural) language of "first quantization".

[1.5] Definition of Mass

The "gravitational mass" is defined using a scale. Since gravitational theory is not includes in this course, we will not use that definition. Another possibility is to define "inertial mass". This type of mass is determined by considering the collision of two bodies:

$$\mathsf{m}_1 v_1 + \mathsf{m}_2 v_2 = \mathsf{m}_1 u_1 + \mathsf{m}_2 u_2 \tag{7}$$

So:

$$\frac{\mathsf{m}_1}{\mathsf{m}_2} = \frac{u_2 - v_2}{v_1 - u_1} \tag{8}$$

In order to be able to measure the inertial mass of an object, we must do so in relation to a reference mass. In other words: we use an arbitrary object as our basic mass unit.

Within the framework of quantum mechanics the above Newtonian definition of inertial mass will not be used. Rather we define mass in an absolute way. We shall define mass as a parameter in the "dispersion relation", and we shall see that the units of mass are:

$$[\mathsf{m}] = \frac{T}{L^2} \tag{9}$$

If we choose to set the units of mass in an arbitrary way to be kg, then a units conversion scheme will be necessary. The conversion scheme is simply a multiplication by the Planck constant:

$$\mathsf{m}[kg] = \hbar\mathsf{m} \tag{10}$$

[1.6] The Dispersion Relation

It is possible to prepare a "monochromatic" beam of (for example) electrons that all have the same velocity, and the same De-Broglie wavelength. The velocity of the particles can be measured by using a pair of rotating circular plates (discs). The wavelength of the beam can be measured by using a diffraction grating. We define the particle's momentum ("wave number") as:

$$p = 2\pi/\text{wavelength} \tag{11}$$

It is possible to find (say by an experiment) the relation between the velocity of the particle and its momentum. This relation is called the "dispersion relation". For low velocities (not relativistic) the relation is approximately linear:

$$v = \frac{1}{\mathsf{m}}p \tag{12}$$

This relation defines the "mass" parameter and also the units of mass.

[1.7] Spin

Apart from the degrees of freedom of being in space, the particles also have an inner degree of freedom called "spin" (Otto Stern and Walter Gerlach 1922). We say that a particle has spin s if its inner degree of freedom is described by a representation of the rotations group of dimension $2s+1$. For example, "spin $\frac{1}{2}$" can be described by a representation of dimension 2, and "spin 1" can be described by a representation of dimension 3. In order to make this abstract statement clearer we will look at several examples.

- Electrons have spin $\frac{1}{2}$, so 180^o difference in polarization ("up" and "down") means orthogonality.
- Photons have spin 1, so 90^o difference in linear polarizations means orthogonality.

If we position two polarizers one after the other in the angles that were noted above, no particles will pass through. We see that an abstract mathematical consideration (representations of the rotational group) has very "realistic" consequences.

[2] Digression: The classical description of nature

[2.1] The Classical Effect of the Electromagnetic Field

The electric field $\mathcal{E}$ and the magnetic field $\mathcal{B}$ can be derived from the vector potential A and the electric potential V:

$$\begin{aligned} \mathcal{E} &= -\nabla V - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \\ \mathcal{B} &= \nabla \times \vec{A} \end{aligned} \tag{13}$$

The electric potential and the vector potential are not uniquely determined, since the electric and the magnetic fields are not affected by the following changes:

$$\begin{aligned} \Phi &\mapsto \tilde{\Phi} = \Phi - \frac{1}{c}\frac{\partial \Lambda}{\partial t} \\ A &\mapsto \tilde{A} = A + \nabla\Lambda \end{aligned} \tag{14}$$

Where $\Lambda(x,t)$ is an arbitrary scalar function. Such a transformation of the potentials is called "gauge". A special case of "gauge" is changing the potential V by an addition of a constant.

Gauge transformations do not affect the classical motion of the particle since the equations of motion contain only the derived fields $\mathcal{E}, \mathcal{B}$.

$$\frac{d^2x}{dt^2} = \frac{1}{\mathsf{m}}\left[e\mathcal{E} - \frac{e}{c}\mathcal{B}\times\dot{x}\right] \tag{15}$$

This equation of motion can be derived from the Langrangian:

$$\mathcal{L}(x,\dot{x}) = \frac{1}{2}\mathsf{m}\dot{x}^2 + \frac{e}{c}\dot{x}A(x,t) - eV(x,t) \tag{16}$$

Or, alternatively, from the Hamiltonian:

$$\mathcal{H}(x,p) = \frac{1}{2\mathsf{m}}(p - \frac{e}{c}A)^2 + eV \tag{17}$$

[2.2] Lorentz Transformation

The Lorentz transformation takes us from one reference frame to the other. A Lorentz boost can be written in matrix form as:

$$S = \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{18}$$

Where β is the velocity of our reference frame relative to the reference frame of the lab, and

$$\gamma = \frac{1}{\sqrt{1-\beta^2}} \tag{19}$$

We use units such that the speed of light is $c = 1$. The position of the particle in space is:

$$\mathbf{x} = \begin{pmatrix} t \\ x \\ y \\ z \end{pmatrix} \tag{20}$$

and we write the transformations as:

$$\mathbf{x}' = S\mathbf{x} \tag{21}$$

We shall see that it is convenient to write the electromagnetic field as:

$$F = \begin{pmatrix} 0 & \mathcal{E}_1 & \mathcal{E}_2 & \mathcal{E}_3 \\ \mathcal{E}_1 & 0 & \mathcal{B}_3 & -\mathcal{B}_2 \\ \mathcal{E}_2 & -\mathcal{B}_3 & 0 & \mathcal{B}_1 \\ \mathcal{E}_3 & \mathcal{B}_2 & -\mathcal{B}_1 & 0 \end{pmatrix} \tag{22}$$

We shall argue that this transforms as:

$$F' = SFS^{-1} \tag{23}$$

or in terms of components:

$$\begin{array}{ll} \mathcal{E}_1' = \mathcal{E}_1 & \mathcal{B}_1' = \mathcal{B}_1 \\ \mathcal{E}_2' = \gamma(\mathcal{E}_2 - \beta\mathcal{B}_3) & \mathcal{B}_2' = \gamma(\mathcal{B}_2 + \beta\mathcal{E}_3) \\ \mathcal{E}_3' = \gamma(\mathcal{E}_3 + \beta\mathcal{B}_2) & \mathcal{B}_3' = \gamma(\mathcal{B}_3 - \beta\mathcal{E}_2) \end{array}$$

[2.3] Momentum and energy of a particle

Let us write the displacement of the particle as:

$$d\mathbf{x} = \begin{pmatrix} dt \\ dx \\ dy \\ dz \end{pmatrix} \tag{24}$$

We also define the proper time (as measured in the particle frame) as:

$$d\tau^2 = dt^2 - dx^2 - dy^2 - dz^2 = (1 - {v_x}^2 - {v_y}^2 - {v_z}^2)dt^2 \tag{25}$$

or:

$$d\tau = \sqrt{1 - v^2}dt \tag{26}$$

The relativistic velocity vector is:

$$\mathbf{u} = \frac{d\mathbf{x}}{d\tau} \tag{27}$$

and obviously:

$$u_t^2 - u_x^2 - u_y^2 - u_z^2 = 1 \tag{28}$$

We also use the notation:

$$\mathbf{p} = \mathsf{m}\mathbf{u} = \begin{pmatrix} E \\ p_x \\ p_y \\ p_z \end{pmatrix} \tag{29}$$

According to the above equations we have:

$$E^2 - p_x^2 - p_y^2 - p_z^2 = \mathsf{m}^2 \tag{30}$$

and we can write the dispersion relation:

$$\begin{aligned} E &= \sqrt{\mathsf{m}^2 + p^2} \\ v &= \frac{p}{\sqrt{\mathsf{m}^2 + p^2}} \end{aligned} \tag{31}$$

We note that for non-relativistic velocities $p_i \approx \mathsf{m}v_i$ for $i = 1, 2, 3$ while:

$$E = \mathsf{m}\frac{dt}{d\tau} = \frac{\mathsf{m}}{\sqrt{1 - v^2}} \approx \mathsf{m} + \frac{1}{2}\mathsf{m}v^2 + \dots \tag{32}$$

═══ [2.4] Equations of Motion for a Particle

The non-relativistic equations of motion for a particle in an electromagnetic field are:

$$\frac{d\vec{p}}{dt} = \mathsf{m}\frac{d\vec{v}}{dt} = e\mathcal{E} - e\mathcal{B} \times \vec{v} \tag{33}$$

The rate of change of the particle's energy E is:

$$\frac{dE}{dt} = \vec{f} \cdot \vec{v} = e\mathcal{E} \cdot \vec{v} \tag{34}$$

The electromagnetic field has equations of motion of its own: Maxwell's equations. As we shall see shortly Maxwell's equations are Lorentz invariant. But Newton's laws as written above are not. In order for the Newtonian equations of motion to be Lorentz invariant we have to adjust them. It is not difficult to see that the obvious way is:

$$\frac{d\mathbf{p}}{dt} = \mathsf{m}\frac{d\mathbf{u}}{dt} = eF\mathbf{u} \tag{35}$$

To prove the invariance under the Lorentz transformation we write:

$$\frac{d\mathbf{p}'}{d\tau} = \frac{d}{d\tau}(S\mathbf{p}) = S\frac{d}{d\tau}\mathbf{p} = S(eF\mathbf{u}) = eSFS^{-1}(S\mathbf{u}) = eF'\mathbf{u}' \tag{36}$$

Hence we have deduced the transformation $F' = SFS^{-1}$ of the electromagnetic field.

═══ [2.5] Equations of Motion of the Field

Back to Maxwell's equations. A simple way of writing them is

$$\partial^\dagger F = 4\pi J^\dagger \tag{37}$$

Where the derivative operator ∂, and the four-current J, are defined as:

$$\partial = \begin{pmatrix} \frac{\partial}{\partial t} \\ -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} \\ -\frac{\partial}{\partial z} \end{pmatrix} \qquad \partial^\dagger = (\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}) \tag{38}$$

and:

$$\mathbf{J} = \begin{pmatrix} \rho \\ J_x \\ J_y \\ J_z \end{pmatrix} \qquad \mathbf{J}^\dagger = (\rho, -J_x, -J_y, -J_z) \tag{39}$$

The Maxwell equations are invariant because $\mathbf{J}$ and ∂ transform as vectors. For more details see Jackson. An important note about notations: in this section we have used what is called a "contravariant" representation for the column vectors. For example $u = \text{column}(u_t, u_x, u_y, u_z)$. For the "adjoint" we use the "covariant" representation $u = \text{row}(u_t, -u_x, -u_y, -u_z)$. Note that $u^\dagger u = (u_t)^2 - (u_x)^2 - (u_y)^2 - (u_z)^2$ is a Lorentz scalar.

[3] Hilbert Space

═══ [3.1] Linear Algebra

In Euclidean geometry, three dimensional vectors can be written as:

$$\vec{u} = u_1\vec{e}_1 + u_2\vec{e}_2 + u_3\vec{e}_3 \tag{40}$$

Using Dirac notation we can write the same as:

$$|u\rangle = u_1|e_1\rangle + u_2|e_2\rangle + u_3|e_3\rangle \tag{41}$$

We say that the vector has the representation:

$$|u\rangle \;\mapsto\; u_i \;=\; \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \tag{42}$$

The operation of a linear operator A is written as $|v\rangle = A|u\rangle$ which is represented by:

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{13} & A_{23} & A_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \tag{43}$$

or shortly as $v_i = A_{ij}u_j$.

Thus the linear operator is represented by a matrix:

$$A \;\mapsto\; A_{ij} \;=\; \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{13} & A_{23} & A_{33} \end{pmatrix} \tag{44}$$

═══ [3.2] Orthonormal Basis

We assume that an inner product $\langle u|v\rangle$ has been defined. From now on we assume that the basis has been chosen to be orthonormal:

$$\langle e_i|e_j\rangle = \delta_{ij} \tag{45}$$

In such a basis the inner product (by linearity) can be calculated as follows:

$$\langle u|v\rangle = u_1^*v_1 + u_2^*v_2 + u_3^*v_3 \tag{46}$$

It can also be easily proved that the elements of the representation vector can be calculated as follows:

$$u_j = \langle e_j|u\rangle \tag{47}$$

And for the matrix elements we can prove:

$$A_{ij} = \langle e_i|A|e_j\rangle \tag{48}$$

[3.3] Completeness of the Basis

In Dirac notation the expansion of a vector is written as:

$$|u\rangle = |e_1\rangle\langle e_1|u\rangle + |e_2\rangle\langle e_2|u\rangle + |e_3\rangle\langle e_3|u\rangle \tag{49}$$

which implies

$$1 = |e_1\rangle\langle e_1| + |e_2\rangle\langle e_2| + |e_3\rangle\langle e_3| \tag{50}$$

Above **1** stands for the identity operator:

$$\mathbf{1} \mapsto \delta_{ij} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{51}$$

Now we can define the "completeness of the basis" as $\sum_j |e_j\rangle\langle e_j| = \mathbf{1}$ where $P^j = |e_j\rangle\langle e_j|$ are called "projector operators". Projector operators have eigenvalues 1 and 0. For example:

$$P^1 \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{52}$$

[3.4] Operators

Definition: an adjoint operator is an operator which satisfies the following relation:

$$\langle u|Av\rangle = \langle A^\dagger u|v\rangle \tag{53}$$

If we substitute the basis vectors in the above relation we get the equivalent matrix-style definition $(A^\dagger)_{ij} = A^*_{ji}$. In what follows we are interested in "normal" operators that are diagonal in some basis. Of particular importance are Hermitian operators. It follows from the definition below that any normal operator can be written as a function $f(H)$ of an Hermitian operator H.

Say that we have a normal operator A. This means that there is a basis $\{|a\rangle\}$ such that A is diagonal. This means that:

$$A = \sum_a |a\rangle a\langle a| = \sum_a aP^a \tag{54}$$

In matrix representation this can be written as:

$$\begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} = a_1 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + a_3 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{55}$$

Thus we see that any normal operator is a combination of projectors.

It is useful to define what is meant by $\hat{B} = f(\hat{A})$ where $f()$ is an arbitrary function. Assuming that $\hat{A} = \sum |a\rangle a\langle a|$, it follows by definition that $\hat{B} = \sum |a\rangle f(a)\langle a|$. Another useful rule to remember is that if $A|k\rangle = B|k\rangle$ for some complete basis k, then it follows by linearity that $A|\psi\rangle = B|\psi\rangle$ for any vector, and therefore $A = B$.

Hermitian operators are of particular importance. By definition they satisfy $H^\dagger = H$ and hence their eigenvalues are real numbers ($\lambda_r^* = \lambda_r$). Another class of important operators are unitary operators. By definition they satisfy $U^\dagger = U^{-1}$ or equivalently $U^\dagger U = \mathbf{1}$. Hence their eigenvalues satisfy $\lambda_r^* \lambda_r = 1$, which means that they can be written as:

$$U \;=\; \sum_r |r\rangle e^{i\varphi_r}\langle r| \;=\; \exp iH \tag{56}$$

where H is Hermitian. In fact it is easy to see that any normal operator can be written a function of some H. We can regard any H with non-degenerate spectrum as providing a specification of a basis, and hence any other operator that is diagonal in that basis can be expressed as a function of that H. An operator which is not "normal" can be expressed as $Q = A + iB$ where A and B are non-commuting Hermitian operators.

[3.5] Notational conventions

In Mathematica there is a clear distinction between dummy indexes and fixed values. For example $f(x\_) = 8$ means that $f(x) = 8$ for any x, hence x is a dummy index. But if $x = 4$ then $f(x) = 8$ means that only one element of the vector $f(x)$ is specified. Unfortunately in the printed mathematical literature there are no clear conventions. How ever the tradition is to use notations such as $f(x)$ and $f(x')$ where x and x' are dummy indexes, while $f(x_0)$ and $f(x_1)$ where x_0 and x_1 are fixed values. Thus

$$\begin{aligned} A_{ij} \;&=\; \begin{pmatrix} 2 & 3 \\ 5 & 7 \end{pmatrix} \\ A_{i_0 j_0} \;&=\; 5 \qquad \text{for } i_0 = 2 \text{ and } j_0 = 1 \end{aligned} \tag{57}$$

Another typical example is

$$\begin{aligned} T_{x,k} \;&=\; \langle x|k\rangle \\ \Psi(x) \;&=\; \langle x|k_0\rangle \\ \Psi^k(x) \;&=\; \langle x|k\rangle \end{aligned} \tag{58}$$

In the first equality we regard $\langle x|k\rangle$ as a matrix: it is the transformation matrix form the position to the momentum basis. In the second equality we regard the same object (with fixed k_0) as a state vector. In the third equality we define a set of "wavefunctions".

We shall keep the following extra convention: representation indexes are always *lower* indexes. The upper indexes are reserved for specification. For example

$$\begin{aligned} Y^{\ell m}(\theta,\varphi) \;&=\; \langle \theta,\varphi|\ell m\rangle \;=\; \text{spherical harmonics} \\ \varphi^n(x) \;&=\; \langle x|n\rangle \;=\; \text{harmonic oscillator eigenfunctions} \end{aligned} \tag{59}$$

Sometime it is convenient to use the Einstein summation convention, where summation over repeated dummy indexes is implicit. For example:

$$f(\theta,\varphi) \;=\; \sum_{\ell m} \langle \theta,\varphi|\ell m\rangle\langle \ell m|f\rangle \;=\; f_{\ell m} Y^{\ell m}(\theta,\varphi) \tag{60}$$

In any case of ambiguity it is best to translate everything into Dirac notations.

[3.6] Digression: change of basis

Definition of T:

Assume we have an "old" basis and a "new" basis for a given vector space. In Dirac notation:

$$\begin{aligned} \text{old basis} &= \{\ |a=1\rangle,\ |a=2\rangle,\ |a=3\rangle,\ \dots\} \\ \text{new basis} &= \{\ |\alpha=1\rangle,\ |\alpha=2\rangle,\ |\alpha=3\rangle,\ \dots\} \end{aligned} \tag{61}$$

The matrix $T_{a,\alpha}$ whose columns represent the vectors of the new basis in the old basis is called the "transformation matrix from the old basis to the new basis". In Dirac notation this may be written as:

$$|\alpha\rangle = \sum_a T_{a,\alpha}\,|a\rangle \tag{62}$$

In general, the bases do not have to be orthonormal. However, if they are orthonormal then T must be unitary and we have

$$T_{a,\alpha} = \langle a|\alpha\rangle \tag{63}$$

In this section we will discuss the general case, not assuming orthonormal basis, but in the future we will always work with orthonormal bases.

Definition of S:

If we have a vector-state then we can represent it in the old basis or in the new basis:

$$\begin{aligned} |\psi\rangle &= \sum_a \psi_a\,|a\rangle \\ |\psi\rangle &= \sum_\alpha \tilde{\psi}_\alpha\,|\alpha\rangle \end{aligned} \tag{64}$$

So, the change of representation can be written as:

$$\tilde{\psi}_\alpha = \sum_a S_{\alpha,a}\psi_a \tag{65}$$

Or, written abstractly:

$$\tilde{\psi} = S\psi \tag{66}$$

The transformation matrix from the old representation to the new representation is: $S = T^{-1}$.

Similarity Transformation:

A unitary operation can be represented in either the new basis or the old basis:

$$\begin{aligned} \varphi_a &= \sum_a A_{a,b}\psi_b \\ \tilde{\varphi}_\alpha &= \sum_\alpha \tilde{A}_{\alpha,\beta}\tilde{\psi}_\beta \end{aligned} \tag{67}$$

The implied transformation between the representations is:

$$\tilde{A} \;=\; SAS^{-1} \;=\; T^{-1}AT \tag{68}$$

This is called a similarity transformation.

======== [3.7] The separation of variables theorem

Assume that the operator $\mathcal{H}$ commutes with an Hermitian operator A. It follows that if $|a,\nu\rangle$ is a basis in which A is diagonalized:

$$\langle a,\nu|A|a',\nu'\rangle = a\delta_{aa'}\delta_{\nu\nu'} \tag{69}$$

then the operator $\mathcal{H}$ is block diagonal in that basis. In other words:

$$\langle a,\nu|\mathcal{H}|a',\nu'\rangle = \delta_{aa'}\mathcal{H}^{(a)}_{\nu\nu'} \tag{70}$$

Where the top index indicates which is the block that belongs to the eigenvalue a.

Proof:

$$\begin{aligned}
&[\mathcal{H},A]=0 \\
&\langle a,\nu|\mathcal{H}A - A\mathcal{H}|a',\nu'\rangle = 0 \\
&a'\langle a,\nu|\mathcal{H}|a',\nu'\rangle - a\langle a,\nu|\mathcal{H}|a',\nu'\rangle = 0 \\
&(a-a')\mathcal{H}_{a\nu,a'\nu'} = 0 \\
&a\neq a' \;\;\Rightarrow\;\; \mathcal{H}_{a\nu,a'\nu'} = 0 \\
&\langle a,\nu|\mathcal{H}|a',\nu'\rangle = \mathcal{H}^{(a)}_{\nu\nu'}\delta_{aa'}
\end{aligned} \tag{71}$$

It follows that there is a basis in which both A and $\mathcal{H}$ are diagonalized. This is trivial since diagonalizing a specific block does not affect the rest of the matrix. Therefore it is possible to diagonalize block by block and eventually get a diagonal matrix.

[4] A particle in an N Site System

[4.1] N Site System

A site is a location where a particle can be located. If we have $N = 5$ sites it means that we have a 5-dimensional Hilbert space of quantum states. Later we shall assume that the particle can "jump" between sites. For mathematical reasons it is conveneint to assume torus topology. This means that the next site after $x = 5$ is $x = 1$. This is also called periodic boundary conditions.

The standard basis is the position basis. For example: $|x\rangle$ with $x = 1, 2, 3, 4, 5$ [mod 5]. So we can define the position operator as follows:

$$\hat{x}|x\rangle = x|x\rangle \tag{72}$$

In this example we get:

$$\hat{x} \mapsto \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix} \tag{73}$$

The operation of this operator on a state vector is for example:

$$\begin{aligned} |\psi\rangle &= 7|3\rangle + 5|2\rangle \\ \hat{x}|\psi\rangle &= 21|3\rangle + 10|2\rangle \end{aligned} \tag{74}$$

[4.2] Translation Operators

The one-step translation operator is defined as follows:

$$\hat{D}|x\rangle = |x + 1\rangle \tag{75}$$

For example:

$$D \mapsto \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{76}$$

and hence $D|1\rangle = |2\rangle$ and $D|2\rangle = |3\rangle$ and $D|5\rangle = |1\rangle$. Let us consider the superposition:

$$|\psi\rangle = \frac{1}{\sqrt{5}}[|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle] \tag{77}$$

It is clear that $D|\psi\rangle = |\psi\rangle$. This means that ψ is an eigenstate of the translation operator (with eigenvalue e^{i0}). The translation operator has other eigenstates that we will discuss in the next section.

[4.3] Momentum States

The momentum states are defined as follows:

$$|k\rangle \to \frac{1}{\sqrt{N}}\mathrm{e}^{ikx} \tag{78}$$
$$k = \frac{2\pi}{N}n, \quad n = \text{integer} \quad \mod (N)$$

In the previous section we have encountered the $k = 0$ momentum state. In Dirac notation this is written as:

$$|k\rangle = \sum_x \frac{1}{\sqrt{N}}\mathrm{e}^{ikx}|x\rangle \tag{79}$$

or equivalently as:

$$\langle x|k\rangle = \frac{1}{\sqrt{N}}\mathrm{e}^{ikx} \tag{80}$$

While in old fashioned notation it is written as:

$$\psi_x^k = \langle x|k\rangle \tag{81}$$

Where the upper index k identifies the state, and the lower index x is the representation index. Note that if x were continuous then it would be written as $\psi^k(x)$.

The k states are eigenstates of the translation operator. This can be proved as follows:

$$D|k\rangle = \sum_x D|x\rangle\langle x|k\rangle = \sum_x |x+1\rangle\frac{1}{\sqrt{N}}\mathrm{e}^{ikx} = \sum_{x'}|x'\rangle\frac{1}{\sqrt{N}}\mathrm{e}^{ik(x'-1)} = \mathrm{e}^{-ik}\sum_{x'}|x'\rangle\frac{1}{\sqrt{N}}\mathrm{e}^{ikx'} = \mathrm{e}^{-ik}|k\rangle \tag{82}$$

Hence we get the result:

$$D|k\rangle = \mathrm{e}^{-ik}|k\rangle \tag{83}$$

and conclude that $|k\rangle$ is an eigenstate of $\hat{D}$ with an eigenvalue e^{-ik}. Note that the number of independent eigenstates is N. For exmaple for a 5-site system we have $\mathrm{e}^{ik_6} = \mathrm{e}^{ik_1}$.

═══ [4.4] Momentum Operator

The momentum operator is defined as: $\hat{p}|k\rangle \equiv k|k\rangle$ From the relation $\hat{D}|k\rangle = \mathrm{e}^{-ik}|k\rangle$ it follows that $\hat{D}|k\rangle = \mathrm{e}^{-i\hat{p}}|k\rangle$. Therefore we get the operator identity:

$$\hat{D} = \mathrm{e}^{-i\hat{p}} \tag{84}$$

We can also define 2-step, 3-step, and r-step translation operators as follows:

$$\hat{D}(2) = (\hat{D})^2 = \mathrm{e}^{-i2\hat{p}} \tag{85}$$
$$\hat{D}(3) = (\hat{D})^3 = \mathrm{e}^{-i3\hat{p}}$$
$$\hat{D}(r) = (\hat{D})^r = \mathrm{e}^{-ir\hat{p}}$$

[5] The Continuum Limit

[5.1] Definition of the Wave Function

Below we will consider a site system in the continuum limit. ϵ is the distance between the sites and L is the length of the system. So, the number of sites is: $N = L/\epsilon$. The eigenvalues of the position operator are: $x = \epsilon \times$ integer We will use the following recipe for changing a sum into an integral:

$$\sum_x \mapsto \int \frac{dx}{\epsilon} \tag{86}$$

The definition of the position operator is:

$$\hat{x}|x\rangle = x|x\rangle \tag{87}$$

The representation of a quantum state is:

$$\psi_x = \langle x|\psi\rangle \tag{88}$$

It is useful to define the "wave function" as:

$$\psi(x) = \frac{1}{\sqrt{\epsilon}}\psi_x \tag{89}$$

So, the normalization of the wave function is:

$$\langle\psi|\psi\rangle = \sum_x |\psi_x|^2 = \int \frac{dx}{\epsilon}|\psi_x|^2 = \int dx|\psi(x)|^2 = 1 \tag{90}$$

[5.2] Momentum States

The definition of the momentum states using this normalization convention is:

$$\psi^k(x) = \frac{1}{\sqrt{L}}\mathrm{e}^{ikx} \tag{91}$$

Where the eigenvalues are:

$$k = \frac{2\pi}{L} \times \text{integer} \tag{92}$$

We will use the following recipe for changing a sum into an integral:

$$\sum_k \mapsto \int \frac{dk}{2\pi/L} \tag{93}$$

We can verify the orthogonality of the momentum states:

$$\langle k_2|k_1\rangle = \sum_x \langle k_2|x\rangle\langle x|k_1\rangle = \sum_x {\psi_x^{k_2}}^* \psi_x^{k_1} = \int dx {\psi^{k_2}(x)}^* \psi^{k_1}(x) = \frac{1}{L}\int dx \mathrm{e}^{i(k_1-k_2)x} = \delta_{k_2,k_1} \tag{94}$$

The transformation from the position basis to the momentum basis is:

$$\Psi_k = \langle k|\psi\rangle = \sum_x \langle k|x\rangle\langle x|\psi\rangle = \int {\psi^k(x)}^* \psi(x) dx = \frac{1}{\sqrt{L}}\int \psi(x)\mathrm{e}^{-ikx} dx \tag{95}$$

For convenience we will define:

$$\Psi(k) = \sqrt{L}\Psi_k \tag{96}$$

Now we can write the above relation as a Fourier transform:

$$\Psi(k) = \int \psi(x)\mathrm{e}^{-ikx} dx \tag{97}$$

Or, in the reverse direction:

$$\psi(x) = \int \frac{dk}{2\pi}\Psi(k)\mathrm{e}^{ikx} \tag{98}$$

═══ [5.3] Translations

We define the translation operator:

$$D(a)|x\rangle = |x+a\rangle \tag{99}$$

If $|\psi\rangle$ is represented by $\psi(x)$ then $D(a)|\psi\rangle$ is represented by $\psi(x-a)$. In Dirac notation we may write:

$$\langle x|D(a)|\psi\rangle = \langle x-a|\psi\rangle \tag{100}$$

This can obviously be proved easily by operating $D^\dagger$ on the "bra". However, for pedagogical reasons we will also present a longer proof: Given

$$|\psi\rangle = \sum_x \psi_x|x\rangle \tag{101}$$

Then

$$D(a)|\psi\rangle = \sum_x \psi(x)|x+a\rangle = \sum_{x'} \psi(x'-a)|x'\rangle = \sum_x \psi(x-a)|x\rangle \tag{102}$$

For an infinitesimal translation we get:

$$D(\delta a)|\psi\rangle \;\mapsto\; \psi(x-\delta a) = \psi(x) - \delta a\frac{d}{dx}\psi(x) \tag{103}$$

[5.4] The Momentum Operator

The momentum states are eigenstates of the translation operators:

$$D(a)|k\rangle = \mathrm{e}^{-iak}|k\rangle \tag{104}$$

The momentum operator is defined the same as in the discrete case:

$$\hat{p}|k\rangle = k|k\rangle \tag{105}$$

Therefore the following operator identity emerges:

$$\hat{D}(a) = \mathrm{e}^{-ia\hat{p}} \tag{106}$$

For an infinitesimal translation:

$$D(\delta a) = 1 - i\delta a\hat{p} \tag{107}$$

We see that the momentum operator is the generator of the translations.

[5.5] The differential representation of the momentum operator

In the continuum limit the operation of p can be realized by a differential operator. We have already proved the identity:

$$\langle x|D(a)|\psi\rangle = \langle x - a|\psi\rangle \tag{108}$$

Therefore:

$$\langle x|p|\psi\rangle = -i\frac{d}{dx}\langle x|\psi\rangle \tag{109}$$

In other words, we have proved the following statement: The operation of p on a wavefunction is realized by the differential operator $-i(d/dx)$.

[5.6] Commutation Relations

If $|x\rangle$ is an eigenstate of $\hat{x}$ with eigenvalue x, then $D|x\rangle$ is an eigenstate of $\hat{x}$ with eigenvalue $x + a$. In Dirac notations:

$$\hat{x}(D|x\rangle) = (x + a)(D|x\rangle) \qquad \text{for any } x \tag{110}$$

Which is equivalent to:

$$\hat{x}(D|x\rangle) = D((\hat{x} + a)|x\rangle) \qquad \text{for any } x \tag{111}$$

Therefore the following operator identity is implied:

$$\hat{x}\ D \ = \ D\ (\hat{x} + a) \tag{112}$$

Which can also be written also in one of the following optional ways:

$$[\hat{x}, D] = aD \tag{113}$$
$$D^{-1}\hat{x}D = \hat{x} + a \tag{114}$$

The opposite is correct too: any operator that fulfills this operator relation, is a translation operator, where a is the translation distance.

If we write the infinitesimal version of this operator relation, by substituting $D(\delta a) = 1 - i\delta a\hat{p}$ and expanding to the first order, then we get the following commutation relation:

$$[\hat{x}, \hat{p}] = i \tag{115}$$

The commutation relations allow us to understand the operation of operators without having to actually use them on wave functions.

[5.7] Vector Operators

Up to now we have discussed the representation of a a particle which is confined to move in a one dimensional geometry. The generalization to a system with three geometrical dimensions is straightforward.

$$\begin{aligned} |x, y, z\rangle &= |x\rangle \otimes |y\rangle \otimes |z\rangle \\ \hat{x}|x, y, z\rangle &= x|x, y, z\rangle \\ \hat{y}|x, y, z\rangle &= y|x, y, z\rangle \\ \hat{z}|x, y, z\rangle &= z|x, y, z\rangle \end{aligned} \tag{116}$$

We define a "vector operator" which is actually a "package" of three operators:

$$\hat{\mathbf{r}} = (\hat{x}, \hat{y}, \hat{z}) \tag{117}$$

And similarly:

$$\begin{aligned} \hat{\mathbf{p}} &= (\hat{p}_x, \hat{p}_y, \hat{p}_z) \\ \hat{\mathbf{v}} &= (\hat{v}_x, \hat{v}_y, \hat{v}_z) \\ \hat{\mathbf{A}} &= (\hat{A}_x, \hat{A}_y, \hat{A}_z) \end{aligned} \tag{118}$$

Sometimes an operator is defined as a function of other operators:

$$\hat{\mathbf{A}} = \mathbf{A}(\hat{\mathbf{r}}) = (A_x(\hat{x}, \hat{y}, \hat{z}), A_y(\hat{x}, \hat{y}, \hat{z}), A_z(\hat{x}, \hat{y}, \hat{z})) \tag{119}$$

For example $\hat{\mathbf{A}} = \hat{\mathbf{r}}/|\hat{\mathbf{r}}|^3$. We also note that the following notation is commonly used:

$$\hat{\mathbf{p}}^2 = \hat{\mathbf{p}} \cdot \hat{\mathbf{p}} = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2 \tag{120}$$

[5.8] The Translation Operator in 3-D

The translation operator in 3-D is defined as:

$$\hat{D}(\mathbf{a})|\mathbf{r}\rangle = |\mathbf{r} + \mathbf{a}\rangle \tag{121}$$

An infinitesimal translation can be written as:

$$\begin{aligned}\hat{D}(\delta\mathbf{a}) &= \mathrm{e}^{-i\delta a_x\hat{p}_x}\mathrm{e}^{-i\delta a_y\hat{p}_y}\mathrm{e}^{-i\delta a_z\hat{p}_z} \\ &= \hat{1} - i\delta a_x\hat{p}_x - i\delta a_y\hat{p}_y - i\delta a_z\hat{p}_z = \hat{1} - i\delta\mathbf{a}\cdot\hat{\mathbf{p}}\end{aligned} \tag{122}$$

The matrix elements of the translation operator are:

$$\langle\mathbf{r}|D(\mathbf{a})|\mathbf{r}'\rangle = \delta^3(\mathbf{r} - (\mathbf{r}' + \mathbf{a})) \tag{123}$$

═══ [5.9] The Matrix Elements of the Momentum Operator

In one dimension, the matrix elements of the translation operator are:

$$\langle x|D(a)|x'\rangle = \delta((x - x') - a) \tag{124}$$

For an infinitesimal translation we write:

$$\langle x|(\hat{1} - i\delta a\hat{p})|x'\rangle = \delta(x - x') - \delta a\delta'(x - x') \tag{125}$$

So that we get:

$$\langle x|\hat{p}|x'\rangle = -i\delta'(x - x') \tag{126}$$

We notice that the delta function is symmetric, so its derivative is anti-symmetric. In analogy to multiplying a matrix with a column vector we write: $\hat{A}|\Psi\rangle \mapsto \sum_j A_{ij}\Psi_j$. Let us examine how the momentum opertor operates on a "wavefunction":

$$\begin{aligned}\hat{p}|\Psi\rangle &\mapsto \sum_{x'}\hat{p}_{xx'}\Psi_{x'} = \int\langle x|\hat{p}|x'\rangle\Psi(x')dx' = \\ &= -i\int\delta'(x - x')\Psi(x')dx' = i\int\delta'(x' - x)\Psi(x')dx' \\ &= -i\int\delta(x' - x)\frac{\partial}{\partial x'}\Psi(x')dx' = -i\frac{\partial}{\partial x}\Psi(x)\end{aligned} \tag{127}$$

Therefore:

$$\hat{p}|\Psi\rangle \mapsto -i\frac{\partial}{\partial x}\Psi(x) \tag{128}$$

The generalization of the previous section to three dimensions is straightforward:

$$\begin{aligned}\hat{\mathbf{p}}|\Psi\rangle &\mapsto \left(-i\frac{\partial}{\partial x}\Psi, -i\frac{\partial}{\partial y}\Psi, -i\frac{\partial}{\partial z}\Psi\right) \\ \hat{\mathbf{p}}|\Psi\rangle &\mapsto -i\nabla\Psi\end{aligned} \tag{129}$$

We also notice that:

$$\mathbf{p}^2|\Psi\rangle \mapsto -\nabla^2\Psi \tag{130}$$

[6] Rotations

[6.1] Euclidean Rotation Matrix

The Euclidean Rotation Matrix $R^E(\vec{\Phi})$ is a 3×3 matrix that rotates the vector $\mathbf{r}$.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} ROTATION \\ MATRIX \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{131}$$

The Euclidean matrices constitute a representation of dimension 3 of the rotation group. The parametrization of a rotation is done using three numbers which are kept in a vector: $\vec{\Phi}$. The three parameters are: Two parameters of the axis of rotation: θ, φ. How much to rotate (the length of the vector): Φ.

$$\vec{\Phi} = \Phi\vec{n} = \Phi(\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta) \tag{132}$$

A 3×3 small angle rotation of $\mathbf{r}$ can be written as:

$$R^E(\delta\vec{\Phi})\mathbf{r} = \mathbf{r} + \delta\vec{\Phi} \times \mathbf{r} \tag{133}$$

[6.2] The Rotation Operator Over the Hilbert Space

The rotation operator over the Hilbert space is defined (in analogy to the translation operator) as:

$$\hat{R}(\vec{\Phi})|\mathbf{r}\rangle \equiv |R^E(\vec{\Phi})\mathbf{r}\rangle \tag{134}$$

This operator operates over an infinite dimension Hilbert space (the standard basis is an infinite number of "sites" in the three-dimensional physical space). Therefore, it is represented by an infinite dimension matrix:

$$R_{r'r} = \langle r'|\hat{R}|r\rangle = \langle r'|R^E_r\rangle = \delta(r' - R^E r) \tag{135}$$

That is in direct analogy to the translation operator which is represented by the matrix:

$$D_{r'r} = \langle r'|\hat{D}|r\rangle = \langle r'|r + a\rangle = \delta(r' - (r + a)) \tag{136}$$

[6.3] Which Operator is the Generator of Rotations?

The generator of rotations (the "angular momentum operator") is defined in analogy to the definition of the generator of translations (the "linear momentum operator"). In order to define the generator of rotations around the axis n we will look at an infinitesimal rotation of an angle $\delta\Phi\vec{n}$. An infinitesimal rotation is written as:

$$R(\delta\Phi\vec{n}) = \mathbf{1} - i\delta\Phi L_n \tag{137}$$

Below we will prove that the generator of rotations around the axis n is:

$$L_n = \vec{n} \cdot (\mathbf{r} \times \mathbf{p}) \tag{138}$$

Where:

$$\begin{aligned} \hat{\mathbf{r}} &= (\hat{x}, \hat{y}, \hat{z}) \\ \hat{\mathbf{p}} &= (\hat{p}_x, \hat{p}_y, \hat{p}_z) \end{aligned} \tag{139}$$

Proof: We shall show that both sides of the equation give the same result if they operate on any basis state $|\mathbf{r}\rangle$. This means that we have an operator identity.

$$\begin{aligned} R(\delta\vec{\Phi})|\mathbf{r}\rangle &= |R^E(\delta\vec{\Phi})\mathbf{r}\rangle = |\mathbf{r} + \delta\vec{\Phi} \times \mathbf{r}\rangle = D(\delta\vec{\Phi} \times \mathbf{r})|\mathbf{r}\rangle \\ &= [\hat{1} - i(\delta\vec{\Phi} \times \mathbf{r}) \cdot \hat{\mathbf{p}}]|\mathbf{r}\rangle = [\hat{1} - i\hat{\mathbf{p}} \cdot \delta\vec{\Phi} \times \mathbf{r}]|\mathbf{r}\rangle = [\hat{1} - i\hat{\mathbf{p}} \cdot \delta\vec{\Phi} \times \hat{\mathbf{r}}]|\mathbf{r}\rangle \end{aligned} \tag{140}$$

So we get the following operator identity:

$$R(\delta\vec{\Phi}) = \hat{1} - i\hat{\mathbf{p}} \cdot \delta\vec{\Phi} \times \hat{\mathbf{r}} \tag{141}$$

Which can also be written (by exploiting the cyclic property of the triple vectorial multiplication):

$$R(\delta\vec{\Phi}) = \hat{1} - i\delta\vec{\Phi} \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \tag{142}$$

From here we get the desired result.

═══ [6.4] Algebraic characterization of rotations

A unitary operator $\hat{D}$ realizes a translation in the basis which is determined by an observable $\hat{x}$ if we have the equality

$$\hat{D}|x\rangle = |x + a\rangle \qquad \text{for any } x \tag{143}$$

This means that $\hat{D}|x\rangle$ is an eigenstate of $\hat{x}$ with an eigenvalue $x + a$, which can be written as $\hat{x}[\hat{D}|x\rangle] = (x + a)[\hat{D}|x\rangle]$, or as $\hat{x}\hat{D}|x\rangle = \hat{D}(\hat{x} + a)|x\rangle$. Therefore an equivalent way to write the defining condition of a translation operator is

$$\hat{x}\hat{D} = \hat{D}(\hat{x} + a) \tag{144}$$

or

$$\hat{D}^{-1}\hat{x}\hat{D} = \hat{x} + a \tag{145}$$

By considering an infinitesimal translation we get another way of writing the same thing:

$$[\hat{p}, \hat{x}] = -i \tag{146}$$

In complete analogy, a unitary operator $\hat{R}$ realizes rotation Φ in the basis which is determined by an observable $\hat{x}$. If we have the equality

$$\hat{R}|\boldsymbol{r}\rangle = |R^E\boldsymbol{r}\rangle \qquad \text{for any } \boldsymbol{r} \tag{147}$$

where R^E is the Euclidean rotation matrix. This can be written as

$$\hat{R}^{-1}\hat{\boldsymbol{r}}_i\hat{R} = R^E_{ij}\hat{\boldsymbol{r}}_j \tag{148}$$

(with implicit summation over j). By considering an infinitesimal rotation we get another way of writing the same thing:

$$[\hat{J}_j, \hat{\boldsymbol{r}}_i] = -i\epsilon_{ijk}\hat{\boldsymbol{r}}_k \tag{149}$$

Thus in order to know if J generates rotations of eigenstates of a 3-component observable A, we have to check if the following algebraic relation is fulfilled:

$$[\hat{J}_i, \hat{A}_j] = i\epsilon_{ijk}\hat{A}_k \tag{150}$$

(for convenience we have interchanged the order of indices).

[6.5] Scalars, Vectors, and Tensor Operators

We can classify operators according to the way that they transform under rotations. The simplest possibility is a scalar operator C. It has the defining property

$$\hat{R}^{-1}\hat{C}\hat{R} = \hat{C} \tag{151}$$

for any rotation, which means that

$$[J_i, C] = 0 \tag{152}$$

Similarly the defining property of a vector is

$$\hat{R}^{-1}\hat{A}_i\hat{R} = R^E_{ij}\hat{A}_j \tag{153}$$

for any rotation, which means that

$$[\hat{J}_i, \hat{A}_j] = i\epsilon_{ijk}\hat{A}_k \tag{154}$$

The generalization of this idea leads to the notion of a tensor. A multicomponent observer is a tensor of rank ℓ, if it transforms according to the R^ℓ_{ij} representation of rotations. Hence a tensor of rank ℓ should have $2\ell+1$ components. In the special case of a 3-component "vector", as discussed above, the transformation is done using the Euclidean matrices R^E_{ij}.

It is easy to prove that if A and B are vector operators, then $C = A \cdot B$ is a scalar operator. We can prove it either directly, or by using the commutation relations. The generalization of this idea to tensors leads to the notion of "contraction of indices".

[6.6] Wigner-Eckart Theorem

If we know the transformation properties of an operator, it has implications on its matrix elements. For scalars it is very simple and follows from the "separation of variables theorem". Namely: the operator C should be diagonal in the basis $|j, m\rangle$:

$$C_{m'm} \;=\; c\,\delta_{m'm} \qquad \text{within a given } j \text{ subspace} \tag{155}$$

We can write $c = \langle C \rangle$, where the expectation value can be taken with any state. A similar theorem applies to a vector operator A. Namely,

$$[A_k]_{m'm} \;=\; g \times [J_k]_{m'm} \qquad \text{within a given } j \text{ subspace} \tag{156}$$

How can we determine the coefficient g? We simply observe that from the last equation it follows that

$$[A \cdot J]_{m'm} \;=\; g\,[J^2]_{m'm} \;=\; g\,j(j+1)\,\delta_{m'm} \tag{157}$$

in agreement with what we had claimed regarding scalars in general. Therefore we get the formula

$$g \;=\; \frac{\langle J \cdot A \rangle}{j(j+1)} \tag{158}$$

where the expectation value of the scalar can be calculated with any state.

Fundamentals (part II)

[7] Quantum states

[7.1] Is the world classical? (EPR, Bell)

We would like to examine whether the world we live in is "classical" or not. The notion of classical world includes mainly two ingredients: (i) realism (ii) determinism. By realism we means that any quantity that can be measured is well defined even if we do not measure it in practice. By determinism we mean that the result of a measurement is determined in a definite way by the state of the system and by the measurement setup. We shall see later that quantum mechanics is not classical in both respects: In the case of spin 1/2 we cannot associate a definite value of $\hat{\sigma}_y$ for a spin which has been polarized in the $\hat{\sigma}_x$ direction. Moreover, if we measure the $\hat{\sigma}_y$ of a $\hat{\sigma}_x$ polarized spin, we get with equal probability ± 1 as the result.

In this section we would like to assume that our world is "classical". Also we would like to assume that interactions cannot travel faster than light. In some textbooks the latter is called "locality of the interactions" or "causality". It has been found by Bell that the two assumptions lead to an inequality that can be tested experimentally. It turns out from actual experiments that Bell's inequality are violated. This means that our world is either non-classical or else we have to assume that interactions can travel faster than light.

If the world is classical it follows that for any set of initial conditions a given measurement would yield a definite result. Whether or not we know how to predict or calculate the outcome of a possible measurement is not assumed. To be specific let us consider a particle of zero spin, which disintegrates into two particles going in opposite directions, each with spin 1/2. Let us assume that each spin is described by a set of state variables.

$$\begin{aligned} \text{state of particle A} &= x_1^A, x_2^A, ... \\ \text{state of particle B} &= x_1^B, x_2^B, ... \end{aligned} \tag{159}$$

The number of state variables might be very big, but it is assumed to be a finite set. Possibly we are not aware or not able to measure some of these "hidden" variables.

Since we possibly do not have total control over the disintegration, the emerging state of the two particles is described by a joint probability function $\rho\left(x_1^A, ..., x_1^B, ...\right)$. We assume that the particles do not affect each other after the disintegration ("causality" assumption). We measure the spin of each of the particles using a Stern-Gerlach apparatus. The measurement can yield either 1 or -1. For the first particle the measurement outcome will be denoted as a, and for the second particle it will be denoted as b. It is assumed that the outcomes a and b are determined in a deterministic fashion. Namely, given the state variables of the particle and the orientation θ of the apparatus we have

$$\begin{aligned} a &= a(\theta_A) = f(\theta_A, x_1^A, x_2^A, ...) = \pm 1 \\ b &= b(\theta_B) = f(\theta_B, x_1^B, x_2^B, ...) = \pm 1 \end{aligned} \tag{160}$$

where the function $f()$ is possibly very complicated. If we put the Stern-Gerlach machine in a different orientation then we will get different results:

$$\begin{aligned} a' &= a(\theta'_A) = f\left(\theta'_A, x_1^A, x_2^A, ...\right) = \pm 1 \\ b' &= b(\theta'_B) = f\left(\theta'_B, x_1^B, x_2^B, ...\right) = \pm 1 \end{aligned} \tag{161}$$

We have following innocent identity:

$$ab + ab' + a'b - a'b' = \pm 2 \tag{162}$$

The proof is as follows: if $b = b'$ the sum is $\pm 2a$, while if $b = -b'$ the sum is $\pm 2a'$. Though this identity looks innocent, it is completely non trivial. It assumes both "reality" and "causality" This becomes more manifest if we write this identity as

$$a(\theta_A)b(\theta_B) + a(\theta_A)b(\theta'_B) + a(\theta'_A)b(\theta_B) - a(\theta'_A)b(\theta'_B) = \pm 2 \tag{163}$$

The realism is reflected by the assumption that both $a(\theta_A)$ and $a(\theta'_A)$ have definite values, though it is clear that in practice we can measure either $a(\theta_A)$ or $a(\theta'_A)$, but not both. The causality is reflected by assuming that a depends on θ_A but not on the distant setup parameter θ_B.

Let us assume that we have conducted this experiment many times. Since we have a joint probability distribution ρ, we can calculate average values, for instance:

$$\langle ab \rangle = \int \rho\left(x_1^A, ..., x_1^B, ...\right) f\left(\theta_A, x_1^A, ...\right) f\left(\theta_B, x_1^B, ...\right) \tag{164}$$

Thus we get that the following inequality should hold:

$$|\langle ab \rangle + \langle ab' \rangle + \langle a'b \rangle - \langle a'b' \rangle| \leq 2 \tag{165}$$

This is called Bell's inequality. Let us see whether it is consistent with quantum mechanics. We assume that all the pairs are generated in a singlet (zero angular momentum) state. It is not difficult to calculate the expectation values. The result is

$$\langle ab \rangle \quad = \quad -\cos(\theta_A - \theta_B) \quad \equiv \quad C(\theta_A - \theta_B) \tag{166}$$

we have for example

$$\begin{aligned} &C(0^o) = -1 \\ &C(45^o) = -\frac{1}{\sqrt{2}} \\ &C(90^o) = 0 \\ &C(180^o) = +1 \end{aligned} \tag{167}$$

If the world were classical the Bell's inequality would imply

$$|C(\theta_A - \theta_B) + C(\theta_A - \theta'_B) + C(\theta'_A - \theta_B) + C(\theta'_A - \theta'_B)| \leq 2 \tag{168}$$

Let us take $\theta_A = 0^o$ and $\theta_B = 45^o$ and $\theta'_A = 90^o$ and $\theta'_B = -45^o$. Assuming that quantum mechanics holds we get

$$\left|\left(-\frac{1}{\sqrt{2}}\right) + \left(-\frac{1}{\sqrt{2}}\right) + \left(-\frac{1}{\sqrt{2}}\right) - \left(+\frac{1}{\sqrt{2}}\right)\right| \;=\; 2\sqrt{2} \;>\; 2 \tag{169}$$

It turns out, on the basis of celebrated experiments that Nature has chosen to violate Bell's inequality. Furthermore it seems that the results of the experiments are consistent with the predictions of quantum mechanics. Assuming that we do not want to admit that interactions can travel faster than light it follows that our world is not classical.

═══ [7.2] The four Postulates of Quantum Mechanics

The 18th century version classical mechanics can be derived from three postulates: The three laws of Newton. The better formulated 19th century version of classical mechanics can be derived from three postulates: (1) The state of classical particles is determined by the specification of their positions and its velocities; (2) The trajectories are

determined by a minimum action principle. (3) The form of the Lagrangian of the theory is determined by symmetry considerations, namely Galilei invariance in the non-relativistic case. See the Mechanics book of Landau and Lifshitz for details.

Quantum mechanically requires four postulates: Two postulates define the notion of quantum state, while the other two postulates, in analogy with classical mechanics, are about the laws that govern the evolution of quantum mechanical systems. The four postulates are:

(1) The collection of "pure" states is a linear space (Hilbert).
(2) The expectation values of observables obey linearity:

$$\langle \alpha \hat{X} + \beta \hat{Y} \rangle = \alpha \langle \hat{X} \rangle + \beta \langle \hat{Y} \rangle \tag{170}$$

(3) The evolution in time obey the superposition principle:

$$\alpha |\Psi^0\rangle + \beta |\Phi^0\rangle \ \rightarrow \ \alpha |\Psi^t\rangle + \beta |\Phi^t\rangle \tag{171}$$

(4) The dynamics of a system is invariant under specific transformations ("gauge", "Galilei").

═══ [7.3] What is a Pure State

"Pure states" are states that have been filtered. The filtering is called "preparation". For example: we take a beam of electrons. Without "filtering" the beam is not polarized. If we measure the spin we will find (in any orientation of the measurement apparatus) that the polarization is zero. On the other hand, if we "filter" the beam (e.g. in the left direction) then there is a direction for which we will get a definite result (in the above example, in the right/left direction). In that case we say that there is full polarization - a pure state. The "uncertainty principle" tells us that if in a specific measurement we get a definite result (in the above example, in the right/left direction), then there are different measurements (in the above example, in the up/down direction) for which the result is uncertain. The uncertainty principle is implied by postulate [1].

═══ [7.4] What is a Measurement

In contrast with classical mechanics, in quantum mechanics measurement only has meaning in a statistical sense. We measure "states" in the following way: we prepare a collection of systems that were all prepared in the same way. We make the measurement on all the "copies". The outcome the measurement is an event $\hat{x} = x$ that can be characterized by a distribution function. The single event has no statistical meaning. For example, if we measured the spin of a single electron and get $\hat{\sigma_z} = 1$, it does not mean that the state is polarized "up". In order to know if the electron is polarized we must measure a large number of electrons that were prepared in an identical way. If only 50% of the events give $\hat{\sigma_z} = 1$ we should conclude that there is no definite polarization in the direction we measured!

═══ [7.5] Random Variables

A random variable is an object that can have any numerical value. In other words $\hat{x} = x$ is an event. Let's assume, for example, that we have a particle that can be in one of five sites: $x = 1, 2, 3, 4, 5$. An experimenter could measure $\text{Prob}(\hat{x} = 3)$ or $\text{Prob}(\hat{p} = 3(2\pi/5))$. Another example is a measurement of the probability $\text{Prob}(\hat{\sigma_z} = 1)$ that the particle will have spin up.

The collection of values of x is called the spectrum of values of the random variable. We make the distinction between random variables with a discrete spectrum, and random variables with a continuous spectrum.

The probability function for a random variable with a discrete spectrum is defined as:

$$f(x) \ = \ \text{Prob}(\hat{x} = x) \tag{172}$$

The probability density function for a random variable with a continuous spectrum is defined as:

$$f(x)dx \ = \ \text{Prob}(x < \hat{x} < x + dx) \tag{173}$$

The expectation value of a variable is defined as:

$$\langle x \rangle = \sum_x f(x)x \tag{174}$$

where the sum should be understood as an integral $\int dx$ in the case the x has a continuous spectrum.

[7.6] Quantum Versus Statistical Mechanics

Quantum mechanics stands opposite classical statistical mechanics. A particle is described in classical statistical mechanics by a probability function:

$$\rho(x,p)dxdp = \text{Prob}(x < \hat{x} < x + dx, p < \hat{p} < p + dp) \tag{175}$$

The expectation value of a random variable $\hat{A} = A(\hat{x}, \hat{p})$ is calculated using the definition:

$$\langle \hat{A} \rangle = \int A(x,p)\rho(x,p)dxdp \tag{176}$$

From this follows the linear relation:

$$\langle \alpha\hat{A} + \beta\hat{B} \rangle = \alpha\langle \hat{A} \rangle + \beta\langle \hat{B} \rangle \tag{177}$$

We see that the linear relation of the expectation values is actually a trivial result of the classical probability theory. As we mentioned earlier, a similar definition of a "quantum state" is impossible since we cannot measure both the location and the momentum simultaneously. For this reason, we have to use a more sophisticated definition of ρ. The more sophisticated definition is based on taking the linearity of the expectation value as a basic assumption (a postulate).

[7.7] Definition of the probability matrix

Any Hermitian operator can be written as a combination of $N \times N$ operators:

$$A = \sum_{i,j} |i\rangle\langle i|A|j\rangle\langle j| = \sum_{i,j} A_{ij}P^{ji} \tag{178}$$

Where $P^{ji} = |i\rangle\langle j|$. We notice that $P^i = P^{ii} = |i\rangle\langle i|$ are a complete set of projectors: They fulfill the completeness relation $\sum_i P^i = \hat{1}$. The rest of the operators can be written as $P^{ij} = X^{ij} + iY^{ij}$. Note that the adjoint operators are $P^{ji} = X^{ij} - iY^{ij}$. We can write $X = 2P - 1$, where P is a projector. The same applies to Y. Thus we see that the operator A is a combination of $N^2 - 1$ independent projectors.

The conclusion is that if we make $N^2 - 1$ independent measurements of projectors then we can predict the result of any other measurement according to the equation:

$$\langle A \rangle = \sum_{i,j} A_{ij}\rho_{ji} = \text{trace}(A\rho) \tag{179}$$

Where ρ is the probability matrix. The probability matrix is a "package" of expectation values of projectors that were defined above. Note that the expectation value of a projector $P = |\psi\rangle\langle\psi|$ is the probability to find the systems in state $|\psi\rangle$.

[7.8] Example: the quantum state of spin $\frac{1}{2}$

We will look at a two-site system, and write the matrix: $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ in the following way:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = a \cdot \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + b \cdot \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + c \cdot \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + d \cdot \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{180}$$

We may write the basis of this space in a more convenient form. For this reason we will define the Pauli matrices:

$$\hat{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{181}$$

We note that these matrices are all Hermitian.

Any operator can be written as a linear combination of the Pauli matrices:

$$\hat{A} = c\hat{1} + \alpha\sigma_x + \beta\sigma_y + \gamma\sigma_z \tag{182}$$

If the operator A is Hermitian then the coefficients of the combination are real. We see that in order to determine the quantum state of spin $\frac{1}{2}$ we must make three independent measurements, say of $\sigma_{x,y,z}$. Then we can predict the result of any *other* measurement by:

$$\langle A \rangle = \alpha + \beta\langle\sigma_x\rangle + \gamma\langle\sigma_y\rangle + \delta\langle\sigma_z\rangle \tag{183}$$

One way of "packaging" the 3 independent measurements is the polarization vector:

$$\vec{M} = (\langle\sigma_x\rangle, \langle\sigma_y\rangle, \langle\sigma_z\rangle) \tag{184}$$

But the standard "package" is the probability matrix whose elements are the expectation values of:

$$\begin{aligned}
P^{\uparrow\uparrow} &= |\uparrow\rangle\langle\uparrow| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(1+\sigma_z) &&= P^Z \\
P^{\downarrow\downarrow} &= |\downarrow\rangle\langle\downarrow| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}(1-\sigma_z) &&= 1 - P^Z \\
P^{\downarrow\uparrow} &= |\uparrow\rangle\langle\downarrow| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x + i\sigma_y) &&= P^X + iP^Y - \mathrm{e}^{i\pi/4} \\
P^{\uparrow\downarrow} &= |\downarrow\rangle\langle\uparrow| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x - i\sigma_y) &&= P^X - iP^Y - \mathrm{e}^{-i\pi/4}
\end{aligned} \tag{185}$$

We get the following relation between the two types of "packages":

$$\rho = \langle P^{ji} \rangle = \begin{pmatrix} \frac{1}{2}(1+M_3) & \frac{1}{2}(M_1 - iM_2) \\ \frac{1}{2}(M_1 + iM_2) & \frac{1}{2}(1-M_3) \end{pmatrix} = \frac{1}{2}(\hat{1} + \vec{M} \cdot \vec{\sigma}) \tag{186}$$

[7.9] Pure states as opposed to mixed states

After diagonalization, the probability matrix can be written as:

$$\rho \to \begin{pmatrix} p_1 & 0 & 0 & . & \\ 0 & p_2 & 0 & . & \\ 0 & 0 & p_3 & . & \\ . & . & . & . & \\ & & & & . \\ & & & & . \end{pmatrix} \tag{187}$$

The convention is to order the diagonal elements in descending order. Using the common jargon we say that the state represented by ρ is a mixture of $|1\rangle, |2\rangle, |3\rangle, \ldots$ with weights $p_1, p_2, p_3, \ldots$. The most well known mixed state is the canonical state:

$$p_r = \frac{1}{Z} \mathrm{e}^{-\beta E_r} \tag{188}$$

Where $\beta = k_B T$. A "pure state" is the special case where the probability matrix after diagonalization is of the form:

$$\rho \rightarrow \begin{pmatrix} 1 & 0 & 0 & . & \\ 0 & 0 & 0 & . & \\ 0 & 0 & 0 & . & \\ . & . & . & . & \\ & & & & . \\ & & & & . \end{pmatrix} \tag{189}$$

This may be written in a more compact way as $\rho = |1\rangle\langle 1| = |\psi\rangle\langle\psi| = P^{\psi}$. Note that $\langle P^{\psi} \rangle = 1$. This means a definite outcome for a measurement that is aimed in checking whether the particle is in state "1". That is why we say that the state is pure.

======= [7.10] Various versions of the expectation value formula

[1] The standard version of the expectation value formula:

$$\langle A \rangle = tr(A\rho) \tag{190}$$

[2] The "mixture" formula:

$$\langle A \rangle = \sum_r p_r \langle r|A|r\rangle \tag{191}$$

[3] The "sandwich" formula:

$$\langle A \rangle_{\psi} = \langle \psi|A|\psi\rangle \tag{192}$$

[4] The "projection" formula:

$$\mathrm{Prob}(\phi|\psi) = |\langle\phi|\psi\rangle|^2 \tag{193}$$

The equivalence of statements 1-4 can be proved. In particular let us see how we go from the fourth statement to the third:

$$\langle A \rangle_{\psi} = \sum_a \mathrm{Prob}(a|\psi) a = \sum_a |\langle a|\psi\rangle|^2 a = \langle\psi|A|\psi\rangle \tag{194}$$

[8] The Evolution of quantum mechanical states

[8.1] The Evolution Operator and the Hamiltonian

We will discuss a particle in site $|1\rangle$. If we multiply the basis vector by a constant, for example -8, we will get a new basis: $|\tilde{1}\rangle = -8|1\rangle$ which isn't normalized and therefore not convenient to work with. Explanation: if we represent the state $|\psi\rangle$ as a linear combination of normalized basis vectors $|\psi\rangle = \sum_j \psi_j |j\rangle$, then we can find the coefficients of the combination by using the following formula: $\psi_i = \langle i|\psi\rangle$.

Even if we decide to work with "normalized" states, there is still a some freedom left which is called "gauge freedom" or "phase freedom". We will consider the state $|\uparrow\rangle$ and the state $\mathrm{e}^{\frac{\pi}{8}i}|\uparrow\rangle$. For these states ρ is the same: Multiplying a vector-state with a phase factor does not change any physical expectation value.

From the superposition principle and what was said above regarding the normalization, it follows that the evolution in quantum mechanics will be described by a unitary operator.

$$\begin{aligned} &|\psi^{t=0}\rangle \to |\psi^t\rangle \\ &|\psi^t\rangle = U|\psi^{t=0}\rangle \end{aligned} \tag{195}$$

In order to simplify the discussion we will assume that the environmental conditions are constant (constant fields in time). In such a case, the evolution operator must fulfill:

$$U(t_2 + t_1) = U(t_2)U(t_1) \tag{196}$$

It follows that the evolution operator can be written as

$$U(t) = \mathrm{e}^{-it\mathcal{H}} \tag{197}$$

Where $\mathcal{H}$ is called the Hamiltonian or "generator" of the evolution.

Proof: The "constructive" way of proving the last formula is as follows: In order to know the evolution of a system from t_1 to t_2 we divide the time interval into many small intervals of equal size $dt = (t_2 - t_1)/N$. This means that:

$$U(t_2, t_1) = U(t_2, t_2 - dt) \cdots U(t_1 + 2dt, t_1 + dt)U(t_1 + dt, t_1) \tag{198}$$

The evolution during an infinitesimal time interval can be written as:

$$U(dt) \;=\; \hat{1} - idt\mathcal{H} \;=\; \mathrm{e}^{-idt\mathcal{H}} \tag{199}$$

In other words, the Hamiltonian is the evolution per unit of time. Or we may say that $\mathcal{H}$ is the derivative of U with respect to time. By multiplying many infinitesimal time steps we get:

$$\hat{U} = (1 - idt\mathcal{H}) \cdots (1 - idt\mathcal{H})(1 - idt\mathcal{H}) = \mathrm{e}^{-idt\mathcal{H}} \cdots \mathrm{e}^{-idt\mathcal{H}}\mathrm{e}^{-idt\mathcal{H}} = \mathrm{e}^{-it\mathcal{H}} \tag{200}$$

Where we have assumed that the Hamiltonian does not change in time, so that the multiplication of exponents can be changed into a single exponent with a sum of powers. We remember that that this is actually the definition of the exponential function in mathematics: $\exp(t) = (1 + t/N)^N$.

[8.2] The Schrödinger Equation

Consider the evolution of a pure state:

$$\begin{aligned} &\psi^{t+dt} = (I - idt\mathcal{H})\psi^t \\ &\frac{d\psi}{dt} = -i\mathcal{H}\psi \end{aligned} \tag{201}$$

This is the Schrödinger equation. For a general mixture

$$\rho = \sum_r |r\rangle p_r \langle r| \tag{202}$$

we have

$$|r\rangle \to U|r\rangle, \;\; \langle r| \to \langle r|U^\dagger \tag{203}$$

Therfore the evolution of ρ in time is:

$$\begin{aligned} &\rho_t = U\rho_{t=0}U^\dagger \\ &\frac{d\rho}{dt} = -i[\mathcal{H}, \rho] \end{aligned} \tag{204}$$

This is Liouville Von-Neumann equation. One of its advantages is that the correspondence between the formalism of statistical mechanics and quantum mechanics becomes explicit. The difference is that in quantum mechanics we deal with a probability matrix whereas in mechanical statistics we deal with a probability function.

[8.3] Stationary States (the "Energy Basis")

We can find the eigenstates $|n\rangle$ and the eigenvalues E_n of a Hamiltonian by diagonalizing it.

$$\begin{aligned} &\mathcal{H}|n\rangle = E_n|n\rangle \\ &U|n\rangle = \mathrm{e}^{-iE_nt}|n\rangle \\ &U \to \delta_{nm}\mathrm{e}^{-iE_nt} \end{aligned} \tag{205}$$

Using Dirac notation:

$$\langle n|U|m\rangle = \delta_{nm}\mathrm{e}^{-iE_nt} \tag{206}$$

If we prepare a state that is a superposition of basis states:

$$|\psi^{t=0}\rangle = \sum_n \psi_n|n\rangle \tag{207}$$

we get after time t

$$|\psi(t)\rangle = \sum_n \mathrm{e}^{-iE_nt}\psi_n|n\rangle \tag{208}$$

[8.4] Rate of change of the expectation value

For any operator $\hat{A}$ we define an operator $\hat{B}$:

$$\hat{B} = i[\hat{\mathcal{H}}, \hat{A}] + \frac{\partial A}{\partial t} \tag{209}$$

such that

$$\frac{d\langle\hat{A}\rangle}{dt} = \langle\hat{B}\rangle \tag{210}$$

proof: From the expectation value formula:

$$\langle \hat{A} \rangle_t = \text{trace}(\hat{A}\rho(t)) \tag{211}$$

We get

$$\begin{aligned} \frac{d}{dt}\langle \hat{A} \rangle_t &= \text{trace}(\frac{\partial A}{\partial t}\rho(t)) + \text{trace}(\hat{A}\frac{d\rho(t)}{dt}) \\ &= \text{trace}(\frac{\partial A}{\partial t}\rho(t)) - i\text{trace}(A[\mathcal{H}, \rho(t)]) \\ &= \text{trace}(\frac{\partial A}{\partial t}\rho(t)) + i\text{trace}([\mathcal{H}, A]\rho(t)) \\ &= \langle \frac{\partial A}{\partial t} \rangle + i\langle [\mathcal{H}, A] \rangle \end{aligned} \tag{212}$$

Where we have used Liouville's equation and the cyclic property of the trace. Alternatively, if the state is pure we can write:

$$\langle \hat{A} \rangle_t = \langle \psi(t)|\hat{A}|\psi(t) \rangle \tag{213}$$

and then we get

$$\begin{aligned} \frac{d}{dt}\langle \hat{A} \rangle &= \langle \frac{d}{dt}\psi|\hat{A}|\psi\rangle + \langle \psi|A|\frac{d}{dt}\psi\rangle + \langle \psi|\frac{\partial A}{\partial t}|\psi\rangle \\ &= i\langle \psi|\mathcal{H}A|\psi\rangle - i\langle \psi|A\mathcal{H}|\psi\rangle + \langle \psi|\frac{\partial A}{\partial t}|\psi\rangle \end{aligned} \tag{214}$$

Where we have used the Schrödinger equation.

We would like to highlight the distinction between a full derivative and a partial derivative. Let's assume that there is an operator that perhaps represents a field that depends on the time t:

$$\hat{A} = \hat{x}^2 + t\hat{x}^8 \tag{215}$$

Then the partial derivative with respect to t is:

$$\frac{\partial A}{\partial t} = \hat{x}^8 \tag{216}$$

While the total derivative of $\langle \hat{A} \rangle$ takes into account the change in the quantum state too.

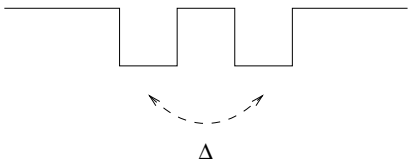
======= [8.5] How do we know what the Hamiltonian is?

We construct the Hamiltonian from "symmetry" considerations. In the next lecture our object will be to show that the Hamiltonian of a non-relativistic particle is of the form:

$$\mathcal{H} = \frac{1}{2\mathsf{m}}(p - A(x))^2 + V(x) \tag{217}$$

In this lecture we will discuss a simpler case: the Hamiltonian of a particle in a two-site system. We will make the following assumptions about the two-site dynamics:

- The system is symmetric with respect to reflection.
- The particle can move from site to site.



These two assumptions determine the form of the Hamiltonian. In addition, we will see how "gauge" considerations can make the Hamiltonian simpler, without loss of generality.

First note that because of gauge considerations, the Hamiltonian can only be determined up to a constant.

$$\mathcal{H} \to \mathcal{H} + \epsilon_0 \hat{1} \tag{218}$$

Namely, if we add a constant to a Hamiltonian, then the evolution operator only changes by a global phase factor:

$$U(t) \to \mathrm{e}^{-it(\mathcal{H}+\epsilon_0\hat{1})} = \mathrm{e}^{-i\epsilon_0 t}\mathrm{e}^{-it\mathcal{H}} \tag{219}$$

This global phase factor can be gauged away by means of time dependent gauge transformation. We shall discuss gauge transformations in the next sections.

[8.6] The Hamiltonian of a two-site system

It would seem that the most general Hamiltonian for a particle in a two-site system includes 4 parameters:

$$\mathcal{H} = \begin{pmatrix} \epsilon_1 & c\mathrm{e}^{-\imath\phi} \\ c\mathrm{e}^{\imath\phi} & \epsilon_2 \end{pmatrix} \tag{220}$$

Because of the assumed reflection symmetry $\epsilon_1 = \epsilon_2 = \epsilon$ it seems that we are left with 3 parameters. But in fact there is only one physical parameter in this model. Thanks to gauge freedom we can define a new basis:

$$\begin{aligned} |\tilde{1}\rangle &= |1\rangle \\ |\tilde{2}\rangle &= \mathrm{e}^{i\phi}|2\rangle \end{aligned} \tag{221}$$

and we see that:

$$\langle\tilde{2}|\mathcal{H}|\tilde{1}\rangle = \mathrm{e}^{-i\phi}\langle 2|\mathcal{H}|1\rangle = \mathrm{e}^{-i\phi}c\mathrm{e}^{i\phi} = c \tag{222}$$

Therefore we can set $\phi = 0$ without loss of generality. Then the Hamiltonian can be written as:

$$\mathcal{H} = \begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon \end{pmatrix} + \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} = \epsilon\hat{1} + c\sigma_1 \tag{223}$$

We also can make a gauge transformation in time. This means that the basis is time t is identified as $|\tilde{1}\rangle = \exp(-i\epsilon t)|1\rangle$ and $|\tilde{2}\rangle = \exp(-i\epsilon t)|2\rangle$. Using this time dependent basis we can get rid of the constant ϵ. In fact, on physical grounds, one cannot say whether the old or new basis is "really" time dependent. All we can say is that the new basis is time dependent relative to the old basis. This is just another example of the relativity principle. The bottom line is that without loss of generality we can set $\epsilon = 0$.

[8.7] The evolution of a two-site system

The eigenstates of the Hamiltonian are the states which are symmetric or anti-symmetric with respect to reflection:

$$|+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \tag{224}$$
$$|-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$

The Hamiltonian in the new basis is:

$$\mathcal{H} = \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} = c\sigma_3 \tag{225}$$

Let us assume that we have prepared the particle in site number one:

$$|\psi^{t=0}\rangle = |1\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \tag{226}$$

The state of the particle, after time t will be:

$$|\psi^{t}\rangle = \frac{1}{\sqrt{2}}(\mathrm{e}^{-ict}|+\rangle + \mathrm{e}^{-i(-c)t}|-\rangle) = \cos(ct)|1\rangle - i\sin(ct)|2\rangle \tag{227}$$

We see that a particle in a two-site system makes coherent oscillations between the two sites. That is in contrast with classical stochastic evolution where the probability to be in each site (if we wait long enough) would become equal. In the future we will see that the ability to pass from site to site is characterized by a parameter called "inertial mass".

[9] The Non-Relativistic Hamiltonian

[9.1] N Site system in the continuum Limit

In the last lesson we found the Hamiltonian $\hat{\mathcal{H}}$ in a two-site system by using gauge and symmetry considerations. Now we will generalize the result for an N-site system. We will give each site a number. The distance between two adjacent sites is a. The basic assumption is that the particle can move from site to site. The generator of the particle's movement is $\hat{\mathcal{H}}$.

$$U_{ij}(dt) = \delta_{ij} - idt\mathcal{H}_{ij} \tag{228}$$

The Hamiltonian should reflect the possibility that the particle will either stay in its place or move one step right or left. Say that $N = 4$. Taking into account that it should be Hermitian it has to be of the form

$$\mathcal{H}_{ij} = \begin{pmatrix} v & c^* & 0 & c \\ c & v & c^* & 0 \\ 0 & c & v & c^* \\ c^* & 0 & c & v \end{pmatrix} \tag{229}$$

For a moment we assume that all the diagonal elements ("on sites energies") are the same, and that also all the hopping amplitudes are the same. Thus for general N we can write

$$\hat{\mathcal{H}} = cD + c^*D^{-1} + \text{Const} = c\mathrm{e}^{-ia\hat{p}} + c^*\mathrm{e}^{ia\hat{p}} + \text{Const} \tag{230}$$

We define $c = c_0\mathrm{e}^{i\phi}$, where c_0 is real, and get:

$$\hat{\mathcal{H}} = c_0\mathrm{e}^{-i(a\hat{p}-\phi)} + c_0\mathrm{e}^{i(a\hat{p}-\phi)} + \text{Const} \tag{231}$$

We define $A = \phi/a$ (phase per unit distance) and get:

$$\hat{\mathcal{H}} = c_0\mathrm{e}^{-ia(\hat{p}-A)} + c_0\mathrm{e}^{ia(\hat{p}-A)} + \text{Const} \tag{232}$$

By using the identity $\mathrm{e}^{ix} \approx 1 + ix - (1/2)x^2$ we get:

$$\hat{\mathcal{H}} = \frac{1}{2\mathsf{m}}(\hat{p} - A)^2 + V \tag{233}$$

Where we have defined $1/(2\mathsf{m}) = -c_0a^2$ and $V = 2c_0 + \text{Const}$. Now $\hat{\mathcal{H}}$ has three constants: m, A, V. If we assume that the space is homogenous then the constants are the same all over space. But, in general, it does not have to be so, therefore:

$$\hat{\mathcal{H}} = \frac{1}{2\mathsf{m}(x)}(\hat{p} - A(x))^2 + V(x) \tag{234}$$

In this situation we say that there is a field in space. Such a general Hamiltonian could perhaps describe an electron in a metal. At this stage we will only discuss a particle whose mass m is the same all over space. This follows if we require the Hamiltonian to be invariant under Galilei transformations. The Galilei group includes translations, rotations and boosts (boost = one system moves at a constant velocity relative to another system). The relativistic version of the Galilei group is the Lorentz group (not included in the syllabus of this course). In addition, we expect the Hamiltonian to be invariant under gauge transformations. This completes our basic requirement for invariance.

[9.2] The Hamiltonian of a Particle in 3-D Space

In analogy to what we did in one dimension, we write:

$$\begin{aligned}\mathcal{H} &= cD_x + c^*D_x^{-1} + cD_y + c^*D_y^{-1} + cD_z + c^*D_z^{-1} = \\ &= c\mathrm{e}^{-ia\hat{p}_x} + c^*\mathrm{e}^{ia\hat{p}_x} + c\mathrm{e}^{-ia\hat{p}_y} + c^*\mathrm{e}^{ia\hat{p}_y} + c\mathrm{e}^{-ia\hat{p}_z} + c^*\mathrm{e}^{ia\hat{p}_z}\end{aligned} \tag{235}$$

After expanding to second order and allowing space dependence we get:

$$\begin{aligned}\mathcal{H} &= \frac{1}{2\mathsf{m}}(\hat{\mathbf{p}} - \hat{\mathbf{A}})^2 + \hat{V} = \frac{1}{2\mathsf{m}}(\hat{\mathbf{p}} - \mathbf{A}(\hat{\mathbf{r}}))^2 + V(\hat{\mathbf{x}}) \\ &= \frac{1}{2\mathsf{m}}(\hat{p}_x - A_x(\hat{x},\hat{y},\hat{z}))^2 + \frac{1}{2\mathsf{m}}(\hat{p}_y - A_y(\hat{x},\hat{y},\hat{z}))^2 + \frac{1}{2\mathsf{m}}(\hat{p}_z - A_z(\hat{x},\hat{y},\hat{z}))^2 + V(\hat{x},\hat{y},\hat{z})\end{aligned} \tag{236}$$

[9.3] Geometric phase and dynamical phase

Consider the case where there is no hopping between sites ($c_0 = 0$), hence the Hamiltonian $\hat{\mathcal{H}}$ does not include a kinetic part:

$$\begin{aligned}&\hat{\mathcal{H}} = V(x) \\ &\hat{U}(t) = \mathrm{e}^{-itV(\hat{x})} \\ &\hat{U}(t)|x_0\rangle = \mathrm{e}^{-itV(x_0)}|x_0\rangle\end{aligned} \tag{237}$$

The particle does not move in space. $\hat{V}$ is the "dynamical phase" that the particle accumulates per unit time. V in a specific site is called "binding energy" or "on site energy" or "potential energy" depending on the physical context. A V that changes from site to site reflects the nonhomogeneity of the space or the presence of an "external field". If the system were homogeneous, we would expect to find no difference between the sites.

Once we assume that the particle can move from site to site we have a hopping amplitude which we write as $c = c_0\mathrm{e}^{i\phi}$. It includes both the geometric phase ϕ and the "inertial" parameter c_0, which tells us how "difficult" it is for the particle to move from site to site. More precisely, in the Hamiltonian matrix we have on the main diagonal the "spatial potential" V_i, whereas on the other diagonals we have the hopping amplitudes $c_{i\to j}\mathrm{e}^{i\phi_{i\to j}}$. If the space in not homogeneous, the hopping coefficients do not have to be identical. For example $|c_{2\to 3}|$ can be different from $|c_{1\to 2}|$. Irrespective of that, as the particle moves from site i to site j it accumalates a geometric phase $\phi_{i\to j}$. By definition the vector potential A is the "geometric phase" that the particle accumulates per unit distance. Hence $\phi_{i\to j} = \vec{A}\cdot(\mathbf{r}_j - \mathbf{r}_i)$.

[9.4] Invariance of the Hamiltonian

The definition of "invariance" is as follows: Given that $\mathcal{H} = h(x,p;V,A)$ is the Hamiltonian of a system in the laboratory reference frame, there exist $\tilde{V}$ and $\tilde{A}$ such that the Hamiltonian in the "new" reference frame is $\tilde{\mathcal{H}} = h(x,p;\tilde{V},\tilde{A})$. The most general Hamiltonian that is invariant under translations, rotations and boosts is:

$$\hat{\mathcal{H}} = h(\hat{x},\hat{p};V,A) = \frac{1}{2\mathsf{m}}(\hat{p} - A(\hat{x}))^2 + V(\hat{x}) \tag{238}$$

Let us demonstrate the invariance of the Hamiltonian under translations: in the original basis $|x\rangle$ we have the fields $V(x)$ and $A(x)$. In the translated reference frame the Hamiltonian looks the same, but with $\tilde{V}(x) = V(x+a)$ and $\tilde{A}(x) = A(x+a)$. We say that the Hamiltonian is "invariant" (keeps its form). In order to make sure that we have not "mixed up" the signs, we will assume for a moment that the potential is $V(x) = \delta(x)$. If we make a translation with $a = 7$, then the basis in the new reference frame will be $|\tilde{x}\rangle = |x+7\rangle$, and we would get $\tilde{V}(x) = V(x+a) = \delta(x+7)$ which means a delta at $x = -7$.

[9.5] Invariance under Gauge Transformation

Let us define a new basis:

$$\begin{aligned} |\tilde{x}_1\rangle &= \mathrm{e}^{-i\Lambda_1}|x_1\rangle \\ |\tilde{x}_2\rangle &= \mathrm{e}^{-i\Lambda_2}|x_2\rangle \end{aligned} \tag{239}$$

and in general:

$$|\tilde{x}\rangle = \mathrm{e}^{-i\Lambda(x)}|x\rangle \tag{240}$$

The hopping amplitudes in the new basis are:

$$\tilde{c}_{1\to 2} = \langle \tilde{x}_2|\hat{\mathcal{H}}|\tilde{x}_1\rangle = \mathrm{e}^{i(\Lambda_2-\Lambda_1)}\langle x_2|\hat{\mathcal{H}}|x_1\rangle = \mathrm{e}^{i(\Lambda_2-\Lambda_1)}c_{1\to 2} \tag{241}$$

We can rewrite this as:

$$\tilde{\phi}_{1\to 2} = \phi_{1\to 2} + (\Lambda_2 - \Lambda_1) \tag{242}$$

Dividing by the size of the step and taking the continuum limit we get:

$$\tilde{A}(x) = A(x) + \frac{d}{dx}\Lambda(x) \tag{243}$$

Or, in three dimensions:

$$\tilde{A}(x) = A(x) + \nabla\Lambda(x) \tag{244}$$

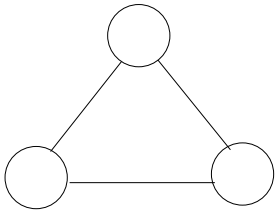
So we see that the Hamiltonian is invariant (keeps its form) under gauge. As we have said, there is also invariance for all the Galilei transformations (notably boosts). This means that it is possible to find transformation laws that connect the fields in the "new" reference frame with the fields in the "laboratory" reference frame.

[9.6] Is it possible to simplify the Hamiltonian further?

Is it possible to find a gauge transformation of the basis so that A will disappear? We have seen that for a two-site system the answer is yes: by choosing $\Lambda(x)$ correctly, we can eliminate A and simplify the Hamiltonian. On the other hand, if there is more than one route that connects two points, the answer becomes no (in other words, for systems with three sites or more). The reason is that in every gauge we may choose, the following expression will always be gauge invariant:

$$\oint \tilde{A}\cdot dl = \oint A\cdot dl = \text{gauge invariant} \tag{245}$$

In other words: it is possible to change each of the phases separately, but the sum of phases along a closed loop will always stay the same. We shall demonstrate this with a three-site system:



$$
\begin{aligned}
&|\tilde{1}\rangle = \mathrm{e}^{-i\Lambda_1}|1\rangle \\
&|\tilde{2}\rangle = \mathrm{e}^{-i\Lambda_2}|2\rangle \\
&|\tilde{3}\rangle = \mathrm{e}^{-i\Lambda_3}|3\rangle \\
&\tilde{\phi}_{1\to 2} = \phi_{1\to 2} + (\Lambda_2 - \Lambda_1) \\
&\tilde{\phi}_{2\to 3} = \phi_{2\to 3} + (\Lambda_3 - \Lambda_2) \\
&\tilde{\phi}_{3\to 1} = \phi_{3\to 1} + (\Lambda_1 - \Lambda_3) \\
&\tilde{\phi}_{1\to 2} + \tilde{\phi}_{2\to 3} + \tilde{\phi}_{3\to 1} = \phi_{1\to 2} + \phi_{2\to 3} + \phi_{3\to 1}
\end{aligned}
\tag{246}
$$

If the system had three sites but with an open topology, then we could have gotten rid of A like in the two-site system. That is also generally true of all the one dimensional problems, if the boundary conditions are "zero" at infinity. Once the one-dimensional topology is closed ("ring" boundary conditions) such a gauge transformation cannot be made. On the other hand, when the motion is in two or three dimensional space, there is always more than one route that connects any two points, without regard to the boundary conditions, so in general one cannot eliminate A.

═══ [9.7] The classical equations of motion

If $\hat{x}$ is the location of a particle, then its rate of change is called velocity. By the rate of change formula we identify v as

$$
\hat{v} = i[\hat{\mathcal{H}}, \hat{x}] = i[\frac{1}{2\mathsf{m}}(\hat{p} - A(\hat{x}))^2, \hat{x}] = \frac{1}{\mathsf{m}}(\hat{p} - A(x)) \tag{247}
$$

and we have:

$$
\frac{d\langle\hat{x}\rangle}{dt} = \langle\hat{v}\rangle \tag{248}
$$

The rate of change of the velocity $\hat{v}$ is called acceleration:

$$
\begin{aligned}
&\frac{d\langle\hat{v}\rangle}{dt} = \langle\hat{a}\rangle \\
&\hat{a} = i[\hat{\mathcal{H}}, \hat{v}] + \frac{\partial\hat{v}}{\partial t} = \frac{1}{\mathsf{m}}\left[\frac{1}{2}(v\times\mathcal{B} - \mathcal{B}\times v) + \mathcal{E}\right]
\end{aligned}
\tag{249}
$$

Where we have defined:

$$
\begin{aligned}
\mathcal{B} &= \nabla\times A \\
\mathcal{E} &= -\frac{\partial A}{\partial t} - \nabla V
\end{aligned}
\tag{250}
$$

We would like to stress stress that the Hamiltonian is the "generator" of the evolution of the system, and therefore all the equations of motion can be derived from it. From the above it follows that in case of a "minimal" wavepacket the expectation values of $\hat{x}$ and $\hat{v}$ and $\hat{a}$ obey the classical equations approximately.

[9.8] Continuity Equation (Conservation of Probability)

The Schrodinger equation is traditionally written as follows:

$$\begin{aligned}
&\hat{\mathcal{H}} = \mathcal{H}(\hat{x}, \hat{p}) \\
&\frac{\partial|\Psi\rangle}{\partial t} = -i\hat{\mathcal{H}}|\Psi\rangle \\
&\frac{\partial\Psi}{\partial t} = -i\mathcal{H}\left(x, -i\frac{\partial}{\partial x}\right)\Psi \\
&\frac{\partial\Psi}{\partial t} = -i\left[\frac{1}{2\mathsf{m}}(-i\nabla - A(x))^2 + V(x)\right]\Psi(x)
\end{aligned} \tag{251}$$

From the Schrödinger equation we can obtain a continuity equation:

$$\frac{\partial\rho(x)}{\partial t} = -\nabla \cdot J(x) \tag{252}$$

Where the probability density is:

$$\rho(x) = |\Psi(x)|^2 \tag{253}$$

And the probability current is:

$$J(x) = Re[\Psi^*(x)\frac{1}{\mathsf{m}}(-i\nabla - A(x))\Psi(x)] \tag{254}$$

We notice that:

$$\begin{aligned}
\rho(x) &= \langle\Psi|\hat{\rho}(x)|\Psi\rangle \\
J(x) &= \langle\Psi|\hat{\mathbf{J}}(x)|\Psi\rangle
\end{aligned} \tag{255}$$

Where we have defined the operators:

$$\begin{aligned}
\hat{\rho}(x) &= \delta(\hat{x} - x) \\
\hat{J}(x) &= \frac{1}{2}(\hat{v}\delta(\hat{x} - x) + \delta(\hat{x} - x)\hat{v}))
\end{aligned} \tag{256}$$

[10] Symmetries and their implications

[10.1] The Concept of Symmetry

Pedagogical remark: In order to motivate and to clarify the abstract discussion in this section it is recommended to consider the problem of finding the Landau levels in Hall geometry, where the system is invariant to x translations and hence p_x is a constant of motion. Later the ideas are extended to discuss motion in centrally symmetrical potentials.

We emphasize that symmetry and invariance are two different concepts. Invariance means that the laws of physics and hence the form of the Hamiltonian do not change. But the fields in the Hamiltonian may change. In contrast to that in case of a symmetry we requite $\tilde{\mathcal{H}} = \mathcal{H}$, meaning that the fields look the literally same. As an example consider a particle that moves in the periodic potential $V(x;R) = \cos(2\pi(x-R)/L)$. The Hamiltonian is invariant under translations: If we make translation a then the new Hamiltonian will be the same but with $R = R - a$. But in the special case that R/L is an integer we have symmetry, because then $V(x;R)$ stays the same.

[10.2] What is the meaning of commutativity?

Let us assume for example that $[\mathcal{H}, p_x] = 0$. We say in such case that the Hamiltonian commutes with the generator of translations. What are the implication of this statement? The answer is that in such case:

- The Hamiltonian is symmetric under translations
- The Hamiltonian is block diagonal in the momentum basis
- The momentum is a constant of motion

The second statement follows from the "separation of variables" theorem. The third statement follows from the expectation value rate of change formula:

$$\frac{d\langle p_x\rangle}{dt} \;=\; \langle i[\mathcal{H}, p_x]\rangle \;=\; 0 \tag{257}$$

For time independent Hamiltonians $E = \langle\mathcal{H}\rangle$ is a constant of the motion because $[\mathcal{H},\mathcal{H}] = 0$. Thus $\langle\mathcal{H}\rangle = \text{const}$ is associated with symmetry with respect to "translations" in time, while $\langle p\rangle = \text{const}$ is associated with symmetry with respect to translations in space, and $\langle L\rangle = \text{const}$ is associated with symmetry with respect to rotations.

[10.3] Symmetry under translations and rotations

If $[\mathcal{H}, p_x] = 0$ then for every translation a:

$$\begin{aligned} &[\mathcal{H}, D(a)] \;=\; \mathcal{H}D - D\mathcal{H} \;=\; 0 \\ &D^{-1}\mathcal{H}D \;=\; \mathcal{H} \end{aligned} \tag{258}$$

If we change to a translated frame of reference, then we have a new basis which is defined as follows:

$$|\tilde{x}\rangle \;=\; |x+a\rangle \;=\; D|x\rangle \tag{259}$$

This means that the transformation matrix is $T = D(a)$, and that the following symmetry is fulfilled:

$$\tilde{\mathcal{H}} \;=\; T^{-1}\mathcal{H}T \;=\; \mathcal{H} \tag{260}$$

We say that the Hamiltonian is symmetric under translations. This can be summarized as follows:

$$[\mathcal{H}, D(\vec{a})] = 0, \quad \text{for any } \vec{a} \tag{261}$$

is equivalent to

$$[\mathcal{H}, p_i] = 0 \quad \text{for } i = x, y, z \tag{262}$$

An analogous statement holds for rotations: Instead of writing:

$$[\mathcal{H}, R(\vec{\Phi})] = 0, \quad \text{for any } \vec{\Phi} \tag{263}$$

We can write:

$$[\mathcal{H}, L_i] = 0 \quad \text{for } i = x, y, z \tag{264}$$

If this holds it means that the Hamiltonian is symmetric under rotations.

Fundamentals (part III)

[11] Group representation theory

═══ [11.1] Groups

A group is a set of elements with a binary operation:

- The operation is defined by a multiplication table for $\tau^1 * \tau^2$.
- There is a unique identity element $\mathbf{1}$.
- Every element has an inverse element so that $\tau\tau^{-1} = \mathbf{1}$
- Associativity: $\tau^1 * (\tau^2 * \tau^3) = (\tau^1 * \tau^2) * \tau^3$

Commutativity does not have to be fulfilled: this means that in general $\tau^1 * \tau^2 \neq \tau^2 * \tau^1$.

The Galilei group is our main interst. It includes translations, rotations, and boosts. A translation is specified uniquely by three parameters (a_1, a_2, a_3), or for short $\mathbf{a}$. Rotations are specified by (θ, φ, Φ), or for short $\mathbf{\Phi}$. A boost is parametrized by the relative velocity (u_1, u_2, u_3). A general element is any translation, rotation, boost, or any combination of them. Such a group, that has a general element that can be defined using a set of parameters is called a Lie group. The Galilei group is a Lie group with 9 parameters. The rotation group (without reflections!) is a Lie group with 3 parameters.

═══ [11.2] Realization of a Group

If there are $\aleph$ elements in a group, then the number of rows in the full multiplication table will be $(\aleph^9)^2 = \aleph^{18}$. The multiplication table is too big for us to construct and use. Instead we will have to make a realization: we must realize the elements of the group using transformations over some space. The realization that defines the Galilei group is over the six dimensional phase space $(\mathbf{x}, \mathbf{v})$. The realization of a translation is

$$\tau_{\mathbf{a}}: \begin{cases} \tilde{\mathbf{x}} = \mathbf{x} + \mathbf{a} \\ \tilde{\mathbf{v}} = \mathbf{v} \end{cases} \tag{265}$$

The realization of a boost is

$$\tau_{\mathbf{u}}: \begin{cases} \tilde{\mathbf{x}} = \mathbf{x} \\ \tilde{\mathbf{v}} = \mathbf{v} + \mathbf{u} \end{cases} \tag{266}$$

and the realization of a rotation is

$$\tau_{\mathbf{\Phi}}: \begin{cases} \tilde{\mathbf{x}} = R^E(\Phi)\mathbf{x} \\ \tilde{\mathbf{v}} = R^E(\Phi)\mathbf{v} \end{cases} \tag{267}$$

A translation by $\mathbf{b}$, and afterward a translation by $\mathbf{a}$, gives a translation by $\tau_{\mathbf{b}+\mathbf{a}}$. This is simple. More generally the "multiplication" of group elements $\tau^3 = \tau^2 * \tau^1$ is realized using a very complicated function:

$$(\mathbf{a}^3, \mathbf{\Phi}^3, \mathbf{u}^3) = f(\mathbf{a}^2, \mathbf{\Phi}^2, \mathbf{u}^2, \mathbf{a}^1, \mathbf{\Phi}^1, \mathbf{u}^1) \tag{268}$$

We notice that this function receives input that includes 18 parameters and gives output that includes 9 parameters.

═══ [11.3] Realization using linear transformations

As mentioned above, a realization means that we regard each element of the group as an operation over a space. We treat the elements as transformations. Below we will discuss the possibility of finding a realization which consists of linear transformations.

First we will discuss the concept of linear transformation, in order to clarify it. As an example, we will check whether $f(x) = x + 5$ is a linear function. A linear function must fulfill the condition:

$$f(\alpha X_1 + \beta X_2) = \alpha f(X_1) + \beta f(X_2) \tag{269}$$

Checking $f(x)$:

$$\begin{aligned} &f(3) = 8, f(5) = 10, f(8) = 13 \\ &f(3+5) \neq f(3) + f(5) \end{aligned} \tag{270}$$

Hence we realize that $f(x)$ is not linear.

In case of the defining realization of the Galilei group over the phase space, rotations are linear transformations, but translations and boosts are not. If we want to realize the Galilei group using linear transformations, the most natural way would be to define a realization over the function space. For example, the translation of a function is defined as:

$$\tau_{\mathbf{a}}: \quad \tilde{\Psi}(x) = \Psi(x - a) \tag{271}$$

The translation of a function is a linear operation. In other words, if we translate $\alpha\Psi_1(x) + \beta\Psi_2(x)$, we get the appropriate linear combination of the translated functions: $\alpha\Psi_1(x-a) + \beta\Psi_2(x-a)$.

Linear transformations are represented by matrices. That leads us to the concept of a "representation".

[11.4] Representation of a group using matrices

A representation is a realization of the elements of a group using matrices. For every element τ of the group, we find an appropriate matrix $U(\tau)$. We demand that the "multiplication table" for the matrices will be one-to-one to the multiplication table of the elements of the group. Below we will "soften" this demand and be satisfied with the requirement that the "multiplication table" will be the same "up to a phase factor". In other words, if $\tau^3 = \tau^2 * \tau^1$, then the appropriate matrices must fulfill:

$$U(\tau^3) \;=\; \mathrm{e}^{i(\text{phase})} U(\tau^2) U(\tau^1) \tag{272}$$

It is natural to realize the group elements using orthogonal transformations (over a real space) or unitary transformations (over a complex space). Any realization using linear transformation is automatically a "representation". The reason for this is that linear transformations are always represented by matrices. For example, we may consider the realization of translations over the function space. Any function can be written as a combination of delta functions:

$$\Psi(x) = \int \Psi(x')\delta(x - x')dx \tag{273}$$

In Dirac notation this can be written as:

$$|\Psi\rangle = \sum_x \Psi_x |x\rangle \tag{274}$$

In this basis, each translation is represented by a matrix:

$$D_{x,x'} \;=\; \langle x|D(a)|x'\rangle \;=\; \delta(x - (x' + a)) \tag{275}$$

Finding a "representation" for a group is very convenient, since the operative meaning of "multiplying group elements" becomes "multiplying matrices". This means that we can deal with groups using linear algebra tools.

[11.5] Commutativity of translations and boosts?

If we make a translation and afterward a boost, then we get the same transformation as we would get if we made the boost before the translation. Therefore, boosts and translations commute. It is not possible to find a representation over function space that shows this commutativity. Therefore, we will have to "soften" the definition of "representation" and demand that the multiplication table will be correct "up to a phase factor". Therefore, from now on we will assume that translations and boosts do not commute!

Proving the last conjecture is very intuitive if we use the physics language. Let's assume that boosts do commute with translations. Say we have a particle in the laboratory reference frame that is described by a wave function that is an eigenstate of the translation operators. In other words, we are talking about a state with a defined momentum k. We will move to a moving reference frame. It is easy to prove that if $\Psi(x)$ is an eigenstate with a specific k, then $\tilde{\Psi}(x)$ is an eigenstate in the moving reference frame, with the same k. This follows from our assumption that boosts and translations commute. From this we come to the absurd conclusion that the particle has the same momentum in all the reference frames... If we don't want to use a trivial representation over the function space, we have to assume that boosts and translations do not commute.

[11.6] Generators

Every element in a Lie group is marked by a set of parameters (3 parameters for the rotation group, 9 parameters for the Galilei group). Below we will assume that we have a "unitary representation" of the group. That means that there is a mapping

$$\tau \mapsto U(\tau_1, \tau_2, ..., \tau_\mu, ...) \tag{276}$$

We will also use the convention:

$$\mathbf{1} \mapsto U(0, 0, ..., 0, ...) = \hat{1} = \text{identity matrix} \tag{277}$$

We define a set of generators $\hat{G}_\mu$ in the following way:

$$U(0, 0, ..., \delta\tau_\mu, 0, ...) \;=\; \hat{1} - i\delta\tau_\mu \hat{G}_\mu \;=\; \mathrm{e}^{-i\delta\tau_\mu \hat{G}_\mu} \tag{278}$$

(there is no summation here) For example:

$$U(\delta\tau_1, 0, 0, ...) \;=\; \hat{1} - i\delta\tau_1 \hat{G}_1 \;=\; \mathrm{e}^{-i\delta\tau_1 \hat{G}_1} \tag{279}$$

The number of basic generators is the same as the number of parameters that marks the elements of the group (3 generators for the rotation group). The generators for the Galieli group are written as:

$$\hat{P}_x, \hat{P}_y, \hat{P}_z, \hat{J}_x, \hat{J}_y, \hat{J}_z, \hat{Q}_x, \hat{Q}_y, \hat{Q}_z \tag{280}$$

The generators of the boosts, when using a representation over the function space, are $\hat{Q}_x = -\mathsf{m}\hat{x}$, etc., where m is the mass. It is physically intuitive, since we may conclude from the commutation relation $[\hat{x}, \hat{p}] = i$ that $-\hat{x}$ is the generator of translations in $\hat{p}$.

[11.7] How to use generators

In general a transformation which is generated by A would not commute with a transformation which is generated by B,

$$\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}} \neq \mathrm{e}^{\hat{B}}\mathrm{e}^{\hat{A}} \neq \mathrm{e}^{\hat{A}+\hat{B}} \tag{281}$$

But if the generated transformations are infinitesimal then:

$$e^{\epsilon\hat{A}}e^{\epsilon\hat{B}} = e^{\epsilon\hat{B}}e^{\epsilon\hat{A}} = \hat{1} + \epsilon\hat{A} + \epsilon\hat{B} + O(\epsilon^2) \tag{282}$$

We can use this in order to show that any transformation $U(\tau)$ can be generated using the complete set of generators that has been defined in the previous section. This means that it is enough to know what are the generators in order to calculate all the matrices of a given representation. The calculation goes as follows:

$$\begin{aligned} U(\tau) &= (U(\delta\tau))^N \\ &= (U(\delta\tau_1)U(\delta\tau_2)...)^N = \\ &= (e^{-i\delta\tau_1\hat{G}_1}e^{-i\delta\tau_2\hat{G}_2}...)^N = \\ &= (e^{-i\delta\tau_1\hat{G}_1 - i\delta\tau_2\hat{G}_2 \cdots})^N = \\ &= (e^{-i\delta\tau\cdot\hat{G}})^N = e^{-i\tau\cdot\hat{G}} \end{aligned} \tag{283}$$

The next issue is how to multiply transformations. For this we have to learn about the algebra of the generators.

[11.8] Combining generators

Statement: Given generators A, B then $G = \alpha A + \beta B$ and $G = i[A, B]$ are also generators.

Proof: by definition G is a generator if $e^{-i\epsilon G}$ is a matrix that represents an element in the group. We will prove the statement by showing that the infinitesimal transformation $e^{-i\epsilon G}$ can be written as a multiplication of matrices that represent elements in the group. In the first case:

$$e^{-i\epsilon(\alpha A+\beta B)} = (e^{-i\epsilon A})^\alpha (e^{-i\epsilon B})^\beta \tag{284}$$

In the second case we write ϵ as a multiplication of small factors $\epsilon = \epsilon_1\epsilon_2$, and use the identity:

$$e^{\epsilon[A,B]} = e^{-i\epsilon_2 B}e^{-i\epsilon_1 A}e^{i\epsilon_2 B}e^{i\epsilon_1 A} + \mathcal{O}(\epsilon^2) \tag{285}$$

This identity can be proved as follows:

$$1 + \epsilon_1\epsilon_2(AB - BA) = (1 - i\epsilon_2 B - \frac{1}{2}\epsilon_2^2 B^2)(1 - i\epsilon_1 A - \frac{1}{2}\epsilon_1^2 A^2)(1 + i\epsilon_2 B - \frac{1}{2}\epsilon_2^2 B^2)(1 + i\epsilon_1 A - \frac{1}{2}\epsilon_1^2 A^2) \tag{286}$$

[11.9] Structure constants

Any element in the group can be written using the set of basic generators:

$$U(\tau) = e^{-i\tau\cdot\hat{G}} \tag{287}$$

From the previous section it follows that $i[\hat{G}_\mu, \hat{G}_\nu]$ is a generator. Therefore, it must be a linear combination of the basic generators. In other words, there exit constants $c_{\mu\nu}^\lambda$ such that the following closure relation is fulfilled:

$$[G_\mu, G_\nu] = i\sum_\lambda c_{\mu\nu}^\lambda G_\lambda \tag{288}$$

The constants $c_{\mu\nu}^\lambda$ are called the "structure constants" of the group. Every "Lie group" has its own structure coefficients. If we know the structure coefficients then we can reconstruct the group's "multiplication table". Below

we will find the structure coefficients of the rotation group, and in the following lectures we will learn how to build all the other representations of the rotation group, from our knowledge of the structure coefficients.

======= [11.10] The structure constants and the multiplication table

In order to find the group's multiplication table from our knowledge of the generators, we must use the formula:

$$\mathrm{e}^{A}\mathrm{e}^{B} \;=\; \mathrm{e}^{A+B+C} \tag{289}$$

Where C is an expression that includes only commutators. There is no simple expression for C. However, it is possible to find ("per request") an explicit expression up to any accuracy wanted. By developing in a Taylor expansion up to the third order, we get:

$$C \;=\; \log(\mathrm{e}^{A}\mathrm{e}^{B}) - A - B \;=\; \frac{1}{2}[A,B] - \frac{1}{12}[[A,B],(A-B)] + ... \tag{290}$$

From this we conclude that:

$$\mathrm{e}^{-i\alpha\cdot G - i\beta\cdot G} \;=\; \mathrm{e}^{-i\gamma\cdot G} \tag{291}$$

Where:

$$\gamma_\lambda = \alpha_\lambda + \beta_\lambda + \frac{1}{2}c^{\lambda}_{\mu\nu}\alpha_\mu\beta_\nu - \frac{1}{12}c^{\lambda}_{\kappa\sigma}c^{\kappa}_{\mu\nu}(\alpha-\beta)_\sigma\alpha_\mu\beta_\nu + ... \tag{292}$$

For more details see paper by Wilcox (1967) available in the course site.

[12] The group of rotations

[12.1] The rotation group SO(3)

The rotation group $SO(3)$ is a non-commutative group. That means that the order of rotations is important. Despite this, it is important to remember that infinitesimal rotations commute. We have already proved this statement in general, but we will prove it once again for the specific case of rotations:

$$R(\delta\mathbf{\Phi})\mathbf{r} = \mathbf{r} + \delta\mathbf{\Phi} \times \mathbf{r} \tag{293}$$

So:

$$\begin{aligned} R(\delta\mathbf{\Phi}^2)R(\delta\mathbf{\Phi}^1)\mathbf{r} &= (\mathbf{r} + \delta\mathbf{\Phi}^1 \times \mathbf{r}) + \delta\mathbf{\Phi}^2 \times (\mathbf{r} + \delta\mathbf{\Phi}^1 \times \mathbf{r}) = \\ &= \mathbf{r} + (\delta\mathbf{\Phi}^1 + \delta\mathbf{\Phi}^2) \times \mathbf{r} = \\ &= R(\delta\mathbf{\Phi}^1)R(\delta\mathbf{\Phi}^2)\mathbf{r} \end{aligned} \tag{294}$$

Obviously, this is not correct when the rotations are not infinitesimal:

$$R(\vec{\Phi}^1)R(\vec{\Phi}^2) \neq R(\vec{\Phi}^1 + \vec{\Phi}^2) \neq R(\vec{\Phi}^2)R(\vec{\Phi}^1) \tag{295}$$

We can construct any infinitesimal rotation from small rotations around the major axes:

$$R(\delta\vec{\Phi}) = R(\delta\Phi_x\vec{e}_x + \delta\Phi_y\vec{e}_y + \delta\Phi_z\vec{e}_z) = R(\delta\Phi_x\vec{e}_x)R(\delta\Phi_y\vec{e}_y)R(\delta\Phi_z\vec{e}_z) \tag{296}$$

If we mark the generators by $\vec{M} = (M_x, M_y, M_z)$, then we conclude that a finite rotation around any axis can be written as:

$$R(\Phi\vec{n}) = R(\vec{\Phi}) = R(\delta\vec{\Phi})^N = (R(\delta\Phi_x)R(\delta\Phi_y)R(\delta\Phi_z))^N = (\mathrm{e}^{-i\delta\vec{\Phi}\cdot\vec{M}})^N = \mathrm{e}^{-i\vec{\Phi}\cdot\vec{M}} = \mathrm{e}^{-i\Phi M_n} \tag{297}$$

We have proved that the matrix $M_n = \vec{n} \cdot \vec{M}$ is the generator of the rotations around the axis $\vec{n}$.

[12.2] How to calculate a general rotation matrix

The general formula for finding a rotation matrix is:

$$R(\vec{\Phi}) = R(\Phi\vec{n}) = \mathrm{e}^{-i\Phi M_n} = 1 - (1 - \cos(\Phi))M_n^2 - i\sin(\Phi)M_n \tag{298}$$

Where $M_n = \vec{n} \cdot \vec{M}$ is the generator of the rotations around the $\vec{n}$ axis. All rotations are "similar" one to the other (moving to another reference frame is done by means of a similarity transformation that represents change of basis). The proof is based on the Taylor expansion. We notice that $M_z^3 = M_z$, from this it follows that for all the odd powers $M_z^k = M_z$, while for all the even powers $M_z^k = M_z^2$ where $k > 0$.

[12.3] Structure constants of the rotation group

Now we will find the structure constants of the rotation group $SO(3)$, which is the defining representation of the rotation group. These matrices induce rotations without performing reflections and all their elements are real. The matrix representation of a rotation around the z axis is:

$$R(\Phi\vec{e}_z) = \begin{pmatrix} \cos(\Phi) & -\sin(\Phi) & 0 \\ \sin(\Phi) & \cos(\Phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{299}$$

For a small rotation:

$$R(\delta\Phi\vec{e}_z) = \begin{pmatrix} 1 & -\delta\Phi & 0 \\ \delta\Phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \hat{1} + \delta\Phi \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \hat{1} - i\delta\Phi M_z \tag{300}$$

Where:

$$M_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{301}$$

We can find the other generators in the same way:

$$M_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \tag{302}$$

$$M_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

Or, written compactly:

$$(M_k)_{ij} = -i\epsilon_{ijk} \tag{303}$$

We have found the 3 generators of rotations. Now we can calculate the structure constants. For example $[M_x, M_y] = iM_z$, and generally:

$$[M_i, M_j] = i\epsilon_{ijk}M_k \tag{304}$$

═══ [12.4] Motivation for finding dim=2 representation

We defined the rotation group by the Euclidean realization over 3D space. Obviously, this representation can be used to make calculations ("to multiply rotations"). The advantage is that it is intuitive, and there is no need for complex numbers. The disadvantage is that they are 3×3 matrices with inconvenient algebraic properties, so a calculation could take hours. It would be convenient if we could "multiply rotations" with simple 2×2 matrices. In other words, we are interested in a dim=2 representation of the rotation group. The mission is to find three simple 2×2 matrices that fulfill:

$$[J_x, J_y] = iJ_z \quad \text{etc.} \tag{305}$$

In the next lecture we will learn a systematic approach to building all the representations of the rotation group. In the present lecture, we will simply find the requested representation by guessing. It is easy to verify that the matrices

$$S_x = \frac{1}{2}\sigma_x,\ S_y = \frac{1}{2}\sigma_y,\ S_z = \frac{1}{2}\sigma_z \tag{306}$$

fulfill the above commutation relations. So, we can use them to create a dim=2 representation of the rotation group. We construct the rotation matrices using the formula:

$$R = \mathrm{e}^{-i\vec{\Phi}\cdot\vec{S}} \tag{307}$$

The matrices that we get will necessarily fulfill the right multiplication table.

We should remember the distinction between a realization and a representation: in a realization it matters what we are rotating. In a representation it only matters to us that the right multiplication table is fulfilled. Is it possible to regard any representation as a realization? Is it possible to say what the rotation matrices rotate? When there is a dim=3 Euclidean rotation matrix we can use it on real vectors that represent points in space. If the matrix operates on complex vectors, then we must look for another interpretation for the vectors. This will lead us to the definition of the concept of spin (spin 1). When we are talking about a dim=2 representation it is possible to give the vectors an interpretation. The interpretation will be another type of spin (spin 1/2).

═══ [12.5] The dim=2 representation

Pauli matrices have a wonderful property. All their even powers are equal to the identity matrix, and all their odd powers are equal to the original matrix. From this (by using the Taylor expansion and separating into two sums), we get the result:

$$\begin{aligned} &R(\Phi) = \cos(\Phi/2)\hat{1} - i\sin(\Phi/2)\sigma_n \\ &\vec{n} = (\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta) \\ &\sigma_n = \vec{n}\cdot\vec{\sigma} = \begin{pmatrix} \cos\theta & \mathrm{e}^{-i\varphi}\sin\theta \\ \mathrm{e}^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix} \end{aligned} \tag{308}$$

Therefore, we get:

$$R(\vec{\Phi}) = \begin{pmatrix} \cos(\Phi/2) - i\cos(\theta)\sin(\Phi/2) & -i\mathrm{e}^{-i\varphi}\sin(\theta)\sin(\Phi/2) \\ -i\mathrm{e}^{i\varphi}\sin(\theta)\sin(\Phi/2) & \cos(\Phi/2) + i\cos(\theta)\sin(\Phi/2) \end{pmatrix} \tag{309}$$

In particular a rotation around the Z axis is given by:

$$R = \mathrm{e}^{-i\Phi S_z} = \begin{pmatrix} \mathrm{e}^{-i\Phi/2} & 0 \\ 0 & \mathrm{e}^{i\Phi/2} \end{pmatrix} \tag{310}$$

And a rotation round the Y axis is given by:

$$R = \mathrm{e}^{-i\Phi S_y} = \begin{pmatrix} \cos(\Phi/2) & -\sin(\Phi/2) \\ \sin(\Phi/2) & \cos(\Phi/2) \end{pmatrix} \tag{311}$$

═══ [12.6] States of Spin 1/2

We will now discuss the interpretation of the "states" that the matrices that we found above rotate. The eigenstates of S_z do not change when we rotate them around the Z axis (aside from a phase factor). Therefore the following interpretation comes to mind:

$$|up\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |down\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{312}$$

This interpretation is confirmed by rotating the "up" state by 180 degrees, and getting the "down" state.

$$R = \mathrm{e}^{-i\pi S_y} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{313}$$

We see that:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \to 180^0 \to \begin{pmatrix} 0 \\ 1 \end{pmatrix} \to 180^0 \to -\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{314}$$

With two rotations of 180^o we get back the "up" state, with a minus sign. Optionally one observes that

$$\mathrm{e}^{-i2\pi S_z} = \mathrm{e}^{-i\pi\sigma_z} = -1 \tag{315}$$

and hence by similarity this holds for any 2π rotation. We see that the representation that we found is not a one-to-one representation of the rotation group. It does not obey the multiplication table in a one-to-one fashion! In fact, we have found a representation of $SU(2)$ and not $SO(3)$. The minus sign has a physical significance. In a two slit experiment it is possible to turn destructive interference into constructive interference by placing a magnetic field in one of the paths. The magnetic field rotates the spin of the electrons. If we induce 360^o rotation, then the relative phase of the interference change sign, and hence constructive interference becomes destructive and vice versa. The relative phase is important! Therefore, we must not ignore the minus sign.

We can get any spin 1/2 polarization state by combining a rotation round the Y axis and a rotation round the Z axis. The result is:

$$|\vec{e}_{\theta,\varphi}\rangle = R(\varphi)R(\theta)|up\rangle = \mathrm{e}^{-i\varphi S_z}\mathrm{e}^{-i\theta S_y}|up\rangle = \begin{pmatrix} \mathrm{e}^{-i\varphi/2}\cos(\theta/2) \\ \mathrm{e}^{i\varphi/2}\sin(\theta/2) \end{pmatrix} \tag{316}$$

======= [12.7] An example for multiplication of rotations

Let us make a 90^o rotation $R(90^0 e_z)$ around the Z axis, followed by a 90^o rotation $R(90^0 e_y)$ around the Y axis. We would like to know what this sequence gives. Using the Euclidean representation

$$R = 1 - i\sin\Phi M_n - (1-\cos\Phi)M_n^2 \tag{317}$$

we get

$$\begin{aligned} R(90^0 e_z) &= 1 - iM_z - M_z^2 \\ R(90^0 e_y) &= 1 - iM_y - M_y^2 \end{aligned} \tag{318}$$

We do not wish to open the parentheses, and add up 9 terms which include multiplications of 3×3 matrices. Therefore, we will leave the Euclidean representation and try and do the same thing with a dim=2 representation, which means we will work with the 2×2 Pauli matrices.

$$\begin{aligned} R(\Phi) &= \cos(\Phi/2)\hat{1} - i\sin(\Phi/2)\sigma_n \\ R(90^0 e_z) &= \frac{1}{\sqrt{2}}(\hat{1} - i\sigma_z) \\ R(90^0 e_y) &= \frac{1}{\sqrt{2}}(\hat{1} - i\sigma_y) \end{aligned} \tag{319}$$

Hence

$$R = R(90^0 e_y)R(90^0 e_z) = (\frac{1}{2} - i\sigma_x - i\sigma_y - i\sigma_z) \tag{320}$$

Where we have used the fact that $\sigma_y\sigma_z = i\sigma_x$. We can write this result as:

$$R = \cos\frac{120^o}{2} - i\sin\frac{120^o}{2}\vec{n}\cdot\vec{\sigma} \tag{321}$$

Where $n = \frac{1}{\sqrt{3}}(1,1,1)$. This defines the equivalent rotation which is obtained by combining the two 90^o rotations.

[12.8] Euler Angles

We can prove the following identity in the same way:

$$R(90^0 e_x) = R(-90^0 e_z) R(90^0 e_y) R(90^0 e_z) \tag{322}$$

This identity is actually trivial: a rotation round the X axis is the same as a rotation round the Y axis, if we change to a different reference frame.

Alternatively, we can look at the above as a special case of a "Euler rotation". Euler showed that any rotation can be assembled from rotations round the Y axis and rotations round the Z axis:

$$R = \mathrm{e}^{-i\alpha J_z} \mathrm{e}^{-i\beta J_y} \mathrm{e}^{-i\gamma J_z} \tag{323}$$

The validity of the idea is obvious, but finding the Euler angles can be complicated.

[13] Building the representations of rotations

[13.1] Irreducible representations

A reducible representation is a representation for which a basis can be found in which each matrix in the group decomposes into blocks. In other words, each matrix can be separated into sub-matrices. Each set of sub-matrices must fulfill the multiplication table of the group. To decompose a representation means that we move to a basis in which all the matrices decompose into blocks. Only in a commutative group a basis can be found in which all the matrices are diagonal. So, we can say that a representation of a commutative group decomposes into one-dimensional representations. The rotation group is not a commutative group. We are interested in finding all the irreducible representations of the rotation group. All the other representations of the rotation group can be found in a trivial way by combining irreducible representations.

We are interested in finding representations of the rotation group. We will assume that someone has given us a "gift": a specific representation of the rotation group. We want to make sure that this is indeed a "good gift". We will check if the representation is reducible. Maybe we have "won the lottery" and had received more than one representation? Without loss of generality, we will assume that we only had received one (irreducible) representation. We will try to discover what are the matrices that we had received. We will see that it is enough to know the dimension of the representation in order to determine what it is. In this way we will convince ourselves that there is only one (irreducible) representation for each dimension, and that we have indeed found all the representations of the rotation group.

[13.2] First Stage - Making Sure that We Got a "Good Gift"

If we had received a representation of the rotation group then we can look at infinitesimal rotations and define generators. For a small rotation around the X axis, we can write:

$$U(\delta\Phi\vec{e}_x) = \hat{1} - i\delta\hat{J}_x \tag{324}$$

In the same way we can write rotations round the Z and Y axes. So, we can find the matrices $\hat{J}_x, \hat{J}_y, \hat{J}_z$. How can we check that the representation that we received is indeed a representation of the rotation group? All we have to do is check that the following equation is fulfilled:

$$[\hat{J}_i, \hat{J}_j] = i\epsilon_{ijk}\hat{J}_k \tag{325}$$

We will also define:

$$\begin{aligned} \hat{J}_\pm &= \hat{J}_x \pm i\hat{J}_y \\ \hat{J}^2 &= \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 = \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) + \hat{J}_z^2 \end{aligned} \tag{326}$$

We notice that the operator $\hat{J}^2$ commutes with all the generators, and therefore also with all the rotation matrices.

[13.3] Second Stage - Determining the Basis

If we have received a representation as a gift, then the first thing we must do is decide in which basis we would like to write it. Without loss of generality, we can decide on a basis that is determined by the operators $\hat{J}^2, \hat{J}_z$:

$$\begin{aligned} \hat{J}^2|\lambda, m\rangle &= \lambda|\lambda, m\rangle \\ \hat{J}_z|\lambda, m\rangle &= m|\lambda, m\rangle \end{aligned} \tag{327}$$

This is the basis in which the matrices $\hat{J}^2, \hat{J}_z$ are diagonalized:

$$\begin{aligned} \langle\lambda m|\hat{J}^2|\lambda' m'\rangle &= \lambda\delta_{\lambda\lambda'}\delta_{mm'} \\ \langle\lambda m|\hat{J}_z|\lambda' m'\rangle &= m\delta_{\lambda\lambda'}\delta_{mm'} \end{aligned} \tag{328}$$

Obviously, the other generators, or a general rotation matrix will not be diagonal in this basis. But, according to the "separation of variables theorem" they will all decompose into blocks. The reason is, as said above, that $\hat{J}^2$ commutes with all of them:

$$\langle \lambda m|R|\lambda' m'\rangle = \delta_{\lambda\lambda'} R^{\lambda}_{mm'} \tag{329}$$

In other words, $\hat{J}^2$ induces a decomposition of the representation that we had received. All the matrices have changed to the same "block structure". Each block corresponds to a specific value of λ, with different values of m.

If we have discovered that the representation has decomposed, it is as if we have "won the lottery" and received more than one representation. From now on we will focus on one of the blocks. In other words, from now on we assume (without loss of generality) that we have one irreducible representation for which $\hat{J}^2 = \lambda$. We will denote the basis elements by $|m\rangle$. We will see that knowing λ makes it possible for us to determine the dimension of the representation that we had received, and what the matrices $R_{mm'}$ look like.

═══ [13.4] Reminder: Ladder Operators

Given an operator $\hat{D}$ (which does not have to be unitary or Hermitian) and an observable $\hat{x}$ that fulfill the commutation relation

$$[\hat{x}, \hat{D}] = a\hat{D} \tag{330}$$

we will prove that the operator $\hat{D}$ is an operator that changes (increments or decrements) eigenstates of $\hat{x}$.

$$\begin{aligned} &\hat{x}\hat{D} - \hat{D}\hat{x} = a\hat{D} \\ &\hat{x}\hat{D} = \hat{D}(\hat{x} + a) \\ &\hat{x}\hat{D}|x\rangle = \hat{D}(\hat{x} + a)|x\rangle \\ &\hat{x}\hat{D}|x\rangle = \hat{D}(x + a)|x\rangle \\ &\hat{x}[\hat{D}|x\rangle] = (x + a)[\hat{D}|x\rangle] \end{aligned} \tag{331}$$

So the state $|\Psi\rangle = \hat{D}|x\rangle$ is an eigenstate of $\hat{x}$ with eigenvalue $(x + a)$. The normalization of $|\Psi\rangle$ is determined by:

$$||\Psi|| = \langle\Psi|\Psi\rangle = \langle x|\hat{D}^{\dagger}\hat{D}|x\rangle \tag{332}$$

═══ [13.5] Third Stage: Finding the ladder operators

It follows from the commutation relations of the generators that:

$$[\hat{J}_z, \hat{J}_{\pm}] \;=\; \pm\hat{J}_{\pm} \tag{333}$$

So $\hat{J}_{\pm}$ are ladder operators in the basis that we are working in. By using them we can move from a given state $|m\rangle$ to other eigenstates: $..., |m-2\rangle, |m-1\rangle, |m+1\rangle, |m+2\rangle, |m+3\rangle, ...$

From the commutation relations of the generators

$$(\hat{J}_+\hat{J}_-) - (\hat{J}_-\hat{J}_+) = [\hat{J}_+, \hat{J}_-] = 2\hat{J}_z \tag{334}$$

From the definition of $\hat{J}^2$

$$(\hat{J}_+\hat{J}_-) + (\hat{J}_-\hat{J}_+) = 2(\hat{J}^2 - (\hat{J}_z)^2) \tag{335}$$

By adding/subtracting these two identities we get:

$$\begin{aligned}\hat{J}_-\hat{J}_+ &= \hat{J}^2 - \hat{J}_z(\hat{J}_z+1) \\ \hat{J}_+\hat{J}_- &= \hat{J}^2 - \hat{J}_z(\hat{J}_z-1)\end{aligned} \tag{336}$$

Now we can find the normalization of the states that are found by using the ladder operators:

$$\begin{aligned}||\hat{J}_+|m\rangle|| &= \langle m|\hat{J}_-\hat{J}_+|m\rangle = \langle m|\hat{J}^2|m\rangle - \langle m|\hat{J}_z(\hat{J}_z+1)|m\rangle = \lambda - m(m+1) \\ ||\hat{J}_-|m\rangle|| &= \langle m|\hat{J}_+\hat{J}_-|m\rangle = \langle m|\hat{J}^2|m\rangle - \langle m|\hat{J}_z(\hat{J}_z-1)|m\rangle = \lambda - m(m-1)\end{aligned} \tag{337}$$

It will be convenient from now on to write the eigenvalue of $\hat{J}^2$ as $\lambda = j(j+1)$. Therefore:

$$\begin{aligned}\hat{J}_+|m\rangle &= \sqrt{j(j+1)-m(m+1)}|m+1\rangle \\ \hat{J}_-|m\rangle &= \sqrt{j(j+1)-m(m-1)}|m-1\rangle\end{aligned} \tag{338}$$

======= [13.6] Fourth Stage - representation of the generators

Since the representation is of a finite dimension, the process of incrementing or decrementing cannot go on forever. By looking at the results of the last section we may conclude that there is only one way that the incrementing could stop: at some stage we get $m = +j$. Similarly, there is only one way that the decrementing could stop: at some stage we get $m = -j$. Hence in the incrementing/decrementing process we get a ladder that includes $2j+1$ states. This number must be an integer number. Therefore j must be either an integer or half integer number.

For a given j the matrix representation of the generators is determined uniquely. This is based on the formulas of the previous section, from which we conclude:

$$\begin{aligned}[\hat{J}_+]_{m'm} &= \sqrt{j(j+1)-m(m+1)}\delta_{m',m+1} \\ [\hat{J}_-]_{m'm} &= \sqrt{j(j+1)-m(m-1)}\delta_{m',m-1}\end{aligned} \tag{339}$$

And all that is left to do is to write:

$$\begin{aligned}[\hat{J}_x]_{m'm} &= \frac{1}{2}\left[(\hat{J}_+)_{m'm} + (\hat{J}_-)_{m'm}\right] \\ [\hat{J}_y]_{m'm} &= \frac{1}{2i}\left[(\hat{J}_+)_{m'm} - (\hat{J}_-)_{m'm}\right] \\ [\hat{J}_z]_{m'm} &= m\delta_{m'm}\end{aligned} \tag{340}$$

And then we get every rotation matrix in the representation by:

$$R_{m'm} = \mathrm{e}^{-i\vec{\Phi}\cdot\vec{J}} \tag{341}$$

A Technical note: In the raising/lowering process described above we got "ladders" of m state. It is possible that we will get either one ladder, or several ladders of the same length. In other words it is possible that the representation will decompose into two identical representations of the same dimension. If we have found only one ladder, then the representation that we have found is irreducible.

[14] Rotations of spin 1/2 and spin 1

======= [14.1] Building the dim=2 representation (Spin $\frac{1}{2}$)

Let us find the representation for $j = 1/2$. This representation can be interpreted as a realization of spin $\frac{1}{2}$.

$$J^2|m\rangle = \frac{1}{2}(\frac{1}{2}+1)|m\rangle \tag{342}$$
$$J_z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

Using formulas of the previous section we find J_+ and J_-:

$$J_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{343}$$
$$J_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Therefore:

$$J_x = \frac{1}{2}\left(\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right) = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} = \frac{1}{2}\sigma_x \tag{344}$$

and

$$J_y = \begin{pmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} = \frac{1}{2}\sigma_y \tag{345}$$

The physical degree of freedom that is called "spin $\frac{1}{2}$" cannot be visualized as a arising from the spinning of small rigid body around some axis like a top. If it were possible, then we could say that the spin can be described by a wave function. In this case, if we would rotate it by 360^o we would get the same state, with the same sign. But in the representation we are discussing we get minus the same state. That is in contradiction with the definition of a (wave) function as a single valued object.

======= [14.2] Building the dim=3 representation (Spin 1)

Let us find the representation for $j = 1$. This representation can be interpreted as a realization of spin 1.

$$\begin{aligned} S^2|m\rangle &= 1(1+1)|m\rangle \\ S_z &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\ S_+ &= \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \end{aligned} \tag{346}$$

So, the standard representation is:

$$S \to \left[\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\right] \tag{347}$$

We remember that the Euclidean representation is:

$$M \to \left[\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] \tag{348}$$

Now we have two different dim=3 representations that represent the rotation group. They are actually the same representation in a different basis. By changing bases (diagonalizing M_z) it is possible to move from the Euclidean representation to the standard representation. It is obvious that diagonalizing M_z is only possible over the complex field. In the defining realization, the matrices of the Euclidean representation rotate points in the real space. But it is possible also to use them on complex vectors. In the latter case it is a realization for spin 1.

For future use we list some useful matrices:

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{349}$$

From this:

$$S_x^2 = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad S_y^2 = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix} \quad S_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{350}$$

And as expected from $\langle \ell, m | S^2 | \ell', m' \rangle = \ell(\ell+1)\delta_{\ell,\ell'}\delta_{m,m'}$ we get

$$S^2 = S_x^2 + S_y^2 + S_z^2 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{351}$$

═══ [14.3] Rotations of Spin 1

Having found the generators we can construct any rotation of spin 1. We notice the following equation:

$$S_i^3 = S_i^2 S_i = S_i \quad \text{for } i = x, y, z \tag{352}$$

From this equation we conclude that all the odd powers $(1, 3, 5, ...)$ are the same and are equal to S_i, and all the even powers $(2, 4, 6, ...)$ are the same and equal to S_i^2. It follows (by way of a Taylor expansion) that:

$$U(\vec{\Phi}) = \mathrm{e}^{-i\vec{\Phi}\cdot\vec{S}} = \hat{1} - i \ \sin(\Phi) S_n - (1 - \cos(\Phi)) S_n^2 \tag{353}$$

Where:

$$S_n = \vec{n} \cdot \vec{S} \tag{354}$$

Any rotation can be given by a combination of a rotation round the z axis and a rotation round the y axis. We will mark the rotation angle round the y axis by θ and the rotation angle round the z axis by φ, and get:

$$U(\varphi \vec{e}_z) = \mathrm{e}^{-i\varphi S_z} = \begin{pmatrix} \mathrm{e}^{-i\varphi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \mathrm{e}^{i\varphi} \end{pmatrix} \tag{355}$$

$$U(\theta \vec{e}_y) = \mathrm{e}^{-i\theta S_y} = \begin{pmatrix} \frac{1}{2}(1+\cos\theta) & -\frac{1}{\sqrt{2}}\sin\theta & \frac{1}{2}(1-\cos\theta) \\ \frac{1}{\sqrt{2}}\sin\theta & \cos\theta & -\frac{1}{\sqrt{2}}\sin\theta \\ \frac{1}{2}(1-\cos\theta) & \frac{1}{\sqrt{2}}\sin\theta & \frac{1}{2}(1+\cos\theta) \end{pmatrix}$$

[14.4] The physical states of a spin

Any state of "spin 1/2" can be specified by an arrow that points to some direction in space. This makes sense because spin 1/2 it is represented by a vector with two complex number. That means we have 4 parameters. After gauge and normalization, we are left with 2 physical parameters which can be associated with the polarization direction (θ, φ). The standard basis is

$$\begin{aligned} |m = \frac{1}{2}\rangle &= |\uparrow\rangle \\ |m = -\frac{1}{2}\rangle &= |\downarrow\rangle \end{aligned} \tag{356}$$

We can get from the "up" state all the other possible states merely by using the appropriate rotation matrix.

The states of "Spin 1" cannot be represented by simple arrows. This should be obvious in advance because it is represented by a vector that has three complex components. That means we have 6 parameters. After gauge and normalization, we will still have 4 physical parameters. Hence it is not possible to find all the possible states of spin 1 by using only rotations. The standard basis is:

$$\begin{aligned} |m = 1\rangle = |\Uparrow\rangle &\mapsto \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |\vec{e}_z\rangle \\ |m = 0\rangle = |\Updownarrow\rangle &\mapsto \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = |\bar{e}_z\rangle \\ |m = -1\rangle = |\Downarrow\rangle &\mapsto \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = |-\vec{e}_z\rangle \end{aligned} \tag{357}$$

The first and the last states represent circular polarizations. By rotating the first state by 180 degrees we get the third state. This means that we have 180 degree orthogonality. However, the middle state is different: it describes linear polarization. Rotating the middle state by 180 degrees gives the same state again! This explains the reason for marking this state with a double headed arrow.

If we rotate the linear polarization state by 90 degrees we get an orthogonal set of states:

$$\begin{aligned} |\bar{e}_x\rangle &= \frac{1}{\sqrt{2}}(-|\Uparrow\rangle + |\Downarrow\rangle) \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \\ |\bar{e}_y\rangle &= \frac{i}{\sqrt{2}}(|\Uparrow\rangle + |\Downarrow\rangle) \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ i \end{pmatrix} \\ |\bar{e}_z\rangle &= |\Updownarrow\rangle \mapsto \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \end{aligned} \tag{358}$$

This basis is called the linear basis. States of "spin 1" can be written either in the standard basis or in the basis of linear polarizations. The latter option, where we have 90 degree orthogonality of the basis vectors, corresponds to the Euclidean representation.

We can rotate the state $|\Uparrow\rangle$ in order to get other circularly polarized states:

$$|\vec{e}_{\theta,\varphi}\rangle = U(\varphi\vec{e}_z)U(\theta\vec{e}_y)|\Uparrow\rangle = \begin{pmatrix} \frac{1}{2}(1+\cos\theta)\mathrm{e}^{-i\varphi} \\ \frac{1}{\sqrt{2}}\sin\theta \\ \frac{1}{2}(1-\cos\theta)\mathrm{e}^{i\varphi} \end{pmatrix} \tag{359}$$

Similarly, we can rotate the state $|\Updownarrow\rangle$ in order to get other linearly polarized states:

$$|\bar{e}_{\theta,\varphi}\rangle = U(\varphi\vec{e}_z)U(\theta\vec{e}_y)|\Updownarrow\rangle = \begin{pmatrix} -\frac{1}{\sqrt{2}}\sin\theta e^{-i\varphi} \\ \cos\theta \\ \frac{1}{\sqrt{2}}\sin\theta e^{i\varphi} \end{pmatrix} \tag{360}$$

We have discussed above circularly polarized states which are obtained by rotating the $|\Uparrow\rangle$ state, and linear polarized states which are obtained by rotating the $|\Updownarrow\rangle$ state. But a general polarization state will not necessarily be a circularly polarized state or a linearly polarized state, but rather a superposition of such. It is possible to find a one-to-one relation between polarization states of spin 1 and ellipses. The direction of the polarization is the orientation of the ellipse. When the ellipse is a circle, the particle is circularly polarized, and when the ellipse shrinks down to a line, the particle is linearly polarized. All the intermediate states are called "elliptical polarization states".

We have claimed that we can match any state vector with components Ψ_1, Ψ_2, Ψ_3 with an ellipse. Let us check if this is reasonable by counting the number of free parameters. The number of parameters that are needed to determine the quantum state is six (three complex numbers). Taking normalization and gauge freedom into account, we actually need only 4 parameters. That is also the number of parameters that are needed to define an ellipse: two angles define the plane the ellipse is in, another parameter determines the ratio between the major axes (this ratio is 1 for a circle), and another parameter defines the angle of the ellipse in the plane.

[15] Multiplying Representations

[15.1] Multiplying representations

Let us assume we have two Hilbert spaces. One is spanned by the basis $|i\rangle$ and the other is spanned by the basis $|\alpha\rangle$. We can multiply the two spaces "externally" and get a space with a basis defined by:

$$|i,\alpha\rangle = |i\rangle \otimes |\alpha\rangle \tag{361}$$

The dimension of the Hilbert space that we obtain is the multiplication of the dimensions. For example, we can multiply the "position" space x by the spin space m. We will assume that the space contains three sites $x = 1, 2, 3$, and that the particle has spin $\frac{1}{2}$ with $m_1 = -\frac{1}{2}, +\frac{1}{2}$. The dimension of the space that we get from the external multiplication is $2 \times 3 = 6$. The basis states are

$$|x,m\rangle = |x\rangle \otimes |m\rangle \tag{362}$$

A general state is represented by a column vector:

$$|\psi\rangle \rightarrow \begin{pmatrix} \psi_{1\uparrow} \\ \psi_{1\downarrow} \\ \psi_{2\uparrow} \\ \psi_{2\downarrow} \\ \psi_{3\uparrow} \\ \psi_{3\downarrow} \end{pmatrix} \tag{363}$$

Or, in Dirac notation:

$$|\psi\rangle = \sum_{x,m} \psi_{x,m} |x,m\rangle \tag{364}$$

If x has a continuous spectrum then the common notational style is

$$|\Psi\rangle = \sum_{x,m} \Psi_m(x) |x,m\rangle \quad \mapsto \quad \Psi_m(x) = \begin{pmatrix} \Psi_\uparrow(x) \\ \Psi_\downarrow(x) \end{pmatrix} \tag{365}$$

[15.2] External multiplication of operators

Let us assume that in the Hilbert space that is spanned by the basis $|\alpha\rangle$, an operator is defined: $\hat{A} \rightarrow A_{\alpha\beta}$. And in another Hilbert space that is spanned by the basis $|i\rangle$, an operator is defined: $\hat{B} \rightarrow B_{ij}$. An operator $\hat{C} = \hat{B} \otimes \hat{A}$ in the new space is defined as follows:

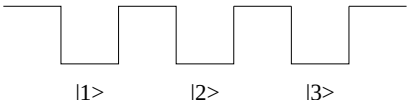
$$C_{i\alpha,j\beta} = B_{ij} A_{\alpha\beta} \tag{366}$$

In Dirac notation:

$$\langle i\alpha|\hat{C}|j\beta\rangle = \langle i|\hat{B}|j\rangle \langle\alpha|\hat{A}|\beta\rangle \tag{367}$$

For example, let us assume that we have a particle in a three-site system:

$$\hat{x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} \tag{368}$$



If the particle has spin $\frac{1}{2}$ we must define the position operator as:

$$\hat{x} = \hat{x} \otimes \hat{1} \tag{369}$$

That means that:

$$\hat{x}|x, m\rangle = x|x, m\rangle \tag{370}$$

And the matrix representation is:

$$\hat{x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix} \tag{371}$$

The system has a 6 dimensional basis. We notice that in physics textbooks there is no distinction between the notation of the operator in the original space and the operator in the space that includes the spin. We must understand the "dimension" of the operator representation by the context. A less trivial example of an external multiplication of operators:

$$\begin{pmatrix} 1 & 0 & 4 \\ 0 & 2 & 0 \\ 4 & 0 & 3 \end{pmatrix} \otimes \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 0 & 0 & 8 & 4 \\ 1 & 2 & 0 & 0 & 4 & 8 \\ 0 & 0 & 4 & 2 & 0 & 0 \\ 0 & 0 & 2 & 4 & 0 & 0 \\ 8 & 4 & 0 & 0 & 6 & 3 \\ 4 & 8 & 0 & 0 & 3 & 6 \end{pmatrix} \tag{372}$$

Specifically, we see that if the operator that we are multiplying externally is diagonal, then we will get a block diagonal matrix.

[15.3] External multiplication of spin spaces

Let us consider two operators in different Hilbert spaces $\hat{L}$ and $\hat{S}$. The bases of the spaces are $|m_\ell\rangle, |m_s\rangle$. The eigenvalues are $m_\ell = 0, \pm 1$ and $m_s = \pm 1/2$. We will mark the new states as follows: $|\Uparrow\uparrow\rangle$, $|\Uparrow\downarrow\rangle$, $|\Updownarrow\uparrow\rangle$, $|\Updownarrow\downarrow\rangle$, $|\Downarrow\uparrow\rangle$, $|\Downarrow\downarrow\rangle$ The system has a basis with 6 states. Therefore, every operator is represented by a 6×6 matrix. We will define, as an example, the operator:

$$\hat{J}_x = \hat{S}_x + \hat{L}_x \tag{373}$$

The three operators operate in 6-D space. A mathematician would write it as follows:

$$\hat{J}_x = \hat{1} \otimes \hat{S}_x + \hat{L}_x \otimes \hat{1} \tag{374}$$

In the next sections we learn how to make the following decompositions:

$$\begin{aligned} &2 \otimes 2 = 1 \oplus 3 \\ &2 \otimes 3 = 2 \oplus 4 \\ &\text{rep. over sphere} = 1 \oplus 3 \oplus 5 \oplus 7 \oplus ... \end{aligned} \tag{375}$$

The first decomposition will be used in connection with the problem of two particles with spin $\frac{1}{2}$, where we can define a basis that includes three symmetrical states (the "triplet") and one anti-symmetric state (the "singlet"). The second example is useful in analyzing the Zeeman splitting of atomic levels. The third example, which is the decomposition of the representation of the rotation group over function space, is best illustrated by considering the motion of a particle on a spherical shell.

======= [15.4] Rotations of a Composite system

We assume that we have a spin ℓ entity whose states are represented by the basis

$$|m_\ell = -\ell ... + \ell\rangle \tag{376}$$

and a spin s entity whose states are represented by the basis

$$|m_s = -s ... + s\rangle \tag{377}$$

The natural $(2\ell+1)\times(2s+1)$ basis for the representation of the composite system is defined as

$$|m_\ell, m_s\rangle = |m_\ell\rangle \otimes |m_s\rangle \tag{378}$$

A rotation of the composite system is represented by the matrices $R^\ell \otimes R^s$, namely

$$\Psi_{m_\ell,m_s} \;=\; R^\ell_{m_\ell,m'_\ell} R^s_{m_s,m'_s} \Psi_{m'_\ell,m'_s} \tag{379}$$

We have

$$R^\ell \otimes R^s \;=\; \mathrm{e}^{-i\Phi\cdot L} \otimes \mathrm{e}^{-i\Phi\cdot S} \;=\; \mathrm{e}^{-i\Phi\cdot J} \tag{380}$$

with the generator

$$J \;=\; L\otimes \hat{1} + \hat{1}\otimes S \;=\; L+S \tag{381}$$

From now on we use the conventional sloppy notations of physicists.

The basis states are eigenstates of J_z. Namely,

$$J_z|m_\ell, m_s\rangle \;=\; (m_\ell + m_s)|m_\ell, m_s\rangle \;\equiv\; m_j|m_\ell, m_s\rangle \tag{382}$$

But we shall see shortly that they are not eigenstates of J^2. This means that the representation is reducible, and can be written as a sum of irreducible representations. Using the conventinal procedure we shall show in the next section that

$$(2\ell+1)\otimes(2s+1) \;=\; (2|\ell+s|+1)\oplus\cdots\oplus(2|l-s|+1) \tag{383}$$

We shall call it the "addition of angular momentum" statement. The output of the "addition of angular momentum" procedure is a new basis $|j, m_j\rangle$ that satisfies

$$J^2|j,m_j\rangle \;=\; j(j+1)|j,m_j\rangle \tag{384}$$
$$J_z|j,m_j\rangle \;=\; m_j|j,m_j\rangle \tag{385}$$

We shall see how to efficiently find the transformation matrix between the "old" and the "new" bases, namely

$$T_{m_\ell m_s, j m_j} = \langle m_\ell, m_s | j, m_j \rangle \tag{386}$$

With this transformation matrix we can transform states and operators between the two optional representations. In particular, note that J^2 is diagonal in the "new" basis, while in the "old basis" it can be calculated as follows:

$$[J^2]_{\text{old basis}} \;\mapsto\; \langle m'_\ell, m'_s | J^2 | m_\ell, m_s \rangle = \langle m'_l, m'_s | j', m'_j \rangle \langle j', m'_j | J^2 | j, m_j \rangle \langle j, m_j | m_\ell, m_s \rangle = T [J^2]_{\text{diagonal}} T^\dagger \tag{387}$$

We shall see that in practical applications each representation has its own advantages.

[15.5] The inefficient decomposition method

Let us discuss as an example the case $\ell = 1$ and $s = 1/2$. In the natural basis we have

$$L_z \;\to\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \tag{388}$$

$$S_z \;\to\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \otimes \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \tag{389}$$

etc. In order to find J^2 we apparently have to do the following calculation:

$$J^2 \;=\; J_x^2 + J_y^2 + J_z^2 \tag{390}$$

The simplest term in this expression is the square of the diagonal matrix

$$J_z \;=\; L_z + S_z \;\to\; [6 \times 6 \;\text{ matrix}] \tag{391}$$

We have two additional terms that contain non-diagonal 6×6 matrices. To find them in a straightforward fashion can be time consuming. Then we have to diagonalize J^2 so as to get the "new" basis.

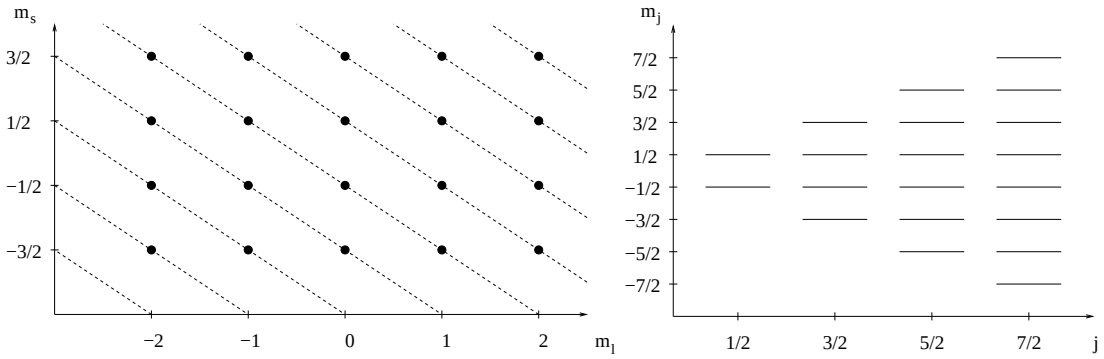
In the next section we explain the efficient procedure to find the "new" basis. Furthermore, it is implied by the "addition of angular momentum" theorem that $3 \otimes 2 = 4 \oplus 2$, meaning that we have a $j = 3/2$ subspace and a $j = 1/2$ subspace. Therefore it is clear that after diagonalization we should get.

$$J^2 \to \begin{pmatrix} (15/4) & 0 & 0 & 0 & 0 & 0 \\ 0 & (15/4) & 0 & 0 & 0 & 0 \\ 0 & 0 & (15/4) & 0 & 0 & 0 \\ 0 & 0 & 0 & (15/4) & 0 & 0 \\ 0 & 0 & 0 & 0 & (3/4) & 0 \\ 0 & 0 & 0 & 0 & 0 & (3/4) \end{pmatrix} \tag{392}$$

This by itself is valuable information. Furthermore, if we know the transformation matrix T we can switch back to the old basis by using a similarity transformation.

[15.6] The efficient decomposition method

In order to explain the procedure to build the new basis we will consider, as an example, the addition of $\ell = 2$ and $s = \frac{3}{2}$. The two graphs below will serve to clarify this example. Each point in the left graph represents a basis state in the $|m_\ell, m_s\rangle$ basis. The diagonal lines connect states that span J_z subspaces. That means $m_\ell + m_s = \text{const} \equiv m_j$. Let us call each such subspace a "floor". The upper floor $m_j = \ell + s$ contains only one state. The lower floor also contains only one state.



We recall that

$$J_z|m_\ell, m_s\rangle = (m_\ell + m_s)|m_\ell, m_s\rangle \tag{393}$$

$$S_-|m_\ell, m_s\rangle = \sqrt{s(s+1) - m_s(m_s-1)}|m_\ell, m_s - 1\rangle \tag{394}$$

$$L_-|m_\ell, m_s\rangle = \sqrt{\ell(\ell+1) - m_\ell(m_\ell-1)}|m_\ell - 1, m_s\rangle \tag{395}$$

$$J_- = S_- + L_- \tag{396}$$

$$J^2 = J_z^2 + \frac{1}{2}(J_+J_- + J_-J_+) \tag{397}$$

Applying J_- or J_+ on a state takes us either one floor down or one floor up. By inspection we see that if J^2 operates on the state in the upper or in the lower floor, then we stay "there". This means that these states are eigenstates of J^2 corresponding to the eigenvalue $j = \ell + s$. Note that they could not belong to an eigenvalue $j > \ell + s$ because this would imply having larger (or smaller) m_j values.

Now we can use J_- in order to obtain the multiplet of $j = \ell + s$ states from the $m_j = \ell + s$ state. Next we look at the second floor from above and notice that we know the $|j = \ell + s, m_j = \ell + s - 1\rangle$ state, so by orthogonalization we can find the $|j = \ell + s - 1, m_j = \ell + s - 1\rangle$ state. Once again we can get the whole multiplet by applying J_-. Going on with this procedure will give us a set of states as arranged in the right graph.

By suggesting the above procedure we have in fact proven the "addition of angular momentum" statement. In the displayed illustration we end up with 4 multiplets ($j = \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}$) so we have $5 \otimes 4 = 8 \oplus 6 \oplus 4 \oplus 2$. In the following sections we review some basic examples in detail.

[15.7] The case of $2 \otimes 2 = 3 \oplus 1$

Consider the addition of $\ell = \frac{1}{2}$ and $s = \frac{1}{2}$ (for example, two electrons). In this case the "old" basis is

$$|m_\ell, m_s\rangle = |\uparrow\uparrow\rangle,\ |\uparrow\downarrow\rangle,\ |\downarrow\uparrow\rangle,\ |\downarrow\downarrow\rangle \tag{398}$$

The "new" basis we want to find is

$$|j, m_j\rangle = \underbrace{|1,1\rangle, |1,0\rangle, |1,-1\rangle}, \underbrace{|0,0\rangle} \tag{399}$$

These states are called triplet and singlet states. It is very easy to apply the procedure as follows:

$$|1,1\rangle \;=\; |\uparrow\uparrow\rangle \tag{400}$$
$$|1,0\rangle \;\propto\; J_-|\uparrow\uparrow\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \tag{401}$$
$$|1,-1\rangle \;\propto\; J_-J_-|\uparrow\uparrow\rangle = 2|\downarrow\downarrow\rangle \tag{402}$$

By orthogonaliztion we get the singlet state, which after normalization is

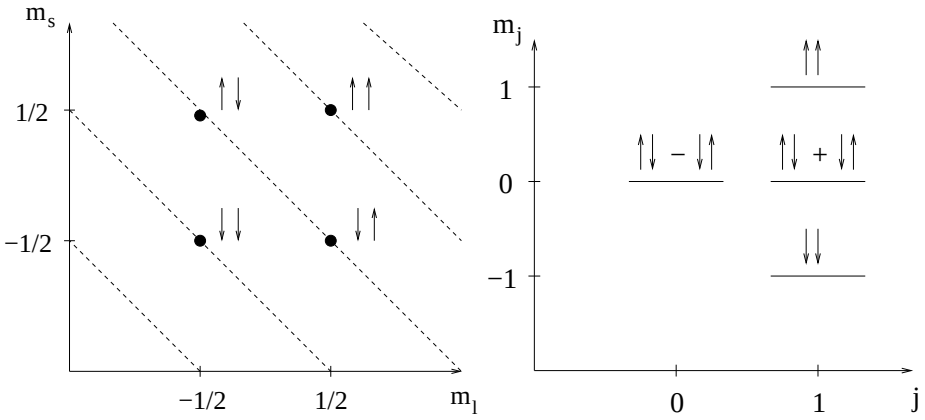
$$|0,0\rangle \;=\; \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{403}$$

Hence the transformation matrix from the old to the new basis is

$$T_{m_\ell,m_s|j,m_j} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{404}$$

The operator J^2 in the $|m_\ell, m_s\rangle$ basis is

$$\langle m'_\ell, m'_s|J^2|m_\ell, m_s\rangle \;=\; T \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} T^\dagger = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \tag{405}$$



═══ [15.8] The case of $3 \otimes 2 = 4 \oplus 2$

Consider the composite system of $\ell = 1$ and $s = \frac{1}{2}$.
In this case the "old" basis is

$$|m_\ell, m_s\rangle = |\Uparrow\uparrow\rangle, |\Uparrow\downarrow\rangle, |\Updownarrow\uparrow\rangle, |\Updownarrow\downarrow\rangle, |\Downarrow\uparrow\rangle, |\Downarrow\downarrow\rangle \tag{406}$$

The "new" basis we want to find is

$$|j,m_j\rangle = \underbrace{|\tfrac{3}{2},\tfrac{3}{2}\rangle, |\tfrac{3}{2},\tfrac{1}{2}\rangle, |\tfrac{3}{2},-\tfrac{1}{2}\rangle, |\tfrac{3}{2},-\tfrac{3}{2}\rangle}, \underbrace{|\tfrac{1}{2},\tfrac{1}{2}\rangle, |\tfrac{1}{2},-\tfrac{1}{2}\rangle} \tag{407}$$

It is very easy to apply the procedure as in the previous section. All we have to remember is that the lowering operator L_- is associated with the $\sqrt{2}$ prefactor:

$$|\tfrac{3}{2},\tfrac{3}{2}\rangle \;=\; |\Uparrow\uparrow\rangle \tag{408}$$

$$|\tfrac{3}{2},\tfrac{1}{2}\rangle \;\propto\; J_-|\Uparrow\uparrow\rangle = |\Uparrow\downarrow\rangle + \sqrt{2}|\Updownarrow\uparrow\rangle \tag{409}$$

$$|\tfrac{3}{2},-\tfrac{1}{2}\rangle \;\propto\; J_-J_-|\Uparrow\uparrow\rangle = 2\sqrt{2}|\Updownarrow\downarrow\rangle + 2|\Downarrow\uparrow\rangle \tag{410}$$

$$|\tfrac{3}{2},-\tfrac{3}{2}\rangle \;\propto\; J_-J_-J_-|\Uparrow\uparrow\rangle = 6|\Downarrow\downarrow\rangle \tag{411}$$

By orthogonalization we get the starting point of the next multiplet, and then we use the lowering operator again:

$$|\tfrac{1}{2},\tfrac{1}{2}\rangle \;\propto\; -\sqrt{2}|\Uparrow\downarrow\rangle + |\Updownarrow\uparrow\rangle \tag{412}$$

$$|\tfrac{1}{2},-\tfrac{1}{2}\rangle \;\propto\; -\sqrt{2}|\Updownarrow\downarrow\rangle + |\Downarrow\uparrow\rangle \tag{413}$$

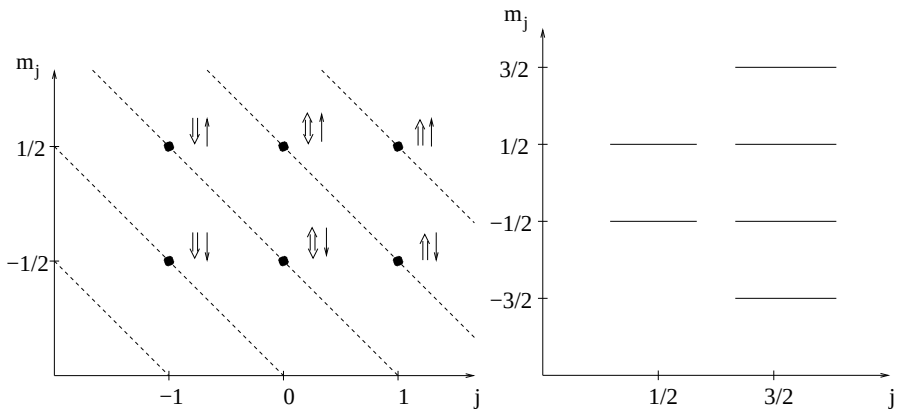
Hence the transformation matrix from the old to the new basis is

$$T_{m_\ell,m_s|j,m_j} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{3}} & 0 & 0 & -\sqrt{\frac{2}{3}} & 0 \\ 0 & \sqrt{\frac{2}{3}} & 0 & 0 & \sqrt{\frac{1}{3}} & 0 \\ 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & -\sqrt{\frac{1}{3}} \\ 0 & 0 & \sqrt{\frac{1}{3}} & 0 & 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \tag{414}$$

and the operator J^2 in the $|m_\ell, m_s\rangle$ basis is

$$\langle m'_\ell, m'_s|J^2|m_\ell, m_s\rangle = T \begin{pmatrix} \frac{15}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{15}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{15}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{15}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{3}{4} \end{pmatrix} T^\dagger = \begin{pmatrix} \frac{15}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{7}{4} & \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & \frac{11}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{11}{4} & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} & \frac{7}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{15}{4} \end{pmatrix} \tag{415}$$

This calculation is done in the Mathematica file *zeeman.nb*.



═══ [15.9] The case of $(2\ell+1)\otimes 2 = (2\ell+2)\oplus(2\ell)$

The last example was a special case of a more general result which is extremely useful in studying the Zeeman Effect in atomic physics. We consider the addition of integer ℓ (angular momentum) and $s = \frac{1}{2}$ (spin). The procedure is exactly as in the previous example, leading to two multiplets: The $j = \ell + \frac{1}{2}$ multiplet and the $j = \ell - \frac{1}{2}$ multiplet. The final expression for the new basis states is:

$$\left| j = \ell \pm \frac{1}{2}, m \right\rangle \;=\; \beta \left| m + \frac{1}{2}, \downarrow \right\rangle + \alpha \left| m - \frac{1}{2}, \uparrow \right\rangle \tag{416}$$

where

$$\alpha \;=\; \sqrt{\frac{\ell + (1/2) \pm m}{2\ell + 1}} \tag{417}$$

$$\beta \;=\; \pm\sqrt{\frac{\ell + (1/2) \mp m}{2\ell + 1}} \tag{418}$$

The $\pm$ signs are for the respective two multiplets. The transformation matrix between the bases has the structure

$$T_{m_l, m_s | j, m_j} = \begin{pmatrix}
1 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & \beta & 0 & \ldots & 0 & 0 & \beta & 0 & \ldots & 0 \\
0 & \alpha & 0. & \ldots & 0 & 0 & \alpha & 0 & \ldots & 0 \\
0 & 0 & \beta & \ldots & 0 & 0 & 0 & \beta & \ldots & 0 \\
0 & 0 & \alpha & \ldots & 0 & 0 & 0 & \alpha & \ldots & 0 \\
0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & \ldots & . \\
. & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . \\
0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & \ldots & \beta & 0 & 0 & 0 & \ldots & \beta \\
0 & 0 & 0 & \ldots & \alpha & 0 & 0 & 0 & \ldots & \alpha \\
0 & 0 & 0 & \ldots & 0 & 1 & 0 & 0 & \ldots & 0
\end{pmatrix} \tag{419}$$

[16] Galilei Group and the Non-Relativistic Hamiltonian

[16.1] The Representation of the Galilei Group

The defining realization of the Galilei group is over phase space. Accordingly, that natural representation is with functions that "live" in phase space. Thus the a-translated $\rho(x,v)$ is $\rho(x-a,v)$ while the u-boosted $\rho(x,v)$ is $\rho(x,v-u)$ etc.

The generators of the displacements are denoted $\mathbf{P}_x, \mathbf{P}_y, \mathbf{P}_z$, the generators of the boosts are denoted $\mathbf{Q}_x, \mathbf{Q}_y, \mathbf{Q}_z$, and the generators of the rotations are denoted $\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z$. Thus we have 9 generators. It is clear that translations and boosts commute, so the only non-trivial structure constants of the Lie algebra have to do with the rotations:

$$[\mathbf{P}_i, \mathbf{P}_j] = \mathbf{0} \tag{420}$$
$$[\mathbf{Q}_i, \mathbf{Q}_j] = \mathbf{0} \tag{421}$$
$$[\mathbf{P}_i, \mathbf{Q}_j] = \mathbf{0} \qquad \text{(to be discussed)} \tag{422}$$
$$[\mathbf{J}_i, \mathbf{A}_j] = i\epsilon_{ijk}\mathbf{A}_k \qquad \text{for } \mathbf{A} = P, Q, J \tag{423}$$

Now we ask the following question: is it possible to find a faithful representation of the Galilei group that "lives" in configuration space. We already know that the answer is "almost" positive: We can represent pure quantum states using "wavefunctions" $\psi(x)$. These wavefunctions can be translated and rotated. On a physical basis it is also clear that we can talk about "boosted" states: this means to give the particle a different velocity. So we can also boost wavefunctions. On physical grounds it is clear that the boost should not change $|\psi(x)|^2$. In fact it is not difficult to figure out that the boost is realized by a multiplication of $\psi(x)$ by $\mathrm{e}^{i(\mathsf{m}u)x}$. Hence we get the identifications $P_x \mapsto -i(d/dx)$ and $Q_x \mapsto -\mathsf{m}x$ for the generators. Still the wise reader should realize that in this "new" representation boosts and translations do not commute, while in case of the strict phase space realization they do commute!

On the mathematical side it would be nice to convince ourselves that the price of not having commutation between translations and boosts is inevitable, and that there is a unique representation (up to a gauge) of the Galilei group using "wavefunctions". This mathematical discussion should clarify that the "compromise" for having such a representation is: (1) The wavefunctions have to be complex; (2) The boosts commute with the translations only up to a phase factor. We shall see that the price that we have to pay is to add $\hat{\mathbf{1}}$ as a tenth generator to the Lie algebra. This is similar to the discussion of the relation between SO(3) and SU(2). The elements of the latter can be regarded as "rotations" provided we ignore an extra "sign factor". Here rather than ignoring a "sign factor" we have to ignore a complex "phase factor".

Finally, we shall see that the most general form of the non-relativistic Hamiltonian of a spinless particle, and in particular its mass, are implied by the structure of the quantum Lie algebra.

[16.2] The Mathematical Concept of Mass

An element τ of the Galilei group is parametrized by 9 parameters. To find a strict (unitary) representation means to associate with each element a linear operator $U(\tau)$ such that $\tau^1 \otimes \tau^2 = \tau^3$ implies

$$U(\tau^1)U(\tau^2) = U(\tau^3) \tag{424}$$

Let us see why this strict requirement cannot be realized if we want a representation with "wavefunctions". Suppose that we have an eigenstate of $\hat{P}$ such that $\hat{P}|k\rangle = k|k\rangle$. since we would like to assume that boosts commute with translations it follows that also $U_{boost}|k\rangle$ is an eigenstate of $\hat{P}$ with the same eigenvalue. This is absurd, because it is like saying that a particle has the same momentum in all reference frames. So we have to replace the strict requirement by

$$U(\tau^1)U(\tau^2) = \mathrm{e}^{i\times\mathrm{phase}}U(\tau^3) \tag{425}$$

This means that now we have an extended group that "covers" the Galilei group, where we have an additional parameter (a phase), and correspondingly an additional generator ($\hat{\mathbf{1}}$). The Lie algebra of the ten generators is characterized by

$$[G_\mu, G_\nu] = i \sum_\lambda c^\lambda_{\mu\nu} G_\lambda \tag{426}$$

where $G_0 = \hat{\mathbf{1}}$ and the other nine generators are P_i, Q_i, J_i with $i = x, y, z$. It is not difficult to convince ourselves that without loss of generality this introduces one "free" parameter into the algebra (the other additional structure constants can be set to zero via appropriate re-definition of the generators). The "free" non-trivial structure constant m appears in the commutation

$$[\mathbf{P}_i, \mathbf{Q}_j] = i\mathsf{m}\delta_{ij} \tag{427}$$

which implies that boosts do not commute with translations.

======== [16.3] Finding the Most General Hamiltonian

Assume that we have a spinless particle for which the standard basis for representation is $|x\rangle$. With appropriate gauge of the x basis the generator of the translations is $P \mapsto -i(d/dx)$. From the commutation relation $[P, Q] = i\mathsf{m}$ we deduce that $Q = -\mathsf{m}\hat{x} + g(\hat{p})$, where $g()$ is an arbitrary function. With appropraite gauge of the momentum basis we can assume $Q = -\mathsf{m}\hat{x}$.

The next step is to observe that the effect of a boost on the velocity operator should be

$$U_{boost}(u)^{-1}\hat{v}U_{boost}(u) = \hat{v} + u \tag{428}$$

which implies that $[Q, \hat{v}] = -i$. The simplest possibility is $\hat{v} = \hat{p}/\mathsf{m}$. But the most general possibility is

$$\hat{v} = \frac{1}{\mathsf{m}}(\hat{p} - A(\hat{x})) \tag{429}$$

where A is an arbitrary function. This time we cannot gauge away A.

The final step is to recall the rate of change formula which implies the relation $\hat{v} = i[\mathcal{H}, \hat{x}]$. The simplest operator that will give the desired result for v is $\mathcal{H} = \frac{1}{2\mathsf{m}}(p - A(x))^2$. But the most general possibility involves a second undetermined function:

$$\mathcal{H} = \frac{1}{2\mathsf{m}}(\hat{p} - A(\hat{x}))^2 + V(x) \tag{430}$$

Thus we have determined the most general Hamiltonian that agrees with the Lie algebra of the Galilei group. In the next sections we shall see that this Hamiltonian is indeed invariant under Galilei transformations.

[17] Transformations and Invariance

[17.1] Transformation of the Hamiltonian

First we would like to make an important distinction between passive ["Heisenberg"] and active ["Schrödinger"] points of view regarding transformations. The failure to appreciate this distinction is an endless source of confusion.

In classical mechanics we are used to the passive point of view. Namely, to go to another reference frame (say a displaced frame) is like a change of basis. Namely, we relate the new coordinates to the old ones (say $\tilde{x} = x - a$), and in complete analogy we relate the new basis $|\tilde{x}\rangle$ to the old basis $|x\rangle$ by a transformation matrix $T = \mathrm{e}^{-ia\tilde{p}}$ such that $|\tilde{x}\rangle = T|x\rangle = |x + a\rangle$.

However we can also use an active point of view. Rather than saying that we "change the basis" we can say that we "transform the wavefunction". It is like saying that "the tree is moving backwards" instead of saying that "the car is moving forward". In this active approach the transformation of the wavefunction is induced by $S = T^{-1}$, while the observables stay the same. So it is meaningless to make a distinction between old (x) and new ($\tilde{x}$) coordinates!

From now on we will use the more convenient active point of view. It is more convenient because it is in the spirit of the Schrödinger (rather than Heisenberg) picture. In this active point of view observables do not transform. Only the wavefunction transforms ("backwards"). Below we discuss the associated transformation of the evolution operator and the Hamiltonian.

Assume that the transformation of the state as we go from the "old frame" to the "new frame" is $\tilde{\psi} = S\psi$. The evolution operator that propagates the state of the system from t_0 to t in the new frame is:

$$\tilde{U}(t, t_0) = S(t)U(t, t_0)S^{-1}(t_0) \tag{431}$$

The idea is that we have to transform the state to the old frame (laboratory) by S^{-1}, then calculate the evolution there, and finally go back to our new frame. We recall that the Hamiltonian is defined as the generator of the evolution. By definition

$$\tilde{U}(t + \delta t, t_0) = (1 - i\delta t\tilde{\mathcal{H}}(t))\tilde{U}(t, t_0) \tag{432}$$

Hence

$$\tilde{\mathcal{H}} \;=\; i\frac{\partial \tilde{U}}{\partial t}\tilde{U}^{-1} \;=\; i\left[\frac{\partial S\,(t)}{\partial t}US\,(t_0)^{-1} + S(t)\frac{\partial U}{\partial t}S(t_0)^{-1}\right]S(t_0)U^{-1}S(t)^{-1} \tag{433}$$

and we get the result

$$\tilde{\mathcal{H}} \;=\; S\mathcal{H}S^{-1} + i\frac{\partial S}{\partial t}S^{-1} \tag{434}$$

In practice we assume a Hamiltonian of the form $\mathcal{H} = h(x, p; V, A)$. Hence we get that the Hamiltonian in the new frame is

$$\tilde{\mathcal{H}} \;=\; h(SxS^{-1}, SpS^{-1}; V, A) + i\frac{\partial S}{\partial t}S^{-1} \tag{435}$$

Recall that "invariance" means that the Hamiltonian keeps its form, but the fields in the Hamiltonian may have changed. So the question is whether we can write the new Hamiltonian as

$$\tilde{\mathcal{H}} = h(x, p; \tilde{A}, \tilde{V}) \tag{436}$$

To have "symmetry" rather than merely "invariance" means that the Hamiltonian remains the same with $\tilde{A} = A$ and $\tilde{V} = V$. We are going to show that the following Hamiltonian is invariant under translations, rotations, boosts and gauge transformations:

$$\mathcal{H} = \frac{1}{2\mathsf{m}} \left(\hat{p} - \vec{A}(x) \right)^2 + V(x) \tag{437}$$

We shall argue that this is the most general non-relativistic Hamiltonian for a spinless particle. We shall also discuss the issue of time reversal (anti-unitary) transformations.

═══ [17.2] Invariance Under Translations

$$\begin{aligned} T &= D(a) = \mathrm{e}^{-ia\hat{p}} \\ S &= T^{-1} = \mathrm{e}^{ia\hat{p}} \end{aligned} \tag{438}$$

The coordinates (basis) transform with T, while the wavefunctions are transformed with S.

$$S\hat{x}S^{-1} = x \hat{+} a \tag{439}$$

$$\begin{aligned} &S\hat{p}S^{-1} = \hat{p} \\ &Sf(\hat{x},\hat{p})S^{-1} = f(S\hat{x}S^{-1}, S\hat{p}S^{-1}) = f(\hat{x}+a,\hat{p}) \end{aligned} \tag{440}$$

Therefore the Hamiltonian is invariant with

$$\begin{aligned} \tilde{V}(x) &= V(x+a) \\ \tilde{A}(x) &= A(x+a) \end{aligned} \tag{441}$$

═══ [17.3] Invariance Under Gauge

$$\begin{aligned} T &= \mathrm{e}^{-i\Lambda(x)} \\ S &= \mathrm{e}^{i\Lambda(x)} \\ &S\hat{x}S^{-1} = \hat{x} \\ &S\hat{p}S^{-1} = \hat{p} - \nabla\Lambda(x) \\ &Sf(\hat{x},\hat{p})S^{-1} = f(S\hat{x}S^{-1}, S\hat{p}S^{-1}) = f(\hat{x},\hat{p}-\nabla\Lambda(x)) \end{aligned} \tag{442}$$

Therefore the Hamiltonian is invariant with

$$\begin{aligned} \tilde{V}(x) &= V(x) \\ \tilde{A}(x) &= A(x) + \nabla\Lambda(x) \end{aligned} \tag{443}$$

Note that the electric and the magnetic fields are not affected by this transformation.

More generally we can consider time dependent gauge transformations with $\Lambda(x,t)$. Then we get in the "new" Hamiltonian an additional term, leading to

$$\begin{aligned} \tilde{V}(x) &= V(x) - (d/dt)\Lambda(x,t) \\ \tilde{A}(x) &= A(x) + \nabla\Lambda(x,t) \end{aligned} \tag{444}$$

In particular we can use the very simple gauge $\Lambda = ct$ in order to change the Hamiltonian by a constant ($\tilde{\mathcal{H}} = \mathcal{H} - c$).

[17.4] Boosts and Transformations to a Moving System

From an algebraic point of view a boost can be regarded as a special case of gauge:

$$\begin{aligned} T &= \mathrm{e}^{i(\mathsf{m}u)x} \\ S &= \mathrm{e}^{-i(\mathsf{m}u)x} \\ S\hat{x}S^{-1} &= \hat{x} \\ S\hat{p}S^{-1} &= \hat{p} + \mathsf{m}u \end{aligned} \tag{445}$$

Hence $\tilde{V}(x) = V(x)$ and $\tilde{A}(x) = A(x) - \mathsf{m}u$. But a transformation to a moving frame is not quite the same thing. The latter combines a boost and a time dependent displacement. The order of these operations is not important because we get the same result up to a constant phase factor that can be gauged away:

$$\begin{aligned} S &= \mathrm{e}^{i\mathrm{phase}(u)}\ \mathrm{e}^{-i(\mathsf{m}u)x}\ \mathrm{e}^{i(ut)p} \\ S\hat{x}S^{-1} &= \hat{x} + ut \\ S\hat{p}S^{-1} &= \hat{p} + \mathsf{m}u \end{aligned} \tag{446}$$

The new Hamiltonian is

$$\tilde{\mathcal{H}} = S\mathcal{H}S^{-1} + i\frac{\partial S}{\partial t}S^{-1} = S\mathcal{H}S^{-1} - u\hat{p} = \frac{1}{2\mathsf{m}}(\hat{p} - \tilde{A}(x))^2 + \tilde{V}(x) + \mathrm{const}(u) \tag{447}$$

where

$$\begin{aligned} \tilde{V}(x,t) &= V(x+ut,t) - u \cdot A(x+ut,t) \\ \tilde{A}(x,t) &= A(x+ut,t) \end{aligned} \tag{448}$$

Thus in the new frame the magnetic field is the same (up to the displacement) while the electric field is:

$$\tilde{\mathcal{E}} = -\frac{\partial \tilde{A}}{\partial t} - \nabla\tilde{V} = \mathcal{E} + u \times \mathcal{B} \tag{449}$$

In the derivation of the latter we used the identity

$$\nabla(u \cdot A) - (u \cdot \nabla)A = u \times (\nabla \times A) \tag{450}$$

Finally we note that if we do not include the boost in S, then we get essentially the same results up to a gauge. By including the boost we keep the same dispersion relation: If in the lab frame $A = 0$ and we have $v = p/\mathsf{m}$, then in the new frame we also have $\tilde{A} = 0$ and therefore $v = p/\mathsf{m}$ still holds.

[17.5] Transformations to a rotating frame

Let us assume that we have a spinless particle held by a a potential $V(x)$. Assume that we transform to a rotating frame. We shall see that the transformed Hamiltonian will have in it a Coriolis force and a centrifugal force.

The transformation that we consider is

$$S = \mathrm{e}^{i(\vec{\Omega}t)\cdot\hat{L}} \tag{451}$$

The new Hamiltonian is

$$\tilde{\mathcal{H}} = S\mathcal{H}S^{-1} + i\frac{\partial S}{\partial t}S^{-1} = \frac{1}{2\mathsf{m}}p^2 + V(x) - \Omega \cdot \hat{L} \tag{452}$$

Without loss of generality we assume $\vec{\Omega} = (0, 0, \Omega)$. Thus we got Hamiltonian that looks very similar to that of a particle in a uniform magnetic field (see appropriate lecture):

$$\mathcal{H} = \frac{1}{2\mathsf{m}}(p - A(x))^2 + V(x) = \frac{p^2}{2\mathsf{m}} - \frac{\mathcal{B}}{2\mathsf{m}}L_z + \frac{\mathcal{B}^2}{8\mathsf{m}}(x^2 + y^2) \tag{453}$$

The Coriolis force is the "magnetic field" $\mathcal{B} = 2\mathsf{m}\Omega$. By adding and subtracting a quadratic term we can write the Hamiltonian $\tilde{\mathcal{H}}$ in the standard way with

$$\begin{aligned} \tilde{V} &= V - \frac{1}{2}\mathsf{m}\Omega^2(x^2 + y^2) \\ \tilde{A} &= A + \mathsf{m}\vec{\Omega} \times r \end{aligned} \tag{454}$$

The extra $-(1/2)\mathsf{m}\Omega^2(x^2 + y^2)$ term is called the centrifugal potential.

======= [17.6] Time Reversal transformations

Assume for simplicity that the Hamiltonian is time independent. The evolution operator is $U = \mathrm{e}^{-i\mathcal{H}t}$. If we make a transformation T we get

$$\tilde{U} = T^{-1}\mathrm{e}^{-i\mathcal{H}t}T = \mathrm{e}^{-i(T^{-1}\mathcal{H}T)t} = \mathrm{e}^{-i\tilde{\mathcal{H}}t} \tag{455}$$

where $\tilde{\mathcal{H}} = T^{-1}\mathcal{H}T$. Suppose we want to reverse the evolution in our laboratory. Apparently we have to engineer T such that $T^{-1}\mathcal{H}T = -\mathcal{H}$. If this can be done the propagator $\tilde{U}$ will take the system backwards in time. We can name such T operation a "Maxwell demon" for historical reasons. Indeed for systems with spins such transformations have been realized using NMR techniques. But for the "standard" Hamiltonian there is a fundamental problem. Consider the simplest case of a free particle $\mathcal{H} = \hat{p}^2/(2\mathsf{m})$. To reverse the sign of the Hamiltonian means to make the mass m negative. This means that there is an unbounded spectrum from below. The feasibility of making such a transformation would imply that a physical system cannot get into thermal equilibrium.

Digression: when Dirac found his Lorentz invariant Hamiltonian, it came out with a spectrum that had an unbounded set of negative energy levels. Dirac's idea to "save" his Hamiltonian was to assume that all the negative energy levels are full of particles. Thus we have a meaningful ground state. If we kick a particle from a negative to a positive energy level we create an electron-positron pair, which requires a positive excitation energy.

But we know from classical mechanics that there is a transformation that reverses the dynamics. All we have to do is to invert the sign of the velocity. Namely $p \mapsto -p$ while $x \mapsto x$. So why not to realize this transformation in the laboratory? This was Loschmidt's claim against Boltzman. Boltzman's answer was "go and do it". Why is it "difficult" to do? Most people will probably say that to reverse the sign of an Avogadro number of particles is tough. But in fact there is a better answer. In a sense it is impossible to reverse the sign even of one particle! If we believe that the dynamics of the system are realized by a Hamiltonian, then *the only physical transformations* are proper canonical transformations. In quantum mechanical language we say that any physical realizable evolution process is described by a unitary operator. We are going to claim that the transformation $p \mapsto -p$ while $x \mapsto x$ cannot be realized by any physical Hamiltonian. The time reversal transformations that we are going to discuss are anti-unitary. They cannot be realized in an actual laboratory experiment. This leads to the distinction between "microreversibility" and actual "reversibility": It is one thing to say that a Hamiltonian has time reversal symmetry. It is a different story to actually reverse the evolution.

Assume that we have a unitary transformation T such that $T\hat{p}T^{-1} = -\hat{p}$ while $T\hat{x}T^{-1} = \hat{x}$. This would imply $T[\hat{x}, \hat{p}]T^{-1} = -[\hat{x}, \hat{p}]$. So we get $i = -i$. This means that such a transformation does not exist. But there is a way out.

Wigner has proved that there are two types of transformations that map states in Hilbert space such that the overalp between states remains the same. These are either unitary transformations or antiunitary transformations. We shall explain in the next section that the "velocity reversal" transformation can be realized by an antiunitary rather than unitary transformation. We also explain that in the case of an antiunitary transformation we get

$$\tilde{U} = T^{-1}\mathrm{e}^{-i\mathcal{H}t}T = \mathrm{e}^{+i(T^{-1}\mathcal{H}T)t} = \mathrm{e}^{-i\tilde{\mathcal{H}}t} \tag{456}$$

where $\tilde{\mathcal{H}} = -T^{-1}\mathcal{H}T$. Thus in order to reverse the evolution we have to engineer T such that $T^{-1}\mathcal{H}T = \mathcal{H}$, or equivalently $[\mathcal{H}, T] = 0$. If such a T exists then we say that $\mathcal{H}$ has time reversal symmetry. In particular we shall explain that in the absence of a magnetic field the non-relativistic Hamiltonian has a time reversal symmetry.

[17.7] Anti-unitary Operators

An anti-unitary operator has an anti-linear rather than linear property. Namely,

$$T\left(\alpha\left|\phi\right\rangle + \beta\left|\psi\right\rangle\right) = \alpha^{*}T\left|\phi\right\rangle + \beta^{*}T\left|\psi\right\rangle \tag{457}$$

The simplest procedure to construct an anti-unitary operator is as follows. We pick an arbitrary basis and define a diagonal anti-unitary operator K. Such operator has the property $K^2 = 1$. In a sense the definition of K is unique. Namely, assume that

$$K\left|r\right\rangle = \mathrm{e}^{i\phi_r}\left|r\right\rangle \tag{458}$$

Without loss of generality we can assume that $\phi_r = 0$. This is because we can gauge the basis. Namely, we can define a new basis $|\tilde{r}\rangle = \mathrm{e}^{i\lambda_r}|r\rangle$ for which

$$K\left|\tilde{r}\right\rangle = \mathrm{e}^{i(\phi_r - 2\lambda_r)}\left|\tilde{r}\right\rangle \tag{459}$$

By setting $\lambda_r = \phi_r/2$ we can make all the eigenvalues equal to one.

Any other antiunitary operator can be written trivially as $T = (TK)K$ where TK is unitary. So in practice any T is represented by complex conjugation followed by a unitary transformation. Disregarding the option of having the "extra" unitary operation, time reversal symmetry $T^{-1}\mathcal{H}T = \mathcal{H}$ means that in the particular basis where T is diagonal the Hamiltonian matrix is real ($\mathcal{H}^{*}_{r,s} = \mathcal{H}_{r,s}$), rather than complex.

Coming back to the the "velocity reversal" transformation it is clear that T should be diagonal in the position basis (x should remain the same). Indeed we can verify that such a T automatically reverses the sign of the momentum:

$$\begin{aligned} \left|k\right\rangle &= \sum_{x} \mathrm{e}^{ikx}\left|x\right\rangle \\ T\left|k\right\rangle &= \sum_{x} T\mathrm{e}^{ikx}\left|x\right\rangle = \sum_{x} \mathrm{e}^{-ikx}\left|x\right\rangle = \left|-k\right\rangle \end{aligned} \tag{460}$$

In the absence of a magnetic field the kinetic term p^2 in the Hamiltonian has symmetry with respect to this T. Therefore we say that in the absence of a magnetic field we have time reversal symmetry. In which case the Hamiltonian is real in the position representation.

What happens if we have a magnetic field? Does it mean that there is no time reversal symmetry? Obviously in particular cases the Hamiltonian may have a different anti-unitary symmetry: if $V(-x) = V(x)$ then the Hamiltonian is symmetric with respect to the transformation $x \mapsto -x$ while $p \mapsto p$. The anti-unitary T in this case is diagonal in the p representation. It can be regarded as a product of "velocity reversal" and "inversion" ($x \mapsto -x$ and $p \mapsto -p$). The former is anti-unitary while the latter is a unitary operation.

If the particle has a spin we can define K with respect to the standard basis. The standard basis is determined by $\hat{x}$ and σ_3. Accordingly

$$K = K_{\text{space}} \otimes K_3 \tag{461}$$

However, $T = K$ is not the standard time reversal symmetry. We would like to have $T^{-1}\sigma T = -\sigma$. This implies that

$$T = \mathrm{e}^{-i\pi S_y} K = -i\sigma_y K \tag{462}$$

Note that $T^2 = (-1)^N$ where N is the number of spin 1/2 particles in the system. This implies Kramers degeneracy for odd N. The issue of time reversal for particles with spin is further discussed in [**Messiah p.669**].

Quantum Mechanics in Practice

[18] Few site system, Fermions and Bosons

[18.1] The Dynamics of a two level system

The most general Hamiltonian for a particle with spin $\frac{1}{2}$ is:

$$\mathcal{H} = \vec{\Omega} \cdot \vec{S} = \Omega_x S_x + \Omega_y S_y + \Omega_z S_z \tag{463}$$

Where $\vec{S} = \frac{1}{2}\vec{\sigma}$.

This means that the evolution operator is:

$$U(t) = \mathrm{e}^{-it\hat{\mathcal{H}}} = \mathrm{e}^{-i(\vec{\Omega}t)\cdot\vec{S}} = R(\vec{\Phi}(t)) \tag{464}$$

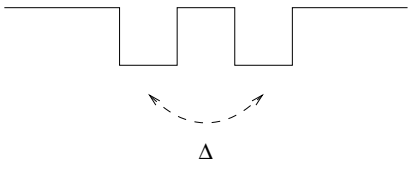
where $\vec{\Phi}(t) = \vec{\Omega}t$. This means that the spin makes precession.

It is best to represent the state of the spin using the polarization vector $\vec{M}$. Then we can describe the precession using a classical picture. The formal derivation of this claim is based on the relation between $M(t)$ and $\rho(t)$. We can write it either as $M(t) = \mathrm{trace}(\sigma\rho(t))$ or as an inverse relation $\rho(t) = (1 + \vec{M}(t)\cdot\sigma)/2$. In the former case the derivation goes as follows:

$$\begin{aligned} M_i(t) &= \mathrm{trace}(\sigma_j\rho(t)) = \mathrm{trace}(\sigma_i(t)\rho) \\ &= \mathrm{trace}((R^{-1}\sigma_i R)\rho) = \mathrm{trace}((R^E_{ij}\sigma_j)\rho) = R^E_{ij}(\Phi(t))\ M_j(0) \end{aligned} \tag{465}$$

where we have used the evolution law $\rho(t) = U(t)\rho(0)U(t)^{-1}$ and the fact that $\vec{\sigma}$ is a vector operator.

We notice that the evolution of any system whose states form a dim=2 Hilbert space can always be described using a precession picture. The purpose of the following section is: (1) To show the power of the precession picture as opposed to diagonalization; (2) To explain the notion of small versus large perturbations.



Above we illustrate a two-site system where c is the probability amplitude (per unit time) to move between the sites. Let us assume without loss of generality that the Hamiltonian is:

$$\mathcal{H} = \begin{pmatrix} \epsilon/2 & c \\ c & -\epsilon/2 \end{pmatrix} = \frac{\epsilon}{2}\sigma_z + c\sigma_x = \vec{\Omega}\cdot\vec{S} \tag{466}$$

Where $\vec{\Omega} = (2c, 0, \epsilon)$. In the case of a symmetric system ($\epsilon = 0$) we can find the eigenstates and then find the evolution by expanding the initial state at that basis. The frequency of the oscillations equals to the energy splitting of the eigen-energies. But once ($\epsilon \neq 0$) this scheme becomes very lengthy and intimidating. It turns out that it is much

much easier to use the analogy with spin 1/2. Then it is clear, just by looking at the Hamiltonian that the oscillation frequency is

$$\Omega = \sqrt{(2c)^2 + \epsilon^2} \tag{467}$$

Also it is clear that the precession axis is tilted relative to the z axis an angle

$$\theta_0 = \arctan(2c/\epsilon) \tag{468}$$

Assuming that initially the system is in state "up", it follows via a simple geometrical inspection that the inclination angle of the polarization $M(t)$ oscillates between the values $\theta = 0$ and $\theta = 2\theta_0$. It follows that $M_z(t)$ oscillates between the maximal value $M_z = 1$ and the minimal value $M_z = \cos(2\theta_0)$.

Let us define $P(t)$ as the probability to find the particle in the left site. We assume that initially $P(0) = 1$. Using the above precession picture and the relation $P(t) = (1 + M_z(t))/2$ we conclude that $P(t)$ oscillates with the frequency Ω between the maximal value 1 and the minimal value $(\cos(\theta_0))^2$.

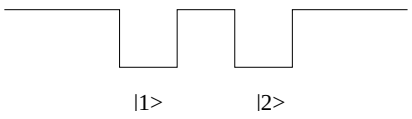
We can easily find an explicit expression for $P(t)$ without having to do any diagonalization of the Hamiltonian. We can use the above precession picture or optionally we can calculate $P(t)$ in a straightforward manner by exploiting well know results for spin 1/2 rotations:

$$P(t) \;=\; |\langle\uparrow|\, \mathrm{e}^{-i\vec{\Omega}t\cdot\vec{S}}|\uparrow\rangle|^2 \;=\; 1 - \cos^2(\theta_0)\sin^2\left(\frac{\Omega t}{2}\right) \tag{469}$$

This result is called Rabi Formula. We see that in order to have nearly complete transitions to the other site after half a period, we need a very strong coupling ($c \gg \epsilon$). In the opposite limit ($c \ll \epsilon$) the particle tends to stay in the same site, indicating that the eigenstates are barely affected.

======== [18.2] A two-site system with one particle

The problem of "positioning a particle of spin $\frac{1}{2}$ in a specific location" is formally identical to the problem of "putting a particle in a two-site system". In both cases the system is described by a two-dimensional Hilbert space dim = 2. Instead of discussing an electron that can be either "up" or "down", we shall discuss a particle that can be either in site 1 or in site 2. In other words, we identify the states as: $|1\rangle = |\uparrow\rangle$ and $|2\rangle = |\downarrow\rangle$.



The standard basis is the position basis $|x = 1\rangle$, $|x = 2\rangle$. The k states are defined in the usual way. We have the even and the odd states with respect to reflection:

$$\begin{aligned} |k = 0\rangle = |+\rangle \;&=\; \frac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right) \\ |k = \pi\rangle = |-\rangle \;&=\; \frac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right) \end{aligned} \tag{470}$$

Note the formal analogy with spin 1/2 system:
$|+\rangle = |\rightarrow\rangle$ represents spin $\frac{1}{2}$ polarized right.
$|-\rangle = |\leftarrow\rangle$ represents spin $\frac{1}{2}$ polarized left.

The representation of the operator $\hat{x}$ is:

$$\hat{x} \to \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} = 1 + \frac{1}{2}\left(1 - \sigma_3\right) \tag{471}$$

where $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the third Pauli matrix. The translation operator is actually a reflection operator:

$$\hat{R} = \hat{D} \rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_1 \tag{472}$$

where σ_1 is the first Pauli matrix. The k states are the eigenstates of the operator D, so they are the eigenstates of σ_1.

[18.3] A two site system with two different particles

In this case the Hilbert space is four dimensional: $\dim = (2 \times 2) = 4$. If the two particles are different (for example, a proton and a neutron) then each state in the Hilbert space is "physical". The standard basis is:

$|1,1\rangle = |1\rangle \otimes |1\rangle$ - particle A in site 1, particle B in site 1
$|1,2\rangle = |1\rangle \otimes |2\rangle$ - particle A in site 1, particle B in site 2
$|2,1\rangle = |2\rangle \otimes |1\rangle$ - particle A in site 2, particle B in site 1
$|2,2\rangle = |2\rangle \otimes |2\rangle$ - particle A in site 2, particle B in site 2

The transposition operator $\hat{T}$ swaps the location of the particles:

$$\hat{T}|i,j\rangle = |j,i\rangle \tag{473}$$

We must not make confusion between the transposition operator and the reflection operators:

$$\begin{aligned} \hat{T} &\mapsto \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ \hat{R} &\mapsto \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \end{aligned} \tag{474}$$

Instead of the basis $|1,1\rangle$, $|1,2\rangle$, $|2,1\rangle$, $|2,2\rangle$, we may use the basis $|A\rangle$, $|1,1\rangle$, $|S\rangle$, $|2,2\rangle$, where we have defined:

$$\begin{aligned} |A\rangle &= \frac{1}{\sqrt{2}}\left(|1,2\rangle - |2,1\rangle\right) \\ |S\rangle &= \frac{1}{\sqrt{2}}\left(|1,2\rangle + |2,1\rangle\right) \end{aligned} \tag{475}$$

The state $|A\rangle$ is anti-symmetric under transposition, and all the others are symmetric under transposition.

[18.4] Placing together two identical particles

The motivation for discussing this system stems from the question: is it possible to place two electrons in the same location so that one of the spins is up and the other is down, or maybe they can be oriented differently. For example, one spin left and one right, or one right and the other up. We shall continue using the terminology of the previous section. We may deduce, from general symmetry considerations that the quantum state of identical particles must be an eigenstate of the transposition operator (otherwise we could conclude that the particles are not identical). It turns out that we must distinguish between two types of identical particles. According to the "spin and statistics theorem", particles with half-odd-integer spins (fermions) must be in an antisymmetric state. Particles with integer spins (bosons) must be in a symmetric state.

Assume that we have two spin zero particles. Such particles are Bosons. There is no problem to place two (or more) Bosons at the same site. If we want to place two such particles in two sites, then the collection of possible states is of dimension 3 (the symmetric states), as discussed in the previous section.

Electrons have spin 1/2, and therefore they are Fermions. Note that the problem of placing "two electron in one site" is formally analogous to the hypothetical system of placing "two spinless electrons in two sites". Thus the physical problem is formally related to the discussion in the previous section, and we can use the same notations. From the requirement of having an antisymmetric state it follows that if we want to place two electrons at the same location then there is only one possible state which is $|A\rangle$. This state is called the "singlet state". We discuss this statement further below.

Let us try to be "wise guys". Maybe there is another way to squeeze to electrons into one site? Rather than placing one electron with spin "up" and the other with spin "down" let us try a superposition of the type $|\rightarrow\leftarrow\rangle - |\leftarrow\rightarrow\rangle$. This state is also antisymmetric under transposition, therefore it is as "good" as $|A\rangle$. Let us see what it looks like in the standard basis. Using the notations of the previous section:

$$\begin{aligned}\frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right) &= \frac{1}{\sqrt{2}}\left(|+\rangle\otimes|-\rangle - |-\rangle\otimes|+\rangle\right) \\ &= \frac{1}{2\sqrt{2}}((|1\rangle+|2\rangle)\otimes(|1\rangle-|2\rangle)) - \frac{1}{2\sqrt{2}}((|1\rangle-|2\rangle)\otimes(|1\rangle+|2\rangle)) \\ &= -\frac{1}{\sqrt{2}}\left(|1\rangle\otimes|2\rangle - |2\rangle\otimes|1\rangle\right) = -|A\rangle\end{aligned} \tag{476}$$

So, we see that mathematically it is in fact the same state. In other words: the antisymmetric state is a single state and it does not matter if we put one electron "up" and the other "down", or one electron "right" and the other "left". Still let us try another possibility. Let us try to put one electron "up" and the other "right". Writing $|\uparrow\rightarrow\rangle$ in the standard basis using the notation of the previous section we get

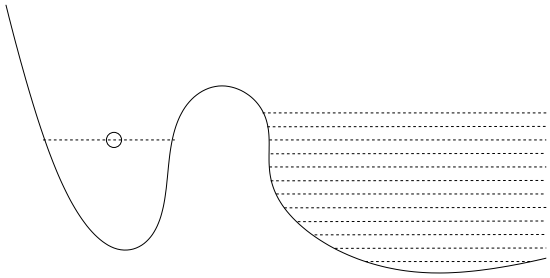
$$|1\rangle\otimes|+\rangle = \frac{1}{\sqrt{2}}|1\rangle\otimes(|1\rangle+|2\rangle) = \frac{1}{\sqrt{2}}(|1,1\rangle+|1,2\rangle) \tag{477}$$

This state is not an eigenstate of the transposition operator, it is neither symmetric nor anti-symmetric state. Therefore it is not physical.

[19] Decay into a continuum

[19.1] Definition of the model

In the problem of a particle in a two site system, we saw that the particle oscillates between the two sites. We will now solve a more complicated problem, where there is one site on one side of the barrier, and on the other side there is a very large number of energy levels (a "continuum").



We will see that the particle "decays" into the continuum. In the two site problem, the Hamiltonian was:

$$\mathcal{H} = \begin{pmatrix} E_0 & \sigma \\ \sigma & E_1 \end{pmatrix} \tag{478}$$

Where σ is the transition amplitude through the barrier. In the new problem, the Hamiltonian is:

$$\mathcal{H} = \begin{pmatrix} E_0 & \sigma & \sigma & \sigma & . & . & . \\ \sigma & E_1 & 0 & 0 & . & . & . \\ \sigma & 0 & E_2 & 0 & . & . & . \\ \sigma & 0 & 0 & E_3 & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{pmatrix} \tag{479}$$

We assume a mean level spacing Δ between the continuum states. If the continuum states are states of a one-dimensional box with length L, then the quantization of the momentum is π/L, and from the relation between the energy and the momentum ($dE = v_E dp$) we get:

$$\Delta = v_E \frac{\pi}{L} \tag{480}$$

From Fermi golden rule we expect to find the decay constant

$$\Gamma \;=\; 2\pi \frac{1}{\Delta} \sigma^2 \tag{481}$$

Below we shall see that this result is exact. We are going to solve both the eigenstate equation

$$(\mathcal{H}_0 + V)_{nn'} \Psi_{n'} = E \Psi_n \tag{482}$$

and the time dependent Schrödinger's equation

$$\frac{d\Psi_n}{dt} \;=\; -i \sum_{n'} (\mathcal{H}_0 + V)_{nn'} \Psi_{n'} \tag{483}$$

where the perturbation term V includes the coupling elements σ.

[19.2] An exact solution for the eigenstates

The unperturbed basis is $|0\rangle, |k\rangle$ with energies E_0 and E_k. The level spacing of the quasi continuum states is Δ. The couplings between the discrete state and the quasi continuum states all equal σ. The system of equations for the eigenstates $|n\rangle$ is

$$E_0\Psi_0 + \sum_k \sigma\Psi_k = E\Psi_0 \tag{484}$$

$$E_k\Psi_k + \sigma\Psi_0 = E\Psi_k \tag{485}$$

From the second line we get how the eigenstates look like:

$$\Psi_k = \frac{\sigma}{E - E_k}\Psi_0 \tag{486}$$

where Ψ_0 should be determined by normalization, while the eigenenergies $E = E_n$ are determined by the equation

$$\sum_k \frac{\sigma^2}{E - E_k} = E - E_0 \tag{487}$$

For equal spacing this can be written as

$$\cot\left(\pi\frac{E}{\Delta}\right) = \frac{1}{\pi}\frac{\Delta}{\sigma^2}(E - E_0) \tag{488}$$

leading to the solution

$$E_n = \left(n + \frac{1}{\pi}\varphi_n\right)\Delta \tag{489}$$

where φ changes monotonically from π to 0. Now we can determine the normalization, leading to

$$\Psi_0 = \frac{\sigma}{\sqrt{(E_n - E_0)^2 + (\Gamma/2)^2}} \tag{490}$$

where

$$\frac{\Gamma}{2} = \sqrt{\sigma^2 + \left(\frac{\pi}{\Delta}\sigma^2\right)^2} \tag{491}$$

This is the Wigner Lorentzian. It gives the overlap of the eigenstates with the unperturbed discrete state. A related result is due to Fano. Assuming that we have an initial state $|F\rangle$ that has coupling Ω to the state $|0\rangle$ and a coupling σ_F to the states $|k\rangle$. Then we get for the decay amplitudes:

$$\langle n|\mathcal{H}|F\rangle = \Omega\langle n|\mathcal{H}|0\rangle + \sigma_F\sum_k \langle n|\mathcal{H}|k\rangle = \frac{\Omega\sigma + (E_n - E_0)\sigma_F}{\sqrt{(E_n - E_0)^2 + (\Gamma/2)^2}} \tag{492}$$

The decay amplitudes to levels E_n that are far away from the resonance is σ_F as in the unperturbed problem. On the other hand, in the vicinity of the resonance we levels to which the decay is suppressed due to destructive interference.

[19.3] An exact solution of the time dependent problem

We switch to the interaction picture:

$$\Psi_n(t) = c_n(t)\mathrm{e}^{-iE_nt} \tag{493}$$

We distinguish between c_k and c_0, and get the system of equations:

$$\begin{aligned} i\frac{dc_0}{dt} &= \sum_k \mathrm{e}^{i(E_0-E_k)t}\, V_{0,k}\, c_k(t) \\ i\frac{dc_k}{dt} &= \mathrm{e}^{i(E_k-E_0)}\, V_{k,0}\, c_0(t) \end{aligned} \tag{494}$$

From the second equation we get:

$$c_k(t) = 0 + \int_0^t \mathrm{e}^{i(E_k-E_0)t'}\, V_{k,0}\, c_0(t')dt' \tag{495}$$

By substituting into the first equation we get:

$$\frac{dc_0}{dt} = -\int_0^t C(t-t')\, c_0(t')\, dt' \tag{496}$$

Where:

$$C(t-t') = \sum_k |V_{k,0}|^2\, \mathrm{e}^{-i(E_k-E_0)(t-t')} \tag{497}$$

The Fourier transform of this function is:

$$\tilde{C}(\omega) = \sum_k |V_{k,0}|^2\, 2\pi\delta(\omega-(E_k-E_0)) \approx \frac{2\pi}{\Delta}\sigma^2 \tag{498}$$

Which means that:

$$C(t-t') \approx \left[\frac{2\pi}{\Delta}\sigma^2\right]\delta(t-t') = \Gamma\delta(t-t') \tag{499}$$

We notice that the time integration only "catches" half of the area of this function. Therefore, the equation for c_0 is:

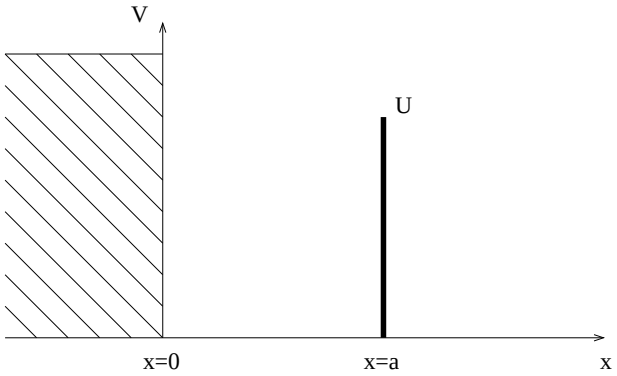
$$\frac{dc_0}{dt} = -\frac{\Gamma}{2}c_0(t) \tag{500}$$

This leads us to the solution:

$$P(t) = |c_0(t)|^2 = \mathrm{e}^{-\Gamma t} \tag{501}$$

[19.4] The Gamow Formula

A particle of mass m in 1D is confined from the left by an infinite potential wall and from the right by a delta function $U(x) = u\delta(x-a)$. We assume large u such that the two regions are weakly coupled. In this section we shall derive an expression for the decay constant Γ. We shall prove that it equals the "attempt frequency" multiplied by the transmission of the barrier. This is called Gamow formula.



We will look for complex energy solutions that satisfy "outgoing wave" boundary conditions. Setting $k = k_r - i\gamma_r$ we write the energy as:

$$\begin{aligned} E &= \frac{k^2}{2\mathsf{m}} = E_r - i\frac{\Gamma_r}{2} \\ E_r &= \frac{1}{2\mathsf{m}}(k_r^2 - \gamma_r^2) \\ \Gamma_r &= \frac{2}{\mathsf{m}} k_r \gamma_r = 2 v_r \gamma_r \end{aligned} \tag{502}$$

In the well the most general solution of $\mathcal{H}\psi = E\psi$ is $\psi(x) = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx}$. Taking the boundary condition $\psi(0) = 0$ at the hard wall, and the outgoing wave boundary condition at infinity we get

$$\begin{aligned} \psi(x) &= C\sin(kx) \qquad \text{for } 0 < x < a \\ \psi(x) &= D\mathrm{e}^{ikx} \qquad \text{for } x > a \end{aligned} \tag{503}$$

The matching conditions across the barrier are:

$$\begin{aligned} \psi(a+0) - \psi(a-0) &= 0 \\ \psi'(a+0) - \psi'(a-0) &= 2\alpha\ \psi(a) \end{aligned} \tag{504}$$

where

$$\alpha = \mathsf{m}\frac{u}{\hbar^2} \tag{505}$$

Thus at $x = a$ the wave functions must fulfill:

$$\frac{\psi'}{\psi}\Big|_+ - \frac{\psi'}{\psi}\Big|_- = 2\alpha \tag{506}$$

leading to

$$ik - k\cot(ka) = 2\alpha \tag{507}$$

We can write last equation as:

$$\tan(ka) = -\frac{\frac{k}{2\alpha}}{1 - i\frac{k}{2\alpha}} \tag{508}$$

The zero order solution in the coupling ($u = \infty$) are the energies of an isolated well corresponding to

$$k = k_n = \frac{\pi}{a} n \tag{509}$$

We assume small coupling c and expand both sides of the equation around k_n. Namely we set $k = (k_n + \delta k) - i\gamma$ where δk and γ are small corrections to the unperturbed energy of the isolated state. To leading order we get:

$$a\delta k - ia\gamma = -\frac{k_n}{2\alpha} - i\left(\frac{k_n}{2\alpha}\right)^2 \tag{510}$$

From the last equation we get:

$$\begin{aligned} k_r &= k_n + \delta k = k_n - \frac{1}{a}\frac{k_n}{2\alpha} \\ \gamma_r &= \frac{1}{a}\left(\frac{k_n}{2\alpha}\right)^2 \end{aligned} \tag{511}$$

From here we can calculate both the shift and the "width" of the energy. To write the result in a more attractive way we recall that the transmission of the delta barrier at the energy $E = E_n$ is

$$g = \frac{1}{1 + (\alpha/k)^2} \approx \left(\frac{k}{\alpha}\right)^2 \tag{512}$$

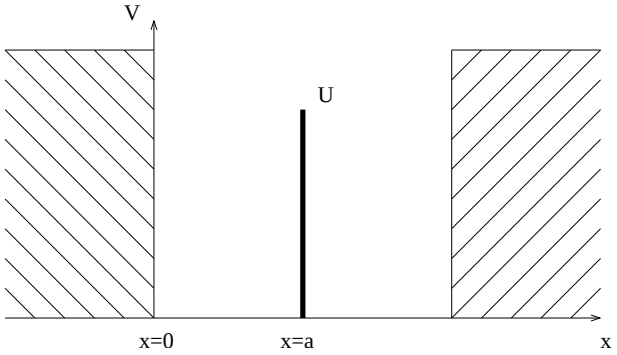
hence

$$\Gamma_r \approx 2v_E \frac{1}{a}\left(\frac{k_n}{2\alpha}\right)^2 \approx \frac{v_E}{2a} g \tag{513}$$

This is called Gamow formula. It reflects the following semiclassical picture: The particle oscillates with velocity $v_E = \sqrt{2E/\mathsf{m}}$ inside the well, hence $v_E/(2a)$ is the number of collisions that it has with the barrier per unit time. The Gamow formula expresses the decay rate as a product of this"attempt frequency" with the transmission of the barrier. It is easy to show that the assumption of weak coupling can be written as $g \ll 1$.

[19.5] From Gamow to the double well problem

Assume a double well which is divided by the same delta function as in the Gamow decay problem. Let us use the solution of the Gamow decay problem in order to deduce the oscillation frequency in the double well.



Going back to the Gamow problem we know that by Fermi golden rule the decay rate is

$$\Gamma = \frac{2\pi}{\Delta_L} |V_{nk}|^2 \tag{514}$$

where V_{nk} is the probability amplitude per unit time to make a transitions form level n inside the well to any of the k states outside of the well. It is assumed that the region outside of the well is very large, namely it has some length L much larger than a. The k states form a quasi-continuum with mean level spacing Δ_L. This expression should be compared with the Gamow formula, which we write as

$$\Gamma = \frac{1}{2\pi} g \Delta_a \tag{515}$$

where g is the transmission of the barrier, and Δ_a is the mean level spacing in the small (length a) region. The Gamow formula should agree with the Fermi golden rule. Hence we deduce that the transition amplitude is

$$|V_{nk}| = \frac{1}{2\pi} \sqrt{g \Delta_a \Delta_L} \tag{516}$$

With some further argumentation we deduce that the coupling between two wavefunctions at the point of a delta junction is:

$$V_{nk} = -\frac{1}{4\mathsf{m}^2 u} [\partial\psi^{(n)}][\partial\psi^{(k)}] \tag{517}$$

where $\partial\psi$ is the radial derivative at the point of the junction. This formula works also if both functions are on the same side of the barrier.

Now we can come back to the double well problem. For simplicity assume a symmetric double well. In the two level approximation n and k are "left" and "right" states with the same unperturbed energy. Due to the coupling we have coherent Bloch oscillation whose frequency is

$$\Omega = 2|V_{nk}| \quad = \quad \frac{1}{\pi} \sqrt{\mathsf{g} \Delta_a \Delta_a} \quad = \quad \frac{v_E}{a} \sqrt{g} \tag{518}$$

[20] The Aharonov-Bohm Effect

[20.1] The Aharonov-Bohm geometry

In the quantum theory it is natural to treat the potentials V, A as basic variables and $\mathcal{E}, \mathcal{B}$ as derived variables. Below we will discuss the case in which $\mathcal{E} = \mathcal{B} = 0$ in the area where the particle is moving. According to the classical theory we expect that the motion of the particle will not be affected by the field, since the Lorentz force is zero. However, we will see that according to the quantum theory the particle will be affected, since $A \neq 0$. This is a topological effect that we are going to clarify.

In what follows we discuss a ring with magnetic flux Φ through it. This is called Aharonov-Bohm geometry. To have flux through the ring means that:

$$\oint \vec{A} \cdot d\vec{l} = \int\int \mathcal{B} \cdot d\vec{s} = \Phi \tag{519}$$

Therefore the simplest possibility is

$$A = \frac{\Phi}{L} \tag{520}$$

where L is the length of the ring. Below we will "spread out" the ring so that we get a particle in the interval $0 < x < L$ with periodical boundary conditions.

$$\hat{\mathcal{H}} = \frac{1}{2\mathsf{m}} \left(\hat{p} - \frac{e\Phi}{cL} \right)^2 \tag{521}$$

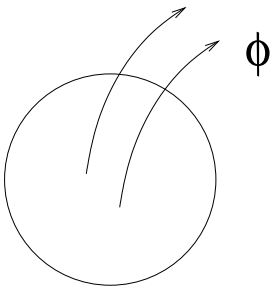
The eigenstates of $\mathcal{H}$ are the momentum states $|k_n\rangle$ where:

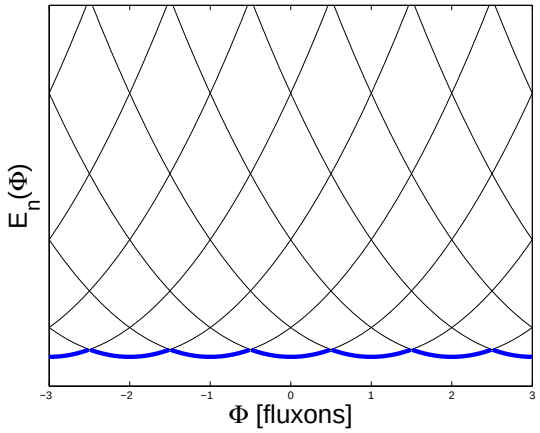
$$k_n = \frac{2\pi}{L} \times \text{integer} \tag{522}$$

The eigenvalues are:

$$E_n = \frac{1}{2\mathsf{m}} \left(\frac{2\pi\hbar}{L} n - \frac{e\Phi}{cL} \right)^2 = \frac{1}{2\mathsf{m}} \left(\frac{2\pi\hbar}{L} \right)^2 \left(n - \frac{e\Phi}{2\pi\hbar c} \right)^2 \tag{523}$$

The unit $2\pi\hbar c/e$ is called "fluxon". It is the basic unit of flux in nature. We see that the energy spectrum is influenced by the presence of the magnetic flux. On the other hand, if we draw a graph of the energies as a function of the flux we see that the energy spectrum repeats itself every time the change in the flux is a whole multiple of a fluxon. (To guide the eye we draw the ground state energy level with thick line).





The fact that the electron is located in an area where there is no Lorentz force $\mathcal{E} = \mathcal{B} = 0$, but is still influenced by the vector potential is called the Aharonov Bohm Effect. This is an example of a topological effect.

[20.2] Digression: energy levels of a ring with a scatterer

Consider an Aharonov-Bohm ring with (say) a delta scatterer:

$$H = \frac{1}{2\mathsf{m}}\left(p - \frac{e\Phi}{L}\right)^2 + u\delta(x) \tag{524}$$

We would like to find the eigenenergies of the ring. The standard approach is to write the general solution in the empty segment, and then to impose the matching condition over the delta scatterer. A simpler method of solution, which is both elegant and also more general, is based on the scattering approach. In order to characterize the scattering within the system, the ring is cut at some arbitrary point and the S matrix of the open segment is specified. It is more convenient to use the row-swapped matrix, such that the transmission amplitudes are along the diagonal:

$$\tilde{\mathbf{S}} = \mathrm{e}^{i\gamma}\begin{pmatrix} \sqrt{g}\mathrm{e}^{i\phi} & -i\sqrt{1-g}\mathrm{e}^{-i\alpha} \\ -i\sqrt{1-g}\mathrm{e}^{i\alpha} & \sqrt{g}\mathrm{e}^{-i\phi} \end{pmatrix} \tag{525}$$

The periodic boundary conditions imply the equation

$$\begin{pmatrix} A \\ B \end{pmatrix} = \tilde{\mathbf{S}}\begin{pmatrix} A \\ B \end{pmatrix} \tag{526}$$

which has a non-trivial solution if and only if

$$\det(\tilde{\mathbf{S}}(E) - \mathbf{1}) = 0 \tag{527}$$

Using

$$\det(\tilde{\mathbf{S}} - I) = \det(\tilde{\mathbf{S}}) - \mathrm{trace}(\tilde{\mathbf{S}}) + 1 \tag{528}$$

$$\det(\tilde{\mathbf{S}}) = (\mathrm{e}^{i\gamma})^2 \tag{529}$$

$$\mathrm{trace}(\tilde{\mathbf{S}}) = 2\sqrt{g}\mathrm{e}^{i\gamma}\cos\phi \tag{530}$$

we get the desired equation:

$$\cos(\gamma(E)) = \sqrt{g(E)}\cos(\phi) \tag{531}$$

where $\phi = e\Phi/\hbar$. With a delta scatterer the transmission of the ring is

$$g(E) = \left[1 + \left(\frac{\mathsf{m}}{\hbar^2 k_E}u\right)^2\right]^{-1} \tag{532}$$

and the associated phase shift is

$$\gamma(E) = k_E L - \arctan\left(\frac{\mathsf{m}}{\hbar^2 k_E}u\right) \tag{533}$$

Note that the free propagation phase is included in γ. In order to find the eigen-energies we plot both sides as a function of E. The left hand side oscillates between -1 and $+1$, while the right hand side is slowly varying monotonically.

[20.3] Digression: The eigenstates of a network system

From geometrical point of view a network (graph) can be regarded as a *ring structure* which is composed of b wires (bonds) that are connected via an $\boldsymbol{S}$ matrix. The wavefunction on a given wire that connects two vertexes i and j is written as

$$|\Psi\rangle \mapsto B_a \mathrm{e}^{ik_a x} + A_a \mathrm{e}^{-ik_{\tilde{a}} x} = A_{\tilde{a}} \mathrm{e}^{ik_a (x-L_a)} + B_{\tilde{a}} \mathrm{e}^{-ik_{\tilde{a}} (x-L_a)} \tag{534}$$

where $0 < x < L_a$ is the position of the particle along the wire, and $k_a = \sqrt{2\mathsf{m}E}/\hbar + (\phi_a/L_a)$ is the wavenumber. The wire index is $a = (i,j)$ if it is regarded as a lead that comes out from $x = 0$ or $\tilde{a} = (j,i)$ if it is regarded as a lead that comes out form the opposite end. The magnetic flux Φ_a along a wire appears via the dimensionless quantity $\phi_a = e\Phi_a/\hbar$. Note that $\phi_{\tilde{a}} = -\phi_a$.

The wavefunction is represented by the vector $A = \{A_a\}$ of length $2b$, or equivalently by the vector $B = \{B_a\}$. The wavefunction and its gradient in the particular point $x = 0$ are

$$\psi = B + A \tag{535}$$
$$\partial\psi = ik \times (B - A) \tag{536}$$

The A and the B vectors are related by

$$B = \boldsymbol{S}\, A \tag{537}$$
$$A = \boldsymbol{J}\, \mathrm{e}^{i\boldsymbol{k}\boldsymbol{L}}\, B \tag{538}$$

where $\boldsymbol{J}$ is a $2b \times 2b$ permutation matrix that that induces the mapping $a \mapsto \tilde{a}$, and $\boldsymbol{L} = \mathrm{diag}\{L_a\}$, and $\boldsymbol{k} = \mathrm{diag}\{k_a\}$. Note that $\boldsymbol{k} = \sqrt{2\mathsf{m}E}/\hbar + \boldsymbol{\phi}/\boldsymbol{L}$, where the fluxes matrix is $\boldsymbol{\phi} = \mathrm{diag}\{\phi_a\}$. If there is a single flux line ϕ one can write $\boldsymbol{\phi} = \phi\boldsymbol{P}$, where $\boldsymbol{P}$ can be expressed as a linear combination of the channel projectors $\boldsymbol{P}_a$. For example, if only one wire a encloses the flux line, then $\boldsymbol{P} = \boldsymbol{P}_a - \boldsymbol{P}_{\tilde{a}}$, while $\phi \equiv \phi_a$. Accordingly

$$\boldsymbol{k} = \frac{1}{\hbar}\sqrt{2\mathsf{m}E} + \phi\frac{\boldsymbol{P}}{\boldsymbol{L}} \tag{539}$$

The equation for the eigenenergies is

$$\left(\boldsymbol{J}\mathrm{e}^{i\boldsymbol{k}\boldsymbol{L}}\boldsymbol{S} - 1\right) A = 0 \tag{540}$$

Given ϕ we can get from this equation a set of eigenvalues E_n with the corresponding eigenvectors $A^{(n)}$ and the associated amplitudes $B^{(n)} = \boldsymbol{S}A^{(n)}$.

In order to define a network system, such as multi-mode ring, we have to specify the following matrices:

$$\boldsymbol{S} \quad \text{(vertexes)} \tag{541}$$
$$\boldsymbol{J} \quad \text{(wires)} \tag{542}$$
$$\boldsymbol{L} \quad \text{(lengths)} \tag{543}$$
$$\boldsymbol{P} \quad \text{(flux)} \tag{544}$$

The $\boldsymbol{S}$ matrix of the network (if appropriately ordered) has a block structure, and can be written as $\boldsymbol{S} = \sum_j \boldsymbol{S}^j$, where S^j is the $v_j \times v_j$ block that describes the scattering in the jth vertex. v_j is the number of leads that stretch out of that vertex. A delta function scatterer is regarded as a $v_j = 2$ vertex. Let us construct a simple example. Consider a ring with two delta barriers. Such ring can be regarded as a network with two wires. The lead indexes are

$12_{\text{L}}, 12_{\text{D}}, 21_{\text{D}}, 21_{\text{L}}$, where L and D distinguish the long wire from the short "dot" segment. The scattering matrix is

$$\boldsymbol{S} = \begin{pmatrix} r_1 & t_1 & 0 & 0 \\ t_1 & r_1 & 0 & 0 \\ 0 & 0 & r_2 & t_2 \\ 0 & 0 & t_2 & r_2 \end{pmatrix} \tag{545}$$

while

$$\boldsymbol{L} = \begin{pmatrix} L & 0 & 0 & 0 \\ 0 & L_0 & 0 & 0 \\ 0 & 0 & L_0 & 0 \\ 0 & 0 & 0 & L \end{pmatrix} \tag{546}$$

and

$$\boldsymbol{J} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{547}$$

═══ [20.4] The Aharonov-Bohm effect in a closed geometry

The eigen-energies of a particle in a closed ring are periodic functions of the flux. In particular in the absence of scattering

$$E_n = \frac{1}{2\mathsf{m}} \left(\frac{2\pi\hbar}{L} \right)^2 \left(n - \frac{e\Phi}{2\pi\hbar c} \right)^2 = \frac{1}{2}\mathsf{m}v_n^2 \tag{548}$$

That is in contrast with classical mechanics, where the energy can have any positive value:

$$E_{\text{classical}} \;=\; \frac{1}{2}\mathsf{m}v^2 \tag{549}$$

According to classical mechanics the lowest state of a magnetic field is energy zero with velocity zero. This is not true in quantum mechanics. In other words: when we add magnetic flux, we can observe its effect on the system. The effect can be described in one of the following ways:

- The spectrum of the system changes (it can be measured using spectroscopy)
- For flux that is not an integer or half integer number there are persistent currents in the system.
- The system has either a diamagnetic or a paramagnetic response (according to the occupancy).

We already have discussed the spectrum of the system. So the next thing is to derive an expression for the current in the ring. The current operator is defined as (see digression):

$$\hat{I} \;=\; -\frac{\partial \mathcal{H}}{\partial \Phi} \;=\; \frac{e}{L}\left[\frac{1}{\mathsf{m}}(\hat{p} - \frac{e\Phi}{L})\right] \;=\; \frac{e}{L}\hat{v} \tag{550}$$

It follows that The current which is created by an electron that occupies the nth level is:

$$I_n \;=\; -\frac{dE_n}{d\Phi} \tag{551}$$

By looking at the plot of the energies $E_n(\Phi)$ as a function of the flux, we can determine (according to the slope) the current that flows in each occupied energy level. For integer or half integer flux all the states "carry current" so that

in equilibrium the net current is not zero. This phenomenon is called "persistent currents". The current in a ring in equilibrium cannot disappear, even if the temperature of the system is zero.

There is a statement in classical statistical mechanics that the equilibrium state of a system is not affected by magnetic fields. The magnetic response of any system is a quantum mechanical effect that has to do with the quantization of the energy levels (Landau magnetism) or with the spins (Pauly magnetism). Definitions:

- Diamagnetic System - in a magnetic field, the system's energy increases.
- Paramagnetic System - in a magnetic field, the system's energy decreases.

The Aharonov Bohm geometry provides the simplest example for magnetic response. If we put one electron in a ring, then when we increase the magnetic flux slightly, the system energy increases. We say that the response is "diamagnetic". The electron cannot "get rid" of its kinetic energy because of the quantization of the momentum.

═══ [20.5] Digression: definition of forces and currents

We would like to know how the system's energy changes when we change one of the parameters (X) that the Hamiltonian ($\mathcal{H}$) depends on. We define the generalized force $\mathcal{F}$ as

$$\mathcal{F} = -\frac{\partial \mathcal{H}}{\partial X} \tag{552}$$

We remember that the rate of change formula for an operator A is:

$$\frac{d\langle \hat{A} \rangle}{dt} = \left\langle i[\hat{\mathcal{H}}, \hat{A}] + \frac{\partial \hat{A}}{\partial t} \right\rangle \tag{553}$$

In particular, the rate of change of the energy is:

$$\frac{dE}{dt} = \frac{d\langle \hat{\mathcal{H}} \rangle}{dt} = \left\langle i[\hat{\mathcal{H}}, \hat{\mathcal{H}}] + \frac{\partial \mathcal{H}}{\partial t} \right\rangle = \left\langle \frac{\partial \mathcal{H}}{\partial t} \right\rangle = \dot{X} \left\langle \frac{\partial \mathcal{H}}{\partial X} \right\rangle = -\dot{X} \langle \mathcal{F} \rangle \tag{554}$$

If $E(0)$ is the energy at time $t = 0$ we can calculate the energy $E(t)$ at a later time, and the work W:

$$W \;=\; -(E(t) - E(0)) \;=\; \int \langle \mathcal{F} \rangle \, \dot{X} dt = \int \langle \mathcal{F} \rangle \, dX \tag{555}$$

A "Newtonian force" is associated with the displacement of a piston. A generalized force called "pressure" is associated with the change of the volume of a box. A generalized force called "polarization" is associated with the change in an electric field. A generalized force called "magnetization" is associated with the change in a magnetic field. Below we will explain why a force called "current" is associated with the change in a magnetic flux.

Lets assume that at a moment t the flux is Φ, and that at the moment $t + dt$ the flux is $\Phi + d\Phi$. The electromotive force (measured in volts) is according to Faraday's law:

$$\text{EMF} \;=\; -\frac{d\Phi}{dt} \tag{556}$$

If the electrical current is I then the amount of charge that has been displaced is:

$$dQ \;=\; I dt \tag{557}$$

Therefore the work which is done is:

$$W \;=\; \text{EMF} \times dQ \;=\; I d\Phi \tag{558}$$

This formula implies that the generalized force which is associated with the change of magnetic flux is in fact the electrical current. Note the analogy between flux and magnetic field, and hence between current and magnetization. In fact one can regard the current in the ring as the "magnetization" of a spinning charge.

[20.6] Digression: Dirac Monopoles

Yet another consequence of the "Aharonov Bohm" effect is the quantization of the magnetic charge. Dirac has claimed that if magnetic monopoles exist, then there must be an elementary magnetic charge. The formal argument can be phrased as follows: If a magnetic monopole exists, it creates a vector potential field in space ($A(x)$). The effect of the field of the monopole on an electron close by is given by the line integral $\oint \vec{A} \cdot d\vec{r}$. We can evaluate the integral by calculating the magnetic flux Φ through a Stokes surface. The result cannot depend on the choice of the surface, otherwise the phase will not be well defined. Therefore the phase $\phi = e\Phi/\hbar c$ must be zero modulo 2π. Specifically, we may choose one Stokes surface that passes over the monopole, and one Stokes surface that passes under the monopole, and conclude that the net flux must be an integer multiple of $2\pi\hbar c/e$. By using "Gauss law" we conclude that the monopole must have a magnetic charge that is an integer multiple of $\hbar c/2e$.

Dirac's original reasoning was somewhat more constructive. Let us assume that a magnetic monopole exist. The magnetic field that would be created by this monopole would be like that of a tip of a solenoid. But we have to *exclude* the region in space where we have the magnetic flux that goes through the solenoid. If we want this "flux line" to be unobservable then it should be quantized in units of $2\pi\hbar c/e$. This shows that Dirac "heard" about the Aharonov Bohm effect, but more importantly this implies that the "tip" would have a charge which equals an integer multiple of $\hbar c/2e$.

[20.7] The Aharonov-Bohm effect: path integral formulation

We can also illustrate the Aharonov-Bohm Effect in an open geometry. In an open geometry the energy is not quantized, but rather it is determined ahead of time. We are looking for stationary states that solve the Schrödinger equation for a given energy. These states are called "scattering states". Below we will discuss the Aharonov-Bohm effect in a "two slit" geometry and then in a "ring" geometry with leads.

First we notice the following rule: if we have a planar wave $\psi(x) = \mathrm{e}^{ikx}$, then if the amplitude at the point $x = x_1$ is $\psi(x_1) = A$, then at another point $x = x_2$ the amplitude is $\psi(x_2) = A\mathrm{e}^{ik(x_2-x_1)}$.

Now we will generalize this rule for the case in which there is a vector potential A. For simplicity's sake, we will assume that the motion is in one-dimension. The eigenstates of the Hamiltonian are the momentum states. If the energy of the particle is E then the wavefunctions that solve the Schrödinger's equation are $\psi(x) = \mathrm{e}^{ik_\pm \cdot x}$. Where:

$$k_\pm \;=\; \pm\sqrt{2\mathsf{m}E} + A \;\equiv\; \pm k_E + A \tag{559}$$

Below we will treat the advancing wave: if at point $x = x_1$ the amplitude is $\psi(x_1) = A$, then at another point $x = x_2$ the amplitude is $\psi(x_2) = A\mathrm{e}^{ik_E(x_2-x_1)+A\cdot(x_2-x_1)}$. It is possible to generalize the idea to three dimensions: if a wave advances along a certain path from point x_1 to point x_2 then the accumulated phase is:

$$\phi \;=\; k_E \times \text{distance} + \int_{x_1}^{x_2} A \cdot dx \tag{560}$$

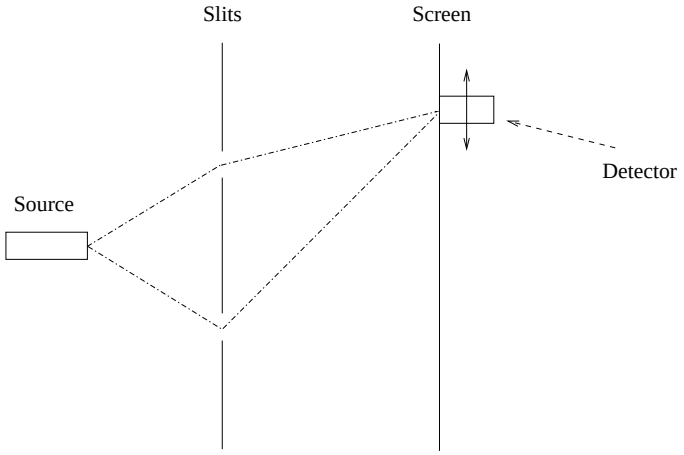
If there are two different paths that connect the points x_1 and x_2, then the phase difference is:

$$\begin{aligned}
\Delta\phi \;&=\; k_E \cdot \Delta\text{distance} + \int_{\text{curve2}} A \cdot dx - \int_{\text{curve1}} A \cdot dx = \\
&=\; k_E \cdot \Delta\text{distance} + \oint A \cdot dx = \\
&=\; k_E \cdot \Delta\text{distance} + \frac{e}{\hbar c}\Phi
\end{aligned} \tag{561}$$

Where in the last term we "bring back" the standard physical units. The approach which was presented above for calculating the probability of the particle to go from one point to another is called "path integrals". This approach was

developed by Feynman, and it leads to what is called "path integral formalism" - an optional approach to calculations in Quantum Mechanics. The conventional method is to solve the Schrödinger's equation with the appropriate boundary conditions.

[20.8] The Aharonov-Bohm effect in a two slits geometry



We will use the path integral point of view in order to analyze the interference in the two slit experiment. A particle that passes through two slits, splits into two partial waves that unite at the detector. Each of these partial waves passes a different optical path. Hence the probability of reaching the detector, and consequently the measures intensity of the beam is

$$\text{intensity} = |1 \times \mathrm{e}^{ikr_1} + 1 \times \mathrm{e}^{ikr_2}|^2 \propto 1 + \cos(k(r_2 - r_1)) \tag{562}$$

If we mark the phase difference as $\phi = k(r_2 - r_1)$, then we can write the result as:

$$\text{intensity} \propto 1 + \cos\phi \tag{563}$$

Changing the location of the detector causes a change in the phase difference ϕ. The "intensity", or more precisely the probability that the particle will reach the detector, as a function of the phase difference ϕ makes an "interference pattern". If we place a solenoid between the slits, then the formula for the phase difference will be:

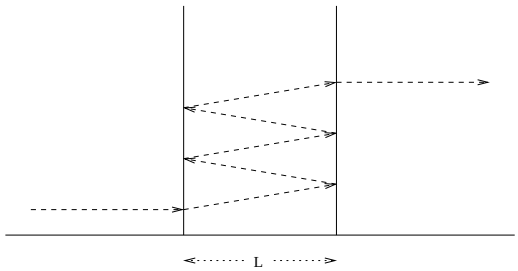
$$\phi = k(r_2 - r_1) + \frac{e}{\hbar c}\Phi \tag{564}$$

If we draw a graph of the "intensity" as a function of the flux we will get the same graph as we would get if we changed the location of the detector. In other words, we will get an "interference pattern" as a function of the flux.

[20.9] Digression: The Fabry Perrot interference problem

If we want to find the transmission of an Aharonov-Bohm device (a ring with two leads) then we must sum all the paths going from the first lead to the second lead. If we only take into account the two shortest paths (the particle can pass through one arm or the other arm), then we get a result that is formally identical to the result for the two slit geometry. In reality we must take into account all the possible paths. That is a very long calculation, so we will demonstrate it with a simpler example. This result is named after Fabry Perrot.

The problem is to find the transmission of a double barrier. We will assume that the barriers are represented by delta functions. The "regular" way of solving this problem is to "sew" together the solutions in the three areas (also known as "matching"). Another way of solving this problem is to "sum over paths", similar to the way we solved the interference problem in the two slit geometry.



We will assume that a delta function's transmission coefficient is $T = |t|^2$, and the reflection coefficient is $R = |r|^2 = 1 - T$. In addition, we will assume that the distance between the two barriers is a so that the partial wave accumulates a phase $\phi = kL$ when going from the one to the other. The transmission of both barriers together is:

$$\text{transmission} = |t \times \mathrm{e}^{i\phi} \times (1 + (r\mathrm{e}^{i\phi})^2 + (r\mathrm{e}^{i\phi})^4 + \dots) \times t|^2 \tag{565}$$

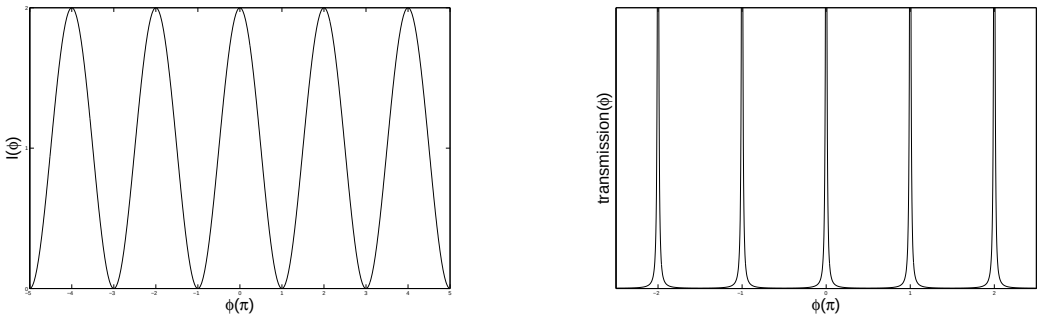
Every round trip between the barriers includes two reflections, so the wave accumulates a phase $(r\mathrm{e}^{i\phi})^2$. We have a geometrical series, and its sum is:

$$\text{transmission} = \left| t \times \frac{\mathrm{e}^{i\phi}}{1 - (r\mathrm{e}^{i\phi})^2} \times t \right|^2 = \tag{566}$$

After some algebra we find the Fabry Perrot expression:

$$\text{transmission} = \frac{1}{1 + 4[R/T^2](\sin(\phi))^2} \tag{567}$$

We notice that this is a very "dramatic" result. If we have two barriers that are almost absolutely opaque $R \sim 1$, then as expected for most energies we get a very low transmission of the order of magnitude of T^2. But there are energies for which $\phi = \pi \times$ integer and then we find that the total transmission is 100%! In the following figure we compare the two slit interference pattern (left) to the Fabry Perrot result (right):



[21] Motion in uniform magnetic field (Landau, Hall)

[21.1] The two-dimensional ring geometry

Let us consider a three-dimensional box with periodic boundary conditions in the x direction, and zero boundary conditions on the other sides. In the absence of magnetic field we assume that the Hamiltonian is:

$$\mathcal{H} = \frac{1}{2\mathsf{m}}\hat{p}_x^2 + \left[\frac{1}{2\mathsf{m}}\hat{p}_y^2 + V(y)\right] + \left[\frac{1}{2\mathsf{m}}\hat{p}_z^2\right] \tag{568}$$

The eigenstates of a particle in such box are labeled as

$$\begin{aligned} &|k_x, n_y, n_z\rangle \\ &k_x = \frac{2\pi}{L} \times \text{integer} \\ &n_y, n_z = 1, 2, 3 \dots \end{aligned} \tag{569}$$

The eigenenergies are:

$$E_{k_x,n_y,n_z} = \frac{k_x^2}{2\mathsf{m}} + \varepsilon_{n_y} + \frac{1}{2\mathsf{m}}(\frac{\pi}{L_z}n_z)^2 \tag{570}$$

We assume L_z to be very small compared to the other dimensions. We will discuss what happens when the system is prepared in low energies such that only $n_z = 1$ states are relevant. So we can ignore the z axis.

[21.2] Classical Motion in a uniform magnetic field

Below we will discuss the motion of electrons on a two-dimensional ring. We assume that the vertical dimension is "narrow", so that we can safely ignore it, as was explained in the previous section. For convenience's sake we will "spread out" the ring so that it forms a rectangle with periodical boundary conditions on $0 < x < L_x$, and an arbitrary potential $V(y)$ on axis y. In addition, we will assume that there is a uniform magnetic field $\mathcal{B}$ along the y axis. Therefore, the electrons will be affected by a Lorentz force $F = -e\mathcal{B} \times v$. If there is no electrical potential, the electrons will perform a circular motion with the cyclotron frequency:

$$\omega_B = \frac{e\mathcal{B}}{\mathsf{m}c} \tag{571}$$

If the particle has a kinetic energy E, then its velocity is:

$$v_E = \sqrt{\frac{2E}{\mathsf{m}}} \tag{572}$$

And then it will move in a circle of radius:

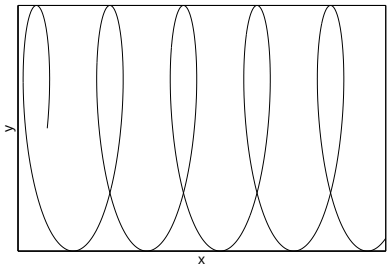
$$r_E = \frac{v_E}{\omega_B} = \frac{\mathsf{m}c}{e\mathcal{B}}v_E \tag{573}$$

If we take into account a non-zero electric field

$$\mathcal{E}_y = -\frac{dV}{dy} \tag{574}$$

we get a motion along a cycloid with the drift velocity (see derivation below):

$$v_{\text{drift}} = c\frac{\mathcal{E}_y}{\mathcal{B}} \tag{575}$$



Let us remind ourselves why the motion is along a cycloid. The Lorentz force in the laboratory reference frame is (from now on we will "swallow" the charge of the electron in the definition of the field):

$$F = \mathcal{E} - \mathcal{B} \times v \tag{576}$$

If we move to a reference frame that is moving at a velocity v_0 we get:

$$F = \mathcal{E} - \mathcal{B} \times (v' + v_0) = (\mathcal{E} + v_0 \times \mathcal{B}) - \mathcal{B} \times v' \tag{577}$$

Therefore, the non-relativistic transformation of the electromagnetic field is:

$$\begin{aligned} \mathcal{E}' &= \mathcal{E} + v_0 \times \mathcal{B} \\ \mathcal{B}' &= \mathcal{B} \end{aligned} \tag{578}$$

If we have a field in the direction of the y axis in the laboratory reference frame, we can move to a "new" reference frame where the field will be zero. From the transformation above we conclude that in order to zero the electrical field, the velocity of the "new" system must be:

$$v_0 = c\frac{\mathcal{E}}{\mathcal{B}} \tag{579}$$

In the "new" reference frame the particle moves in a circle. Therefore, in the laboratory reference frame it moves along a cycloid.

═══ [21.3] The Hall Effect

If we have particles spread out in a uniform density ρ per unit area, then the density of current per unit length as:

$$J_x = e\rho v_{\text{drift}} = \rho\frac{ec}{\mathcal{B}}\mathcal{E}_y = -\rho\frac{e^2c}{\mathcal{B}}\frac{dV}{dy} \tag{580}$$

where V is the electrical potential (measured in Volts) and hence the extra e. The total current is:

$$I_x = \int J_x dy = -\rho\frac{e^2c}{\mathcal{B}}(V_2 - V_1) \tag{581}$$

So that the Hall conductance is:

$$G_{\text{Hall}} = -\rho\frac{e^2c}{\mathcal{B}} \tag{582}$$

Classically we have seen that $J_x \propto (dV/dy)$. We would like to derive this result in a quantum mechanical way and to find the quantum Hall conductance. In the quantum analysis we shall see that the electrons occupy "Landau levels". The density of electrons in each Landau Level is $\mathcal{B}/2\pi\hbar c$. From this it follows that the Hall conductance is quantized in units of $e^2/2\pi\hbar$, which is the universal unit of conductance in quantum mechanics.

We note that both Ohm's law and Hall's law should be written as:

$$I = G \times \frac{1}{e}(\mu_2 - \mu_1) \tag{583}$$

and not as:

$$I = G \times (V_2 - V_1) \tag{584}$$

Where μ is the electrochemical potential. When the electrical force is the only cause for current, then the electrochemical potential is simply the electrical potential (multiplied by the charge of the electron). At zero absolute temperature μ can be identified with the Fermi energy. In metals in equilibrium, according to classical mechanics, there are no currents inside the metal. This means that the electrochemical potential must be uniform. This does not mean that the electrical potential is uniform! For example: when there is a difference in concentrations of the electrons (e.g. different metals) then there should be a "contact potential" to balance the concentration gradient, so as to have a uniform electrochemical potential. Another example: in order to balance the gravitation force in equilibrium, there must be an electrical force such that the total potential is uniform. In general, the electrical field in a metal in equilibrium cannot be zero!

[21.4] Hamiltonian treatment via canonical transformation

In this section we will see that there is an elegant and formal way of treating the problem within the framework of the Hamiltonian formalism. This method of solution is valid both in classical mechanics and in quantum mechanics (all one has to do is swap the Poisson brackets with commutators). In the next lecture we will solve the quantum problem again, using the conventional method of "separation of variables". Below we will use the Landau gauge:

$$\begin{aligned} \vec{A} &= (-\mathcal{B}y, 0, 0) \\ \mathcal{B} &= \nabla \times \vec{A} = (0, 0, \mathcal{B}) \end{aligned} \tag{585}$$

Therefore, the Hamiltonian is (from here we will "swallow" the charge of the electron in the definition of the field):

$$\mathcal{H} = \frac{1}{2\mathsf{m}}(\hat{p}_x + \mathcal{B}y)^2 + \frac{1}{2\mathsf{m}}(\hat{p}_y)^2 + V(y) \tag{586}$$

We define a new set of operators:

$$\begin{aligned} v_x &= \frac{1}{\mathsf{m}}(p_x + \mathcal{B}y) \\ v_y &= \frac{1}{\mathsf{m}}p_y \\ X &= x + \frac{1}{\omega_B}v_y = x + \frac{1}{\mathcal{B}}p_y \\ Y &= y - \frac{1}{\omega_B}v_x = -\frac{1}{\mathcal{B}}p_x \end{aligned} \tag{587}$$

We notice that from a geometrical perspective, X, Y represent the "center of the circle" that the particle moves in. We also notice the commutation relations: the operators X, Y commute with v_x, v_y. On the other hand:

$$\begin{aligned} [X, Y] &= i\frac{1}{\mathsf{m}^2}\frac{e\mathcal{B}}{c} \\ [v_x, v_y] &= -i(\frac{e\mathcal{B}}{c})^{-1} \end{aligned} \tag{588}$$

So that we can define a new set of canonical coordinates:

$$\begin{aligned} Q_1 &= \frac{\mathsf{m}c}{e\mathcal{B}} v_x \\ P_1 &= \mathsf{m} v_y \\ Q_2 &= Y \\ P_2 &= \frac{e\mathcal{B}}{c} X \end{aligned} \tag{589}$$

And rewrite the Hamiltonian as:

$$\mathcal{H}(Q_1, P_1, Q_2, P_2) = \frac{1}{2\mathsf{m}} P_1^2 + \frac{1}{2}\mathsf{m}\omega_B^2 Q_1^2 + V(Q_1 + Q_2) \tag{590}$$

We see (as expected) that $Q_2 = Y$ is a constant of motion. We also see that the kinetic energy is quantized in units of ω_B. Therefore, it is natural to mark the eigenstates as $|Y, \nu\rangle$, where: $\nu = 0, 1, 2, 3 \ldots$, is the kinetic energy index.

======= [21.5] Hamiltonian treatment: the Landau procedure

The Hamiltonian that describes the motion of a particle in the Hall bar geometry is:

$$\hat{\mathcal{H}} = \frac{1}{2\mathsf{m}}(\hat{p}_x + \mathcal{B}\hat{y})^2 + \frac{1}{2\mathsf{m}}(\hat{p}_y)^2 + V(\hat{y}) \tag{591}$$

Recall that we have periodic boundary conditions in the x axis, and an arbitrary confining potential $V(y)$ in the y direction. We also incorporate a homogeneous magnetic field $\mathcal{B} = (0, 0, \mathcal{B})$. The vector potential in the Landau gauge is $\vec{A} = (-\mathcal{B}y, 0, 0)$. We would like to find the eigenstates and the eigenvalues of the Hamiltonian.

The key observation is that in the Landau gauge the momentum operator p_x is a constant of motion. It is more physical to re-phrase this statement in a gauge independent way. Namely, the constant of motion is in fact

$$Y = \hat{y} - \frac{1}{\omega_B}\hat{v}_x = -\frac{1}{\mathcal{B}}\hat{p}_x \tag{592}$$

which represents the y location of the classical cycloid. In fact the eigenstates that we are going to find are the quantum mechanical analog of the classical cycloids. The eigenvalues of $\hat{p}_x$ are $\frac{2\pi}{L_x}\ell$, where $\ell =$ integer. Or, equivalently, we may write that the eigenvalues of $\hat{Y}$ are:

$$Y_\ell \;=\; \frac{2\pi}{\mathcal{B}L_x}\ell \tag{593}$$

That means that the y distance between the eigenstates is quantized. According to the "separation of variables theorem" the Hamiltonian matrix is a block diagonal matrix in the basis in which the $\hat{Y}$ matrix is diagonal. It is natural to choose the basis $|\ell, y\rangle$ which is determined by the operators $\hat{p}_x,\ \hat{y}$.

$$\langle \ell, y|\hat{\mathcal{H}}|\ell', y'\rangle \;=\; \delta_{\ell,\ell'}\,\mathcal{H}^\ell_{yy'} \tag{594}$$

It is convenient to write the Hamiltonian of the block ℓ in abstract notation (without indexes):

$$\hat{\mathcal{H}}^\ell = \frac{1}{2\mathsf{m}}\hat{p}_y^2 + \frac{\mathcal{B}^2}{2\mathsf{m}}(\hat{y} - Y_\ell)^2 + V(\hat{y}) \tag{595}$$

Or, in another notation:

$$\hat{\mathcal{H}}^\ell = \frac{1}{2\mathsf{m}}\hat{p}_y^2 + V_\ell(\hat{y}) \tag{596}$$

where the effective potential is:

$$V_\ell(y) = V(y) + \frac{1}{2}\mathsf{m}\omega_{\mathcal{B}}^2(y - Y_\ell)^2 \tag{597}$$

For a given ℓ, we find the eigenvalues $|\ell,\nu\rangle$ of the one-dimensional Hamiltonian $\hat{\mathcal{H}}^\ell$. The running index is $\nu = 0, 1, 2, 3, \ldots$.

For a constant electric field we notice that this is the Schrödinger equation of a displaced harmonic oscillator. More generally, the harmonic approximation for the effective potential is valid if the potential $V(y)$ is wide compared to the quadratic potential which is contributed by the magnetic field. In other words, we assume that the magnetic field is strong. We write the wave functions as:

$$|\ell,\nu\rangle \;\; \rightarrow \;\; \frac{1}{\sqrt{L_x}}\, \mathrm{e}^{-i(\mathcal{B}Y_\ell)x}\, \varphi^{(\nu)}(y - Y_\ell) \tag{598}$$

We notice that $\mathcal{B}Y_\ell$ are the eigenvalues of the momentum operator. If there is no electrical field then the harmonic approximation is exact, and then $\varphi^{(\nu)}$ are the eigenfunctions of a harmonic oscillator. In the general case, we must "correct" them (in case of a constant electric field they are simply shifted). If we use the harmonic approximation then the energies are:

$$E_{\ell,\nu} \;\approx\; V(Y_\ell) + (\frac{1}{2} + \nu)\omega_B \tag{599}$$

Plotting $E_{\ell,\nu}$ against Y_ℓ we get a picture of "energy levels" that are called "Landau levels" (or more precisely they should be called "energy bands"). The first Landau level is the collection of states with $\nu = 0$. We notice that the physical significance of the term with ν is the kinetic energy. The Landau levels are "parallel" to the bottom of the potential $V(y)$. If there is an area of width L_y where the electric potential is flat (no electric field), then the eigenstates in that area (for a given ν) will be degenerate in the energy (they will have the same energy). Because of the quantization of Y_ℓ the number of particles that can occupy a band of width L_y in each Landau level is finite:

$$g_{landau} \;=\; \frac{L_y}{2\pi/(\mathcal{B}L_x)} \;=\; \frac{L_x L_y}{2\pi}\mathcal{B} \tag{600}$$

Generalization: Here we discuss a trivial generalization of the above solution which will help us in the next section. Let us assume that we add a magnetic flux Φ through the ring, as in the case of Aharonov-Bohm geometry. In this case, the vector potential is:

$$\vec{A} = \left(\frac{\Phi}{L_x} - \mathcal{B}y, 0, 0\right) \tag{601}$$

We can separate the variables in the same way, and get:

$$E_{\ell,\nu} \;\approx\; V\left(Y_\ell + \frac{1}{\mathcal{B}L_x}\Phi\right) + (\frac{1}{2} + \nu)\omega_B \tag{602}$$

═══ [21.6] The Quantum Hall current

We would like to calculate the current for an electron that occupies a Landau state $|\ell,\nu\rangle$:

$$\begin{aligned}
\hat{J}_x(x,y) \;&=\; \frac{1}{2}(ev_x\delta(\hat{x} - x)\delta(\hat{y} - y) + h.c.) \\
\hat{J}_x(y) \;&=\; \frac{1}{L_x}\int \hat{J}_x(x,y)dx \;=\; \frac{e}{L_x}\hat{v}_x\delta(\hat{y} - y) \\
\hat{I}_x \;&=\; -\frac{\partial\mathcal{H}}{\partial\Phi} \;=\; \frac{e}{L_x}v_x \;=\; \int \hat{J}_x(y)dy
\end{aligned} \tag{603}$$

Recall that $v_x = (e\mathcal{B}/\mathsf{m})(\hat{y} - \hat{Y})$, and that the Landau states are eigenstates of $\hat{Y}$. Therefore, the current density of an occupied state is given by:

$$J_x^{\nu\ell}(y) = \langle \ell\nu | \hat{J}_x(y) | \ell\nu \rangle = \frac{e^2\mathcal{B}}{L_x \mathsf{m}} \left\langle (\hat{y} - \hat{Y})\, \delta(\hat{y} - y) \right\rangle = \frac{e^2\mathcal{B}}{\mathsf{m} L_x} (y - Y_\ell)\ |\varphi^\nu(y - Y_\ell)|^2 \tag{604}$$

If we are in the region ($Y_\ell < y$) we observe current that flows to the right (in the direction of the positive x axis), and the opposite if we are on the other side. This is consistent with the classical picture of a particle moving clockwise in a circle. If there is no electric field, the wave function is symmetric around Y_ℓ, so we get zero net current. If there is a non-zero electric field, it shifts the wave function and then we get a net current that is not zero. The current is given by:

$$I_x^{\ell\nu} = \int J_x^{\ell\nu}(y) dy = -\frac{\partial E_{\ell\nu}}{\partial \Phi} = -\frac{1}{\mathcal{B} L_x} \left. \frac{dV(y)}{dy} \right|_{y=Y_\ell} \tag{605}$$

For a Fermi occupation of the Landau level we get:

$$\begin{aligned} I_x &= \sum_\ell I_x^{\ell\nu} = \int_{y_1}^{y_2} \frac{dy}{2\pi/(BL_x)} \left(-\frac{1}{\mathcal{B} L_x} \frac{dV(y)}{dy} \right) \\ &= -\frac{1}{2\pi}(V(y_2) - V(y_1)) = -\frac{e}{2\pi\hbar}(\mu_2 - \mu_1) \end{aligned} \tag{606}$$

In the last equation we have restored the standard physical units. We see that if there is a chemical potential difference we get a current I_x. The Hall coefficient is $e/2\pi\hbar$ times the number of full Landau levels. In other words: the Hall coefficient is quantized in units of $e/2\pi\hbar$.

[22] The Hamiltonian of a spin 1/2 particle

[22.1] The Hamiltonian of a spinless particle

The Hamiltonian of a spinless particle can be written as:

$$\mathcal{H} = \frac{1}{2\mathsf{m}}(\vec{p} - e\vec{A}(r))^2 + eV(r) = \frac{p^2}{2\mathsf{m}} - \frac{e}{2\mathsf{m}}(\vec{A}\cdot\vec{p} + \vec{p}\cdot\vec{A}) + \frac{e^2}{2\mathsf{m}}A^2 + eV(r) \tag{607}$$

We assume that the field is uniform $\mathcal{B} = (0, 0, \mathcal{B}_0)$. In the previous lectures we saw that this field can be derived from $\vec{A} = (-\mathcal{B}_0 y, 0, 0)$, but this time we will use a different gauge, called "symmetrical gauge":

$$\vec{A} = \left(-\frac{1}{2}\mathcal{B}_0 y, \frac{1}{2}\mathcal{B}_0 x, 0\right) = \frac{1}{2}\mathcal{B}\times\vec{r} \tag{608}$$

We will also use the identity (note that triple multiplications are commutative):

$$\vec{A}\cdot\vec{p} = \frac{1}{2}(\mathcal{B}\times\vec{r})\cdot\vec{p} = \frac{1}{2}\mathcal{B}\cdot(\vec{r}\times\vec{p}) = \frac{1}{2}\mathcal{B}\cdot\vec{L} \tag{609}$$

Substitution into the Hamiltonian gives:

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} + eV(r) - \frac{e}{2\mathsf{m}}\mathcal{B}\cdot\vec{L} + \frac{e^2}{8\mathsf{m}}(r^2\mathcal{B}^2 - (\vec{r}\cdot\mathcal{B})^2) \tag{610}$$

Specifically for a homogeneous field in the z axis we get

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} + eV(r) - \frac{e}{2\mathsf{m}}\mathcal{B}_0 L_z + \frac{e^2}{8\mathsf{m}}\mathcal{B}_0^2(x^2 + y^2) \tag{611}$$

The two last terms are called the "Zeeman term" and the "diamagnetic term".

$$\mathcal{H}_{\text{Zeeman,orbital motion}} = -\frac{e}{2\mathsf{m}}\mathcal{B}\cdot\vec{L} \tag{612}$$

[22.2] The additional Zeeman term for the spin

Spectroscopic measurements on atoms have shown, in the presence of a magnetic field, a double (even) Zeeman splitting of the levels, and not just the expected "orbital" splitting (which is always odd). From this Zeeman has concluded that the electron has another degree of freedomwhich is called "spin 1/2". The Hamiltonian should include an additional term:

$$\mathcal{H}_{\text{Zeeman,spin}} = -g\frac{e}{2\mathsf{m}}\mathcal{B}\cdot\vec{S} \tag{613}$$

where $e = -|e|$ is the elementary unit charge. The spectroscopic measurements of the splitting make it possible to determine the gyromagnetic coefficient to a high precision. The same measurements were conducted also for protons, neutrons (a neutral particle!) and other particles:

Electron: $g_e = 2.0023$
Proton: $g_p = -5.5854$
Neutron: $g_n = 3.8271$

The implication of the Zeeman term in the Hamiltonian is that the spin of the particle precesses with the frequency

$$\Omega = -g\frac{e}{2\mathsf{m}}\mathcal{B} \tag{614}$$

whereas the wavefunction of the particle precesses with a different frequency:

$$\Omega = -\frac{e}{2\mathsf{m}}\mathcal{B} \tag{615}$$

======== [22.3] The spin orbit term

The added Zeeman term describes the interaction of the spin with the magnetic field. In fact, the "spin" degree of freedom (and the existence of anti-particles) is inevitable because of relativistic considerations of invariance under the Lorentz transformation. These considerations lead to Dirac's Hamiltonian. There are further "corrections" to the non-relativistic Hamiltonian that are needed in order to make it "closer" to Dirac's Hamiltonian. The most important of these corrections is the "spin orbit interaction":

$$\mathcal{H}_{spin-orbit} = -\frac{e}{2\mathsf{m}^2}(\mathcal{E}\times\vec{p})\cdot\vec{S} \tag{616}$$

where we implicitly use $g \approx 2$. In other words, the spin interacts with the electric field. This interaction depends on its velocity. This is why the interaction is called spin-orbit interaction. If there is also a magnetic field then we have the additional interaction which is described by the Zeeman term.

We can interpret the "spin-orbit" interaction in the following way: even if there is no magnetic field in the "laboratory" reference frame, still there is a magnetic field in the reference frame of the particle, which is a moving reference frame. This follows from Lorentz transformation:

$$\tilde{\mathcal{B}} = \mathcal{B} - \vec{\mathbf{v}}_{\text{frame}}\times\mathcal{E} \tag{617}$$

It looks by this argument that there is a missing factor $g \approx 2$ in the spin-orbit term. But it turn out that this factor is canceled by another factor of $1/2$ that comes from the so called "Thomas precession".

We summarize this lecture by writing the common non-relativistic approximation to the Hamiltonian of a particle with spin $1/2$.

$$\mathcal{H} = \frac{1}{2\mathsf{m}}(\vec{p} - e\vec{A}(r))^2 + eV(r) - g\frac{e}{2\mathsf{m}}\mathcal{B}\cdot\vec{S} - \frac{e}{2\mathsf{m}^2}(\mathcal{E}\times\vec{p})\cdot\vec{S} \tag{618}$$

[23] Motion in a Central Potential

[23.1] The Hamiltonian

We will assume that the only field in space is a central potential which depends only on the distance from the origin. We will write the Hamiltonian in spherical coordinates. For completeness of the discussion we include also the spin-orbit interaction:

$$\begin{aligned}\mathcal{H} &= \frac{1}{2\mathsf{m}}p^2 + eV(r) - \frac{e}{2\mathsf{m}^2}(\mathcal{E}\times\vec{p})\cdot\vec{S} \\ &= \frac{1}{2\mathsf{m}}(p_r^2 + \frac{1}{r^2}L^2) + eV(r) + \frac{e}{2\mathsf{m}^2}\frac{V'(r)}{r}\vec{L}\cdot\vec{S}\end{aligned} \tag{619}$$

Where we have used the following facts:

$$\begin{aligned}&\mathcal{E} = -\frac{V'(r)}{r}\vec{r} \\ &\vec{L} = \vec{r}\times\vec{p} \\ &p_r^2 \to -\frac{1}{r}\frac{\partial^2}{\partial r^2}r\end{aligned} \tag{620}$$

Below, we will neglect the spin-orbit interaction. Later on we will treat it as a "perturbation". In order to find the eigenstates we carry out a separation of variables. The Hamiltonian commutes with rotations:

$$[\hat{\mathcal{H}}, \hat{R}] = 0 \tag{621}$$

And in particular:

$$\begin{aligned}&[\hat{\mathcal{H}}, L^2] = 0 \\ &[\hat{\mathcal{H}}, L_z] = 0\end{aligned} \tag{622}$$

The natural basis for the separation of variables is $|r,\ell,m\rangle$

$$\langle r,\theta,\varphi|r_0,\ell_0,m_0\rangle = Y_{\ell_0,m_0}(\theta,\varphi)\frac{1}{r}\delta(r-r_0) \tag{623}$$

These are states that "live" on spherical shells, and any wave function can be written as a linear combination of the states of this basis. Note that the normalization is correct (the volume element in spherical coordinates includes r^2). According to the "separation of variables theorem" a matrix in this basis has a block structure. And indeed:

$$\begin{aligned}&\langle r,\ell,m|\mathcal{H}|r',\ell',m'\rangle = \delta_{\ell,\ell'}\delta_{m,m'}\mathcal{H}^{(\ell,m)}_{r,r'} \\ &\mathcal{H}^{(\ell,m)} = \frac{1}{2\mathsf{m}}\hat{p}^2 + \left(\frac{\ell(\ell+1)}{2\mathsf{m}r^2} + V(r)\right) = \frac{1}{2\mathsf{m}}p^2 + V^{(\ell)}(r)\end{aligned} \tag{624}$$

Where $p \to -i(d/dr)$.

Note: in the derivation above we have made a "shortcut". In the approach popular in textbooks the basis is not normalized in the separation of variables basis, and the wave function is written as: $R(r)Y_{\ell,m}(\theta,\varphi)$. At a later stage they define $u(r) = rR(r)$, and then get the result that we got. By using the right normalization of the basis we saved ourselves an algebraic stage.

By the separation of variables the problem has turned into a semi-one-dimensional Schrödinger equation for the wave function $u(r)$. By "semi-one-dimensional" we mean that $0 < r < \infty$. In order to get a wave function $\Psi(r,\theta,\varphi)$ that

is continuous at the origin, we must demand that the radial function $R(r)$ be finite, or alternatively that the function $u(r)$ is zero at $r = 0$.

The effective potential $V^(\ell)(r)$ that appears in the semi-one-dimensional problem includes the original potential plus a centrifugal potential (for $\ell \neq 0$). Typically, the centrifugal potential $+1/r^2$ causes a "potential barrier" (positive). But in the case of the Hydrogen atom the attractive potential $-1/r$ wins and there is no such barrier. Moreover, unlike typical short range potentials, the potential has an infinite number of bound states in the $E < 0$ range. In addition, there are also "resonance" states in the range $E > 0$, that can "leak" out through the centrifugal barrier (by tunneling) into the continuum of states outside. Another special property of the Hydrogen atom is the high degree of symmetry (the Hamiltonian commutes with the Runge-Lentz operators). This is manifested in the degeneracy of energy levels that have different ℓ.

[23.2] Reminder: motion on the surface of a torus

First we recapitulate the problem of a particle in a 2-D box. If we demand (as is customary) periodical boundary conditions, this means that the particle moves on the surface of a "torus" (a bagel). For sake of simplicity we assume that the dimensions of the surface are $L_x = L_y = 1$.

The representation of the particle in the standard basis is:

$$|\Psi\rangle = \sum_{x,y} \psi(x,y)|x,y\rangle \tag{625}$$

The representation in the momentum basis is:

$$|\Psi\rangle = \sum_{k_x,k_y} \Psi_{k_x,k_y}|k_x,k_y\rangle \tag{626}$$

If we want to move between the bases, the transformation matrix is:

$$\langle x,y|k_x,k_y\rangle = \mathrm{e}^{ik_x x + ik_y y} \tag{627}$$

The displacement operators in the space basis are not diagonal:

$$D_{\mathbf{x},\mathbf{x}'} = \delta(x-(x'+a_x))\delta(y-(y'+a_y)) \tag{628}$$

However, in the momentum basis we will get diagonal matrices:

$$D_{k,k'} = \delta_{k_x,k'_x}\delta_{k_y,k'_y}\,\mathrm{e}^{-ia_x k_x - ia_y k_y} \tag{629}$$

In other words, we have decomposed the translations group into 1-D representations. This is possible because the group is commutative. If a group is not commutative it is not possible to find a basis in which all the matrices of the group are diagonal simultaneously.

[23.3] Motion on a spherical shell

In full analogy with the case of a torus, the standard representation of the states of a particle that moves on the surface of a sphere is:

$$|\Psi\rangle = \sum_{\theta,\varphi} \psi(\theta,\varphi)|\theta,\varphi\rangle \tag{630}$$

Alternatively, we can work with a different basis:

$$|\Psi\rangle = \sum_{\ell m} \Psi_{\ell m}|\ell,m\rangle \tag{631}$$

If we want to move between the bases, the transformation matrix is:

$$\langle \theta, \varphi | \ell, m \rangle \; = \; Y^{\ell m}(\theta, \varphi) \tag{632}$$

The "displacement" matrices are actually "rotation" matrices. They are not diagonal in the space basis:

$$R_{\mathbf{x},\mathbf{x}'} \; = \; \delta(\theta - f(\theta', \varphi'))\delta(\varphi - g(\theta', \varphi')) \tag{633}$$

But in the new basis the representation of rotations becomes simpler:

$$R_{\ell m, \ell' m'} \; = \; \begin{pmatrix} 1 \times 1 & 0 & 0 & 0 \\ 0 & 3 \times 3 & 0 & 0 \\ 0 & 0 & 5 \times 5 & 0 \\ 0 & 0 & 0 & \ldots \end{pmatrix} \; = \; \text{block diagonal} \tag{634}$$

When we rotate a function, each block stays "within itself". Each group in each block is a sub-space of rotations. The rotation does not mix states that have different ℓ. In other words: in the basis $|\ell, m\rangle$ the representation of the rotation group over the function space decomposes into a sum of representations of finite dimension:

$$1 \oplus 3 \oplus 5 \oplus \ldots \tag{635}$$

In the next section we show how the general procedure we have learned for decomposing representations, does indeed help us to find the $Y^{\ell m}(\theta, \varphi)$ functions.

======= [23.4] The spherical harmonics

We have already found the differential representation of the rotation generators over function space:

$$\begin{aligned} \vec{L} \; &= \; \vec{r} \times \vec{p} \\ L_z &= -i \frac{\partial}{\partial \varphi} \\ L_{\pm} &= \mathrm{e}^{\pm i\varphi} \left(\pm \frac{\partial}{\partial \theta} + i \cot(\theta) \frac{\partial}{\partial \varphi} \right) \\ L^2 &\to \left[\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} (\sin(\theta) \frac{\partial}{\partial \theta}) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] \end{aligned} \tag{636}$$

We must find the eigenstates:

$$\begin{aligned} L^2 \psi &= \ell(\ell+1)\psi \\ L_z \psi &= m\psi \end{aligned} \tag{637}$$

The solution is:

$$Y^{\ell m}(\theta, \phi) \; = \; \left[\frac{2\ell + 1}{4\pi} \frac{(\ell - m)!}{(\ell + m)!} \right]^{1/2} \; [(-1)^m P_{\ell m}(\cos(\theta))] \; \mathrm{e}^{im\varphi} \tag{638}$$

It is customary in physics textbooks to "swallow" the factor $(-1)^m$ in the definition of the Legendre polynomials. We note that it is convenient to start with

$$Y_{\ell\ell}(\theta, \phi) \; \propto \; (\sin(\theta))^{\ell} \, \mathrm{e}^{i\ell\varphi} \tag{639}$$

and then to find the rest of the functions using the lowering operator:

$$|\ell, m\rangle \ \propto \ L_{-}^{(\ell-m)} \, |\ell, \ell\rangle \tag{640}$$

Let us give some examples for Spherical Functions. The simplest function is spread uniformly over the surface of the sphere:

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \tag{641}$$

A linear polarization state along the Z axis is represented by a function that is concentrated mostly at the poles:

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos(\theta) \tag{642}$$

If we rotate this wave function by 90 degrees we get:

$$\begin{aligned} Y_{1,x} &= \sqrt{\frac{3}{4\pi}} \sin(\theta) \cos(\varphi) \\ Y_{1,y} &= \sqrt{\frac{3}{4\pi}} \sin(\theta) \sin(\varphi) \end{aligned} \tag{643}$$

While according to the "recipe" the circular polarizations are:

$$\begin{aligned} Y_{1,1} &= -\sqrt{\frac{3}{8\pi}} \sin(\theta) \mathrm{e}^{i\varphi} \\ Y_{1,-1} &= +\sqrt{\frac{3}{8\pi}} \sin(\theta) \mathrm{e}^{-i\varphi} \end{aligned} \tag{644}$$

[23.5] Eigenstates of a particle on a spherical surface

We set the ground state as the reference energy, and find that the energy levels are:

$$E_{\ell m} \ = \ \frac{1}{2\mathsf{m} R^2} \ell(\ell+1) \tag{645}$$

Where R is the radius of the spherical shell. We remind ourselves of the considerations leading to the degeneracies. In the most symmetrical state Y_{00}, the symmetry of the state is the same as the symmetry of the Hamiltonian since they are both invariant under rotations. In this state there are no degeneracies. On the other hand, the state Y_{10} has a lower symmetry and by rotating it we get 3 orthogonal states with the same energy. The degeneracy is a "compensation" for the low symmetry of the state, so that the symmetry of the energy level is conserved globally.

We mark the number of states up to energy E by $N(E)$. It is easy to prove that the density of states is:

$$\frac{dN}{dE} \ \approx \ \frac{\mathsf{m}}{2\pi\hbar^2} \mathrm{A} \tag{646}$$

Where A is the surface area. It can be proved that this formula is also valid for other surfaces. The most trivial example is obviously a rectangular surface:

$$E_{n_x, n_y} \ = \ \frac{\pi^2}{2\mathsf{m} L_x^2} n_x^2 + \frac{\pi^2}{2\mathsf{m} L_y^2} n_y^2 \tag{647}$$

For a 3-D box it is possible to show that the density of states is proportional to the volume.

[23.6] The Hydrogen Atom

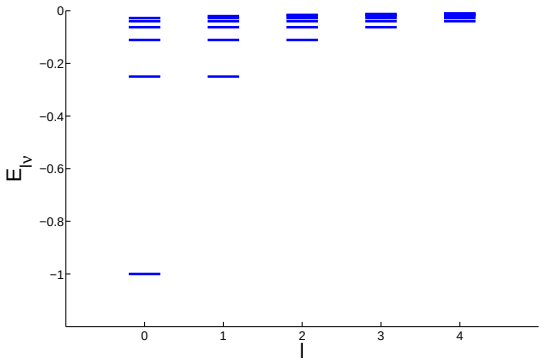
The potential is:

$$V(r) = -\frac{\alpha}{r} \tag{648}$$

We solve the radial equation (for each ℓ separately) and get:

$$E_{\ell,m,\nu} = -\frac{\alpha^2 \mathsf{m}}{2(\ell+\nu)^2} \tag{649}$$

Where $\nu = 1, 2, 3, \ldots$. The energy levels are illustrated in the diagram below:



[23.7] Why are there degeneracies in the energy spectrum

When the Hamiltonian has a single constant of motion, there will usually not be a degeneracy. According to the separation of variables theorem it is possible to move to a basis in which the Hamiltonian will have a block structure, and then diagonalize each block separately. There is no reason for a conspiracy amongst the blocks. Therefore there is no reason for a degeneracy. If we still get a degeneracy it is called an accidental degeneracy.

But, if the Hamiltonian commutes with a "non-commutative group" then there are necessarily degeneracies that are determined by the dimensions of the irreducible representations. In the case of a central potential, the symmetry group is the "rotation group". In the special case of the potential $-1/r$ a larger symmetry group exists.

Statements:

- A degeneracy is compensation for the fact that the eigenstates of the Hamiltonian have a lower symmetry.
- The degree of degeneracy is determined by the dimensions of the irreducible representations.

There are several ways of explaining why there must be a degeneracy. The most intuitive way is as follows: let us assume that we have found an eigenstate of the Hamiltonian. If it has the same degree of symmetry (spherical symmetry) then there is no reason for degeneracy. These are the states with $\ell = 0$. But, if we have found a state with a lower symmetry (the states with $\ell \neq 0$) then we can rotate it and get another state with the same energy level. Therefore, in this case there must be a degeneracy.

Instead of "rotating" an eigenstate, it is simpler (technically) to find other states with the same energy by using ladder operators. This already gives an explanation why the degree of the degeneracy is determined by the dimension of the irreducible representations. Below, we will offer an alternative explanation for this statement.

The Hamiltonian $\mathcal{H}$ commutes with all the rotations, and therefore it also commutes with all their generators and also with L^2. We choose a basis $|n, \ell, \nu\rangle$ in which both $\mathcal{H}$ and L^2 are diagonal. The index of the energy levels n is

determined by $\mathcal{H}$, while the index ℓ is determined by L^2. The index ν differentiates states with the same energy and the same ℓ. According to the "separation of variables theorem" every rotation matrix will have a "block structure" in this basis: each level that is determined by the quantum numbers (n, ℓ) is an invariant subspace of the induced representation. In other words, $\mathcal{H}$ together with L^2 induce a primary decomposition of the group. Now we can continue using the standard procedure in order to conclude that the dimension of the (sub) representation which is characterized by the quantum number ℓ, is $2\ell + 1$. In other words, we have discovered that the degree of the degeneracy must be $2\ell + 1$ (or a multiple of this number).

[24] Implications of having "spin"

[24.1] The Stern-Gerlach effect

We first discuss the effect that the Zeeman term has on the dynamics of a "free" particle. We will see that because of this term, there is a force on the particle if the magnetic field is not homogeneous. For simplicity's sake, we will assume that there is a magnetic field in the direction of the Z axis (note that this can be true only as an approximation). If we keep only the Zeeman term then the Hamiltonian is:

$$\mathcal{H} = \frac{\vec{p}^2}{2\mathsf{m}} - g_s \frac{e}{2\mathsf{m}} \mathcal{B}_z(x) S_z \tag{650}$$

We see that S_z is a constant of motion. That means that if we have prepared a particle in the "up" state, it sees an effective potential:

$$\mathcal{V}_{\text{eff}} = -\frac{1}{2} g_s \frac{e}{2\mathsf{m}} \mathcal{B}_z(x) \tag{651}$$

While a particle with spin "down" sees an inverted potential (with the opposite sign). That means that the direction of the force depends on the the direction of the spin. We can come to the conclusions by looking at the equations of motion. As we have seen before:

$$\frac{d}{dt}\langle x \rangle = \langle i[\mathcal{H}, x] \rangle = \langle \frac{1}{\mathsf{m}} (\vec{p} - A(x)) \rangle \tag{652}$$

This still holds with no change. But what about the acceleration? We see that there is a new term:

$$\frac{d}{dt}\langle v \rangle = \langle i[\mathcal{H}, v] \rangle = \frac{1}{\mathsf{m}} \left\langle \text{ Lorentz force } + \; g_s \frac{e}{2\mathsf{m}} (\nabla \mathcal{B}_z) S_z \right\rangle \tag{653}$$

The observation that in inhomogeneous magnetic field the force on the particle depends on the spin orientation is used in order to measure the spin using a Stern-Gerlach apparatus.

[24.2] The reduced Hamiltonian in a central potential

The reduced Hamiltonian for with the ℓ sub-space of a particle moving in a central potential can be written as:

$$\mathcal{H}^{(\ell)} = \mathcal{H}_0^{(\ell)} - \frac{e}{2\mathsf{m}} \mathcal{B} L_z - g_s \frac{e}{2\mathsf{m}} \mathcal{B} S_z + f(r) L \cdot S \tag{654}$$

The interaction $L \cdot S$ commutes with L^2, therefore ℓ is still a good quantum number. If we assume that the last terms in the Hamiltonian are a weak perturbation that does not "mix" energy levels, then we can make an approximation(!) and reduce further by taking the states that have the same energy:

$$\mathcal{H}^{(\ell\nu)} = -h L_z - g_S h S_z + v L \cdot S + \text{const} \tag{655}$$

Where the first term with $h = e\mathcal{B}/(2\mathsf{m})$ is responsible for the orbital Zeeman splitting, and the second term with $g_S h$ is responsible to the spin-related Zeeman splitting. We also use the notation

$$v = \langle \ell, \nu | f(r) | \ell, \nu \rangle \tag{656}$$

If the spin-orbit interaction did not exist, the dynamics of the spin would become independent of the dynamics of the wave function. But even when there is a spin-orbit interaction, the situation is not so bad. $L \cdot S$ couples only states

with the same ℓ. We will focus on the second state of the Hydrogen atom. The Hamiltonian matrix is 8×8. But it decomposes trivially into matrix blocks of 2×2 and 6×6. We notice that the 2×2 block is already diagonalized: the only term that could destroy the diagonalization (to couple states in the block) is $L \cdot S$, but it is zero in this block since $\ell = 0$. So, we only have to diagonalize the 6×6 block.

Why does $L \cdot S$ couple only states with the same ℓ? The full rotation generator $J = L + S$ rotates both the wave equation and the spin. The system is symmetrical to rotations. So, it is obvious that $[\mathcal{H}, J] = 0$ and specifically $[L \cdot S, J] = 0$. On the other hand, the symmetry: $[\mathcal{H}, L^2] = [L \cdot S, L^2] = 0$ is less trivial. The Hamiltonian is not symmetrical under rotations generated by L. We must rotate both the wave function and the spin together, in order for the Hamiltonian to stay the same. In order to prove the commutation relation with L^2, we notice that:

$$\vec{L} \cdot \vec{S} = \frac{1}{2}\left(J^2 - L^2 - S^2\right) \tag{657}$$

We consider the reduced Hamiltonian for the state $\ell = 1, \nu = 1$, in the standard basis $|\ell = 1, \nu = 1, m_\ell, m_s\rangle$. As mentioned above, the Hamiltonian is represented by a 6×6 matrix. It is easy to write the matrices for the Zeeman terms:

$$\begin{aligned} L_z &\to \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \\ S_z &\to \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \otimes \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \end{aligned} \tag{658}$$

But the spin-orbit term is not diagonal. In principle, we must make the following calculation:

$$\vec{L} \cdot \vec{S} = \frac{1}{2}\left(J^2 - L^2 - S^2\right) = \frac{1}{2}\left(J_x^2 + J_y^2 + J_z^2 \; - \; 2 \; - \; \frac{3}{4}\right) \tag{659}$$

Where the most simple term in this expression includes the diagonal matrix:

$$J_z \; = \; L_z + S_z \; \to \; [6 \times 6 \text{ matrix}] \tag{660}$$

And there are two additional terms that include 6×6 matrices that are not diagonal ... We will see later on that there is a relatively simple way to find the representation of J^2 in the "normal" basis. In fact, it is very easy to "predict" what it will look like after diagonalization:

$$J^2 \to \begin{pmatrix} (15/4) & 0 & 0 & 0 & 0 & 0 \\ 0 & (15/4) & 0 & 0 & 0 & 0 \\ 0 & 0 & (15/4) & 0 & 0 & 0 \\ 0 & 0 & 0 & (15/4) & 0 & 0 \\ 0 & 0 & 0 & 0 & (3/4) & 0 \\ 0 & 0 & 0 & 0 & 0 & (3/4) \end{pmatrix} \tag{661}$$

It follows that the eigenenergies of the Hamiltonian in the absence of a magnetic field are:

$$\begin{aligned} &E_{j=\frac{3}{2}} = v/2 \quad \text{degeneracy} = 4 \\ &E_{j=\frac{1}{2}} = -v \quad \text{degeneracy} = 2 \end{aligned} \tag{662}$$

On the other hand, in a strong magnetic field the spin-orbit term is negligible, and we get:

$$E_{m_\ell,m_s} = -(m_\ell + g_s m_s)h \tag{663}$$

[24.3] Detailed analysis of the Zeeman effect

The reduced Hamiltonian that describes (for example) the first $\ell = 1$ level of the Hydrogen atom is the 6×6 matrix

$$\mathcal{H} \;=\; hL_z + g_s h S_z + v\vec{L}\cdot\vec{S} \tag{664}$$

where $h = \frac{|e|}{2\mathsf{m}}\mathcal{B}$ is the magnetic field in appropriate units, and v is determined by the spin orbit interaction. Also we have $g_s = 2.0023$. Using the identity

$$\vec{L}\cdot\vec{S} = \frac{1}{2}\left(J^2 - L^2 - S^2\right) = \frac{1}{2}\left(J^2 \,-\, 2 \,-\, \frac{3}{4}\right) \tag{665}$$

the Hamiltonain can be written in the alternate form:

$$\mathcal{H} \;=\; hL_z + g_s h S_z + \frac{v}{2}\left(J^2 - \frac{11}{4}\right) \tag{666}$$

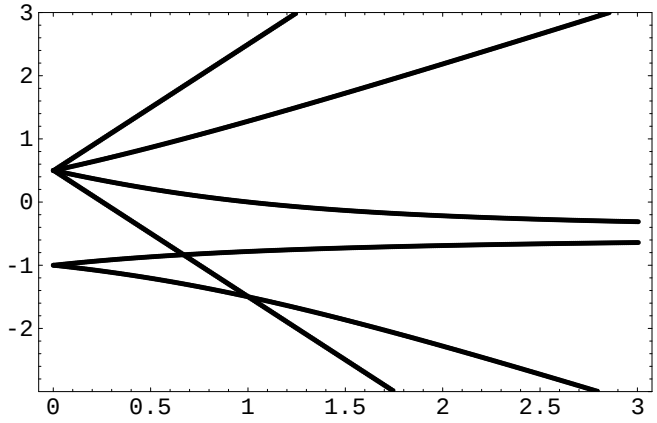
Using the results of previous sections we see that the Hamiltonian matrix in the $|m_\ell, m_s\rangle$ basis is:

$$\mathcal{H} = h\begin{pmatrix} 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&-1&0\\ 0&0&0&0&0&-1 \end{pmatrix} + g_s h\begin{pmatrix} \frac{1}{2}&0&0&0&0&0\\ 0&-\frac{1}{2}&0&0&0&0\\ 0&0&\frac{1}{2}&0&0&0\\ 0&0&0&-\frac{1}{2}&0&0\\ 0&0&0&0&\frac{1}{2}&0\\ 0&0&0&0&0&-\frac{1}{2} \end{pmatrix} + v\begin{pmatrix} \frac{1}{2}&0&0&0&0&0\\ 0&-\frac{1}{2}&\frac{1}{\sqrt{2}}&0&0&0\\ 0&\frac{1}{\sqrt{2}}&0&0&0&0\\ 0&0&0&0&\frac{1}{\sqrt{2}}&0\\ 0&0&0&\frac{1}{\sqrt{2}}&-\frac{1}{2}&0\\ 0&0&0&0&0&\frac{1}{2} \end{pmatrix} \tag{667}$$

while in the $|j, m_j\rangle$ basis we have

$$\mathcal{H} = \frac{h}{3}\begin{pmatrix} 3&0&0&0&0&0\\ 0&1&0&0&-\sqrt{2}&0\\ 0&0&-1&0&0&-\sqrt{2}\\ 0&0&0&-3&0&0\\ 0&-\sqrt{2}&0&0&2&0\\ 0&0&-\sqrt{2}&0&0&-2 \end{pmatrix} + g_s\frac{h}{6}\begin{pmatrix} 3&0&0&0&0&0\\ 0&1&0&0&2\sqrt{2}&0\\ 0&0&-1&0&0&2\sqrt{2}\\ 0&0&0&-3&0&0\\ 0&2\sqrt{2}&0&0&-1&0\\ 0&0&2\sqrt{2}&0&0&1 \end{pmatrix} + \frac{v}{2}\begin{pmatrix} 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&-2&0\\ 0&0&0&0&0&-2 \end{pmatrix}$$

The spectrum of $\mathcal{H}$ can be found for a range of h values. See again the Mathematica file zeeman.nb. The results (in units such that $v = 1$) are illustrated in the following figure:



If the field is zero the Hamiltonian is diagonal in the $|j, m_j\rangle$ basis and we find that

$$E_{j=\frac{3}{2}} = \frac{v}{2} \quad \text{degeneracy} = 4 \tag{668}$$

$$E_{j=\frac{1}{2}} = -v \quad \text{degeneracy} = 2 \tag{669}$$

In a very strong magnetic field we can make a rough approximation by neglecting the spin-orbit coupling. With this approximation the Hamiltonian is diagonal in the $|m_\ell, m_s\rangle$ basis and we get

$$E_{m_\ell, m_s} = (m_\ell + g_s m_s)h \tag{670}$$

In fact there are two levels that are exact eigensates of the Hamiltonian for any h. These are:

$$E_{j=\frac{3}{2}, m_j=\pm\frac{3}{2}} \;=\; \frac{v}{2} \pm (1 + \frac{g_s}{2})h \tag{671}$$

For a weak magnetic field it is better to write the Hamiltonian in the $|j, m_j\rangle$ basis, so as to have $\vec{L} \cdot \vec{S}$ diagonal, while the Zeeman terms are treated as a perturbation. We can determine (approximately) the splitting of the j multiplets by using degenerate perturbation theory. In order to do so we only need to find the j sub-matrices of the the Hamiltonian. We already know that they should obey the Wigner Eckart theorem. By inspection of the Hamiltonian we see that this is indeed the case. We have $g_L = \frac{2}{3}$ and $g_S = \frac{1}{3}$ for $j = \frac{3}{2}$, while $g_L = \frac{4}{3}$ and $g_S = -\frac{1}{3}$ for $j = \frac{1}{2}$. Hence we can write

$$E_{j,m_j} = E_{j=\frac{3}{2}} + (g_M m_j)h \tag{672}$$

where $g_M = g_L + g_s g_S$ is associated with the vector operator $\vec{M} = \vec{L} + g_s \vec{S}$. In order to calculate g_L and g_S we do not need to calculate the multiplication of the 6×6 matrices. We can simply can use the formulas

$$g_L \;=\; \frac{\langle \vec{J} \cdot \vec{L} \rangle}{j(j+1)} \;=\; \frac{j(j+1) + \ell(\ell+1) - s(s+1)}{2j(j+1)} \tag{673}$$

$$g_S \;=\; \frac{\langle \vec{J} \cdot \vec{S} \rangle}{j(j+1)} \;=\; \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)} \tag{674}$$

Approximations

[25] Introduction to Perturbation Theory

[25.1] Perturbation theory - a mathematical example

Let us use perturbation theory to find a solution to the following equation:

$$x + \lambda x^5 = 3 \tag{675}$$

We assume that the magnitude of the perturbation (λ) is small. The Taylor expansion of x with respect to λ is:

$$x(\lambda) = x^{(0)} + x^{(1)}\lambda + x^{(2)}\lambda^2 + x^{(3)}\lambda^3 + \dots \tag{676}$$

The zero-order solution gives us the solution for the case $\lambda = 0$:

$$x^{(0)} = 3 \tag{677}$$

For the first-order solution we substitute $x(\lambda) = x^{(0)} + x^{(1)}\lambda$ in the equation, and get:

$$\begin{aligned} &[x^{(0)} + x^{(1)}\lambda] + \lambda[x^{(0)} + x^{(1)}\lambda]^5 = 3 \\ &[x^{(0)} - 3] + \lambda[x^{(1)} + (x^{(0)})^5] + \mathcal{O}(\lambda^2) = 0 \end{aligned} \tag{678}$$

By comparing coefficients we get:

$$\begin{aligned} &x^{(0)} - 3 = 0 \\ &x^{(1)} + (x^{(0)})^5 = 0 \end{aligned} \tag{679}$$

Therefore:

$$x^{(1)} = -(x^{(0)})^5 = -3^5 \tag{680}$$

For the second-order solution, we substitute $x(\lambda) = x^{(0)} + x^{(1)}\lambda + x^{(2)}\lambda^2$ in the equation, and get:

$$[x^{(0)} + x^{(1)}\lambda + x^{(2)}\lambda^2] + \lambda[x^{(0)} + x^{(1)}\lambda + x^{(2)}\lambda^2]^5 = 3 \tag{681}$$

Once again, after comparing coefficients (of λ^2), we get:

$$x^{(2)} = -5(x^{(0)})^5 x^{(1)} = 5 \times 3^{10} \tag{682}$$

It is obviously possible to find the corrections for higher orders by continuing in the same way.

[25.2] Perturbation theory - physical motivation

Let us consider a particle in a two dimensional box. On the left a rectangular box, and on the right a chaotic box.

For a regular box (with straight walls) we found: $E_{n_x,n_y} \propto (n_x/L_x)^2 + (n_y/L_y)^2$, so if we change L_x we get the energy level scheme which is drawn in the left panel of the following figure. But if we consider a chaotic box, we shall get energy level scheme as on the right panel.

The spectrum is a function of a control parameter, which in the example above is the position of a wall. For generality let us call this parameter X. The Hamiltonian is $\mathcal{H}(\hat{Q},\hat{P};X)$. Let us assume that we have calculated the levels either analytically or numerically for $X = X_0$. Next we change the control parameter to the value $X = X_0 + \lambda$. Possibly, if δX is small enough, we can linearize the Hamiltonian as follows:

$$\mathcal{H} \quad = \quad \mathcal{H}(\hat{Q},\hat{P};X_0) + \lambda V(\hat{Q},\hat{P}) \quad = \quad \mathcal{H}_0 + \lambda\hat{V} \tag{683}$$

With or without this approximation we can try to calculate the new energy levels. But if we do not want or cannot diagonalize $\mathcal{H}$ for the new value of X we can try to use a perturbation theory scheme. Obviously this scheme will work only for small enough λ that do not "mix" the levels too much. There is some "radius of convergence" (in λ) beyond which perturbation theory fails completely. In many practical cases $X = X_0$ is taken as the value for which the Hamiltonian is simple and can be handled analytically. In atomic physics the control parameter X is usually either the prefactor of the spin-orbit term, or an electric field or a magnetic field which are turned on.

There is another context in which perturbation theory is very useful. Given (say) a chaotic system, we would like to predict its response to a small change in one of its parameters. For example we may ask what is the response of the system to an external driving by either an electric or a magnetic field. This response is characterized by a quantity called "susceptibility". In such case, finding the energies without the perturbation is not an easy task (it is actually impossible analytically, so if one insists heavy numerics must be used). Instead of "solving" for the eigenstates it turns out that for any practical purpose it is enough to characterize the spectrum and the eigenstates in a statistical way. Then we can use perturbation theory in order to calculate the "susceptibility" of the system.

[25.3] Digression: perturbation caused by displacing a wall

Let us assume that we have a particle in a one dimensional box of length L, such that $0 < x < L$. For $L = L_0$ the unperturbed Hamiltonian after digonalization is

$$[\mathcal{H}_0]_{nm} \quad = \quad \frac{1}{2\mathsf{m}}\left(\frac{\pi}{L_0}n\right)^2 \delta_{nm} \tag{684}$$

If we displace the wall a distance dL the new Hamiltonian would become $\mathcal{H} = \mathcal{H}_0 + dLV$. We ask what are the matrix elements V_{nm} of this perturbation. At first sight it looks as if to displace an "infinite wall" constitutes "infinite

perturbation" and hence $V_{nm} = \infty$. But in fact it is not like that. We shall show that

$$V_{nm} = -\frac{\pi^2}{\mathsf{m}L_0^3}nm \tag{685}$$

Let us recall what does it mean "infinite wall". The wall is in fact a potential barrier of height $U_0 \to \infty$ located at $x = L$. We assume that the left (fixed) wall is literally an infinite barrier, which forces Dirichlet boundary conditions on the wavefunction. But for the right wall, which we want to displace, we assume that U_0 is very very large but finite. We shall take the limit $U_0 \to \infty$ only at the end of the calculation. The wavefunction of nth eigenstate is

$$\psi(x) = \begin{cases} A\sin(kx) & \text{for } 0 < x < L \\ B\mathrm{e}^{-\alpha x} & \text{for } x > L \end{cases} \tag{686}$$

Where

$$\begin{aligned} k &= \sqrt{2\mathsf{m}E} \\ \alpha &= \sqrt{2\mathsf{m}(U_0 - E)} \approx \sqrt{2\mathsf{m}U_0} \end{aligned} \tag{687}$$

and the normalization factor at the limit $U_0 \to \infty$ is $A = (2/L)^{1/2}$. The matching conditions are:

$$\left.\frac{\psi`(x)}{\psi(x)}\right|_{x=L-0} = \left.\frac{\psi`(x)}{\psi(x)}\right|_{x=L+0} = -\alpha \tag{688}$$

So the eigenvalue equation is

$$k\cot(kL) = -\alpha \tag{689}$$

In the limit $U_0 \to \infty$ the equation becomes $\sin(kL) = 0$ leading to the unperturbed eigen-energies. For the following calculation we point out that for very large U_0 the derivative of the $n$the wavefunction at the wall is

$$\left.\frac{d}{dx}\psi^{(n)}(x)\right|_{x=L} = \sqrt{\frac{2}{L}}k_n \tag{690}$$

where $k_n = (\pi/L)n$. The Hamiltonian of the original system (before we displace the wall) is:

$$\mathcal{H}_0 = \frac{p^2}{2\mathsf{m}} + U_1(x) \tag{691}$$

The Hamiltonian after we have displaced the wall a distance dL is:

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} + U_2(x) \tag{692}$$

So the perturbation is:

$$\delta U(x) = U_2(x) - U_1(x) \equiv dL \times V \tag{693}$$

which is a rectangle of width dL and height $-U_0$. It follows that the matrix elements of the perturbation are

$$V_{nm} = \frac{1}{dL}\int_L^{L+dL} \psi^{(n)}(x)[-U_0]\psi^{(m)}(x)dx = -U_0\psi^{(n)}(L)\psi^{(m)}(L) = -U_0\frac{1}{\alpha^2}\left(\frac{d}{dx}\psi^{(n)}(L)\right)\left(\frac{d}{dx}\psi^{(m)}(L)\right)$$

where in the last step we have used the "matching conditions". Now there is no problem to take the limit $U_0 \to \infty$

$$V_{nm} = -U_0 \frac{1}{2\mathsf{m}U_0} \left(\sqrt{\frac{2}{L}} k_n\right) \left(\sqrt{\frac{2}{L}} k_m\right) = -\left(\frac{1}{\mathsf{m}L}\right) k_n k_m = -\frac{\pi^2}{\mathsf{m}L^3}\, n\; m \tag{694}$$

[26] Perturbation theory for the eigenstates

[26.1] Degenerate perturbation theory (zero-order)

We will take a general Hamiltonian after diagonalization, and add a small perturbation that spoils the diagonalization:

$$\mathcal{H} = \begin{pmatrix} 2 & 0.03 & 0 & 0 & 0 & 0.5 & 0 \\ 0.03 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0.1 & 0.4 & 0 & 0 \\ 0 & 0 & 0.1 & 5 & 0 & 0.02 & 0 \\ 0 & 0 & 0.4 & 0 & 6 & 0 & 0 \\ 0.5 & 0 & 0 & 0.02 & 0 & 8 & 0.3 \\ 0 & 0 & 0 & 0 & 0 & 0.3 & 9 \end{pmatrix} \tag{695}$$

The eigenvectors without the perturbation are:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \cdots \tag{696}$$

The perturbation spoils the diagonalization. The question we would like to answer is what are the new eigenvalues and eigenstates of the Hamiltonian. We would like to find them "approximately", without having to diagonalize the Hamiltonian again. First we will take care of the degenerated blocks. The perturbation can remove the existing degeneracy. In the above example we make the following diagonalization:

$$2 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + 0.03 \cdot \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \rightarrow \quad \begin{pmatrix} 1.97 & 0 & 0 \\ 0 & 2.03 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{697}$$

We see that the perturbation has removed the degeneracy. At this stage our achievement is that there are no matrix elements that couple degenerate states. This is essential for the next steps: we want to ensure that the perturbative calculation would not diverge.

For the next stage we have to transform the Hamiltonian to the new basis. See the calculation in the Mathematica file "diagonalize.nb". If we diagonalize numerically the new matrix we find that the eigenvector that corresponds to the eigenvalue $E \approx 5.003$ is

$$|\Psi\rangle \quad \rightarrow \quad \begin{pmatrix} 0.0008 \\ 0.03 \\ 0.0008 \\ 1 \\ -0.01 \\ -0.007 \\ 0.0005 \end{pmatrix} \quad = \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0.0008 \\ 0.03 \\ 0.0008 \\ 0 \\ -0.01 \\ -0.007 \\ 0.0005 \end{pmatrix} \quad \equiv \quad \Psi_n^{[0]} + \Psi_n^{[1,2,3,\dots]} \tag{698}$$

We note that within the scheme of perturbation theory it is convenient to normalize the eigenvectors according to the zero order approximation. We also use the convention that all the higher order corrections have zero overlap with the the zero order solution. Else the scheme of the solution becomes ill defined.

[26.2] Perturbation theory to arbitrary order

We write the Hamiltonian as $\mathcal{H} = \mathcal{H}_0 + \lambda V$ where V is the perturbation and λ is the control parameter. Note that λ can be "swallowed" in V. We keep it during the derivation in order to have clear indication for the "order" of the

terms in the expansion. The Hamiltonian is represented in the unperturbed basis as follows:

$$\mathcal{H} = \mathcal{H}_0 + \lambda V = \sum_n |n\rangle \varepsilon_n \langle n| \;\; + \;\; \lambda \sum_{n,m} |n\rangle V_{n,m} \langle m| \tag{699}$$

which means

$$\mathcal{H} \quad \rightarrow \quad \begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 \\ 0 & \varepsilon_2 & 0 & 0 \\ 0 & 0 & \varepsilon_3 & 0 \\ 0 & 0 & 0 & \ldots \end{pmatrix} + \begin{pmatrix} V_{1,1} & V_{1,2} & \ldots & \ldots \\ V_{2,1} & V_{2,2} & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots \end{pmatrix} \tag{700}$$

In fact we can assume without loss of generality that $V_{n,m} = 0$ for $n = m$, because these terms can be swallowed into the diagonal part. Most importantly we assume that none of the matrix element couples degenerated states. Such couplings should be treated in the preliminary "zero order" step that has been discussed in the previous section.

We would like to introduce a perturbative scheme for finding the eigenvalues and the eigenstates of the equation

$$(\mathcal{H}_0 + \lambda V)|\Psi\rangle = E|\Psi\rangle \tag{701}$$

The eigenvalues and the eigenvectors are expanded as follows:

$$\begin{aligned} E &= E^{[0]} + \lambda E^{[1]} + \lambda^2 E^{[2]} + \cdots \\ \Psi_n &= \Psi_n^{[0]} + \lambda \Psi_n^{[1]} + \lambda^2 \Psi_n^{[2]} \end{aligned} \tag{702}$$

where it is implicit that the zero order solution and the normalization are such that

$$\begin{aligned} &E^{[0]} = \varepsilon_{n_0} \\ &\Psi_n^{[0]} = \delta_{n,n_0} \\ &\Psi_n^{[1,2,3,\ldots]} = 0 \quad \text{for} \quad n = n_0 \end{aligned} \tag{703}$$

It is more illuminating to rewrite the expansion of the eigenvector using Dirac notations:

$$|n_0\rangle = |n_0^{[0]}\rangle + \lambda |n_0^{[1]}\rangle + \lambda^2 |n_0^{[2]}\rangle + \cdots \tag{704}$$

hence

$$\langle n^{[0]}|n_0\rangle = \langle n^{[0]}|n_0^{[0]}\rangle + \lambda \langle n^{[0]}|n_0^{[1]}\rangle + \lambda^2 \langle n^{[0]}|n_0^{[2]}\rangle + \cdots \tag{705}$$

which coincides with the traditional notation. In the next section we introduce a derivation that leads to the following practical results:

$$\begin{aligned} \Psi_n^{[0]} &= \delta_{n,n_0} \\ \Psi_n^{[1]} &= \frac{V_{n,n_0}}{\varepsilon_{n_0} - \varepsilon_n} \\ E^{[0]} &= \varepsilon_{n_0} \\ E^{[1]} &= V_{n_0,n_0} \\ E^{[2]} &= \sum_{m(\neq n_0)} \frac{V_{n_0,m} V_{m,n_0}}{\varepsilon_{n_0} - \varepsilon_m} \end{aligned} \tag{706}$$

The calculation can be illustrated graphically using a "Feynman diagram". For the calculation of the second order correction to the energy we should sum all the paths that begin with the state n_0 and also end with the state n_0. We see that the influence of the nearer levels is much greater than the far ones. This clarifies why we cared to treat the couplings between degenerated levels in the zero order stage of the calculation. The closer the level the stronger the influence. This influence is described as "level repulsion". Note that in the absence of first order correction the ground state level always shifts down.

═══ [26.3] Derivation of the results

The equation we would like to solve is

$$\begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 \\ 0 & \varepsilon_2 & 0 & 0 \\ 0 & 0 & \varepsilon_3 & 0 \\ 0 & 0 & 0 & \dots \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \dots \end{pmatrix} + \lambda \begin{pmatrix} V_{1,1} & V_{1,2} & \dots & \dots \\ V_{2,1} & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \dots \end{pmatrix} = E \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \dots \end{pmatrix} \tag{707}$$

Or, in index notation:

$$\varepsilon_n \Psi_n \; + \; \lambda \sum_m V_{n,m} \Psi_m \; = \; E \Psi_n \tag{708}$$

This can be rewritten as

$$(E - \varepsilon_n)\Psi_n = \lambda \sum_m V_{n,m} \Psi_m \tag{709}$$

We substitute the Taylor expansion:

$$\begin{aligned} E = \sum_{k=0} \lambda^k E^{[k])} \;\; &= \;\; E^{[0]} + \lambda E^{[1]} + \dots \\ \Psi_n = \sum_{k=0} \lambda^k \Psi_n^{[k]} \;\; &= \;\; \Psi_n^{[0]} + \lambda \Psi_n^{[1]} + \dots \end{aligned} \tag{710}$$

We recall that

$$E^{[0]} = \varepsilon_{n_0} \tag{711}$$

$$\Psi_n^{(0)} = \delta_{n,n_0} \; \rightarrow \; \begin{pmatrix} \dots \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \dots \end{pmatrix}$$

$$\Psi_n^{[k \neq 0]} \; \rightarrow \; \begin{pmatrix} \dots \\ ? \\ ? \\ 0 \\ ? \\ ? \\ \dots \end{pmatrix}$$

After substitution of the expansion we use on the left side the identity

$$(a_0 + \lambda a_1 + \lambda^2 a_2 + \dots)(b_0 + \lambda b_1 + \lambda^2 b_2 + \dots) = \sum_k \lambda^k \sum_{k'=0}^{k} a_{k'} b_{k-k'} \tag{712}$$

Comparing the coefficients of λ^k we get a system of equations $k = 1, 2, 3...$

$$\sum_{k'=0}^{k} E^{[k']}\Psi_n^{[k-k']} - \varepsilon_n \Psi_n^{[k]} \;=\; \sum_m V_{n,m}\Psi_m^{[k-1]} \tag{713}$$

We write the kth equation in a more expanded way:

$$(E^{[0]} - \varepsilon_n)\Psi_n^{(k)} + E^{[1]}\Psi_n^{[k-1]} + E^{[2]}\Psi_n^{[k-2]} + \cdots + E^{[k]}\Psi_n^{[0]} = \sum_m V_{n,m}\Psi_m^{[k-1]} \tag{714}$$

If we substitute $n = n_0$ in this equation we get:

$$0 \;+\; 0 \;+ \cdots + E^{[k]} = \sum_m V_{n_0,m}\Psi_m^{[k-1]} \tag{715}$$

If we substitute $n \neq n_0$ in this equation we get:

$$(\varepsilon_{n_0} - \varepsilon_n)\Psi_n^{[k]} = \sum_m V_{n,m}\Psi_m^{[k-1]} - \sum_{k'=1}^{k} E^{[k']}\Psi_n^{[k-k']} \tag{716}$$

Now we see that we can solve the system of equations that we got in the following order:

$$\Psi^{[0]} \to E^{[1]} \to \Psi^{[1]} \to E^{[2]} \to \dots \tag{717}$$

Where:

$$\begin{aligned} E^{[k]} \;&=\; \sum_m V_{n_0,m}\Psi_n^{[k-1]} \\ \Psi_n^{[k]} \;&=\; \frac{1}{(\varepsilon_{n_0} - \varepsilon_n)}\left[\sum_m V_{n,m}\Psi_m^{[k-1]} - \sum_{k'=1}^{k} E^{[k']}\Psi_n^{[k-k']}\right] \end{aligned} \tag{718}$$

The practical results that were cited in the previous sections are easily obtained from this iteration scheme.

═══ [26.4] Perturbation theory for a ring + scatterer + flux

Let us consider a particle with mass m on a 1D ring. A flux Φ flows through the ring. In addition, there is a scatterer on the ring, described by a delta function. The Hamiltonian that describes the system is:

$$\mathcal{H} = \frac{1}{2\mathsf{m}}\left(p - \frac{\Phi}{L}\right)^2 + \epsilon\delta(x) \tag{719}$$

This Hamiltonian's symmetry group is $O(2)$. This means symmetry with respect to rotations and reflections. In fact, in one dimension, rotations and reflections are the same (since a 1D ring = a circle). Only in higher dimensions they are different (torus $\neq$ sphere).

Degeneracies are an indication for symmetries of the Hamiltonian. If the eigenstate has a lower symmetry than the Hamiltonian, a degeneracy appears. Rotations and reflections do not commute, that is why we have degeneracies. When we add flux or a scatterer, the degeneracies open up. Adding flux breaks the reflection symmetry, and adding a scatterer breaks the rotation symmetry. Without a scatterer ($\epsilon = 0$) the eigenenergies are:

$$E_n = \frac{1}{2\mathsf{m}}\left(\frac{2\pi}{L}n - \frac{\Phi}{L}\right)^2 = \frac{1}{2\mathsf{m}}\left(\frac{2\pi}{L}\right)^2\left(n - \frac{\Phi}{2\pi}\right)^2 \tag{720}$$

On the other hand, in the limit $\epsilon \to \infty$ the system does not "feel" the flux, and the ring becomes a one-dimensional potential. The eigenenergies in this limit are:

$$E_n = \frac{1}{2\mathsf{m}}(\frac{\pi}{L} \times \text{integer})^2 \tag{721}$$

The number of the energy levels does not change, they just move. If $\Phi = 0$ and $\epsilon = 0$, the Hamiltonian commutes with translations and reflections. Therefore there are two bases that can be used.

The First Basis:

The first basis complies with the rotation (=translations) symmetry:

$$\begin{aligned} |n=0\rangle &= \frac{1}{\sqrt{L}} \\ |n, \text{anticlockwise}\rangle &= \frac{1}{\sqrt{L}}\mathrm{e}^{ik_n x} \\ |n, \text{clockwise}\rangle &= \frac{1}{\sqrt{L}}\mathrm{e}^{-ik_n x} \end{aligned} \tag{722}$$

Where $k_n = \frac{2\pi}{L}n$ with $n = 1, 2, 3, \ldots$. The degenerate states are different under reflection. Only the ground state $|n=0\rangle$ is symmetrical under both reflection and rotation, and therefore it does not need to be degenerate.

It is very easy to calculate the perturbation matrix elements in this basis, since:

$$\langle n|\delta(x)|m\rangle = \int \Psi^n(x)\delta(x)\Psi^m(x)dx = \Psi^n(0)\Psi^m(0) = \frac{1}{L} \tag{723}$$

So that we get:

$$V_{nm} = \frac{\epsilon}{L}\begin{pmatrix} 1 & 1 & 1 & 1 & \ldots \\ 1 & 1 & 1 & 1 & \ldots \\ 1 & 1 & 1 & 1 & \ldots \\ 1 & 1 & 1 & 1 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix} \tag{724}$$

The Second Basis:

The second basis complies with the reflection symmetry:

$$\begin{aligned} |n=0\rangle &= \frac{1}{\sqrt{L}} \\ |n,+\rangle &= \sqrt{\frac{2}{L}}\cos(k_n x) \\ |n,-\rangle &= \sqrt{\frac{2}{L}}\sin(k_n x) \end{aligned} \tag{725}$$

The degeneracy is between the even states and the odd states that are displaced by half a wavelength with respect to each other.

If the perturbation is not the flux but rather the scatterer, then it is better to work with the second basis, which complies with the potential's symmetry. The odd states are not influenced by the delta function, and they are also not "coupled" to the even states. The reason is that:

$$\langle m|\delta(x)|n\rangle = \int \Psi^m(x)\delta(x)\Psi^n(x)dx = 0 \tag{726}$$

if one of the states is odd. (the sine function is not influenced by the barrier, because it is zero at the barrier). Consequently the subspace of odd states is not influenced by the perturbation, and we only need to diagonalize the block that belongs to the even states. It is very easy to write the perturbation matrix for this block:

$$V_{nm} = \frac{\epsilon}{L} \begin{pmatrix} 1 & \sqrt{2} & \sqrt{2} & \sqrt{2} & \dots \\ \sqrt{2} & 2 & 2 & 2 & \dots \\ \sqrt{2} & 2 & 2 & 2 & \dots \\ \sqrt{2} & 2 & 2 & 2 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{727}$$

The Corrections To The Energy

The first-order correction to the energy of the states is:

$$\begin{aligned} E_{n=0} &= E^{[0]}_{n=0} + \frac{\epsilon}{L} \\ E_{n=2,4,\dots} &= E^{[0]}_{n} + \frac{2\epsilon}{L} \end{aligned} \tag{728}$$

The correction to the ground state energy, up to the second order is:

$$E_{n=0} = 0 + \frac{\epsilon}{L} + \left(\frac{\epsilon}{L}\right)^2 \sum_{k=1}^{\infty} \frac{(\sqrt{2})^2}{0 - \frac{1}{2\mathsf{m}}\left(\frac{2\pi}{L}k\right)^2} = \frac{\epsilon}{L}\left(1 - \frac{1}{6}\epsilon \mathsf{m} L\right) \tag{729}$$

Where we have used the identity:

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6} \tag{730}$$

What Happens If We Choose the First Basis?

We will now assume that we did not notice the symmetry of the problem, and we chose to work with the first basis. Using perturbation theory on the ground state energy is simple in this basis:

$$E_{n=0} = 0 + \frac{\epsilon}{L} + \left(\frac{\epsilon}{L}\right)^2 2\sum_{k=1}^{\infty} \frac{(1)^2}{0 - \frac{1}{2\mathsf{m}}\left(\frac{2\pi}{L}k\right)^2} = \frac{\epsilon}{L}\left(1 - \frac{1}{6}\epsilon \mathsf{m} L\right) \tag{731}$$

But using perturbation theory on the rest of the states is difficult because there are degeneracies. The first thing we must do is "degenerate perturbation theory". The diagonalization of each degenerate energy level is:

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} \tag{732}$$

Now we must move to the "new" basis, where the degeneracy is removed. This is exactly the "second" basis that we chose to work with because of symmetry considerations. The moral is: understanding the symmetries in the system can save us work in the calculations of perturbation theory.

[27] Perturbation Theory / Wigner

[27.1] The overlap between the old and the new states

We have found that the perturbed eigenstates to first-order are given by the expression

$$|n_0\rangle \approx |n_0^{[0]}\rangle + \sum_n \frac{V_{n,n_0}}{\varepsilon_{n_0} - \varepsilon_n} |n^{[0]}\rangle \tag{733}$$

So, it is possible to write:

$$\langle n^{[0]}|n_0\rangle \approx \frac{V_{nn_0}}{\varepsilon_{n_0} - \varepsilon_n} \qquad \text{for } n \neq n_0 \tag{734}$$

which implies

$$P(n|m) \equiv |\langle n^{[0]}|m\rangle|^2 \approx \frac{|V_{nm}|^2}{(E_m - E_n)^2} \qquad \text{for } n \neq n_0 \tag{735}$$

We notice that since the difference between the original spectrum and the perturbed spectrum is very small, we can write in the denominator the perturbed energies instead of the corrected energies. In order for our perturbation theory to be valid, we demand that:

$$|V| \ll \Delta \tag{736}$$

In other words, the perturbation must be much smaller than the mean level spacing. We observe that once this condition breaks down the sum $\sum_m P(n|m)$ becomes much larger then one, whereas the exact value is exactly one due to normalization. This means that if $|V| \gg \Delta$ the above first order expression cannot be trusted.

Can we do better? In principle we have to go to higher orders of perturbation theory, which might be very complicated. But in fact the generic result that comes out is quite simple:

$$P(n|m) \approx \frac{|V_{n,m}|^2}{(E_n - E_m)^2 + (\Gamma/2)^2} \tag{737}$$

This is called "Wigner Lorentzian". As we shall see later, it is related to the exponential decay law that is also named after Wigner ("Wigner decay"). The expression for the "width" of this Lorentzian is implied by normalization:

$$\Gamma = \frac{2\pi}{\Delta}|V|^2 \tag{738}$$

The Lorentzian expression is not exact. It is implicit that we assume a dense spectrum (high density of states). We also assume that all the matrix elements are of the same order of magnitude. Such assumption can be justified e.g. in case of chaotic systems. In order to show that $\sum_m P(n|m) = 1$ one use the recipe:

$$\sum_n f(E_n) \approx \int \frac{dE}{\Delta} f(E) \tag{739}$$

where Δ is the mean level spacing. In the following we shall discuss further the notion Density of States (DOS) and Local Density of States (LDOS) which are helpful in further clarifying the significance of the Wigner Lorentzian.

[27.2] The DOS and the LDOS

When we have a dense spectrum, we can characterize it with a density of states (DOS) function:

$$g(E) = \sum_n \delta(E - E_n) \tag{740}$$

We notice that according to this definition:

$$\int_E^{E+dE} g(E')dE' = \text{number of states with energy } E < E_n < E + dE \tag{741}$$

If the mean level spacing Δ is approximately constant within some energy interval then $g(E) = 1/\Delta$.

The local density of states (LDOS) is a weighted version of the DOS. Each level has a weight which is proportional to its overlap with a reference state:

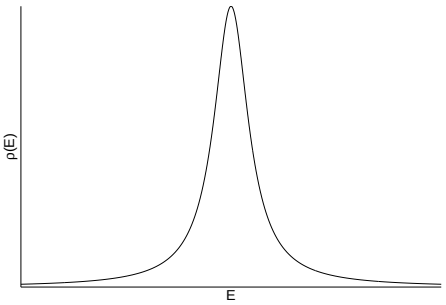
$$\rho(E) = \sum_n |\langle \Psi | n \rangle|^2 \delta(E - E_n) \tag{742}$$

The index n labels as before the eigenstates of the Hamiltonian, while Ψ is the reference state. In particular Ψ can be one of the eigenstates of the unperturbed Hamiltonian. In such case the Wigner Lorentzian approximation implies

$$\rho(E) = \frac{1}{\pi} \frac{(\Gamma/2)}{(E - E_{n_0})^2 + (\Gamma/2)^2} \tag{743}$$

It should be clear that by definition we have

$$\int_{-\infty}^{\infty} \rho(E)dE = \sum_n |\langle \Psi | n \rangle|^2 = 1 \tag{744}$$



[27.3] Wigner decay and its connection to the LDOS

Let us assume that we have a system with many energy states. We prepare the system in the state $|\Psi\rangle$. Now we apply a field for a certain amount of time, and then turn it off. What is the probability $P(t)$ that the system will remain in the same state? This probability is called the survival probability. By definition:

$$P(t) = |\langle \Psi(0) | \Psi(t) \rangle|^2 \tag{745}$$

Let $\mathcal{H}_0$ be the unperturbed Hamiltonian, while $\mathcal{H}$ is the perturbed Hamiltonian (while the field is "on"). In what follows the index n labels the eigenstates of the perturbed Hamiltonian $\mathcal{H}$. We would like to calculate the survival

amplitude:

$$\langle\Psi(0)|\Psi(t)\rangle = \langle\Psi|U(t)|\Psi\rangle = \sum_n \langle n|\Psi\rangle|^2 \mathrm{e}^{-iE_n t} \tag{746}$$

We notice that:

$$\langle\Psi(0)|\Psi(t)\rangle = \mathrm{FT}\left[\sum_n \langle n|\Psi\rangle|^2 2\pi\delta(\omega - E_n)\right] = \mathrm{FT}\left[2\pi\rho(\omega)\right] \tag{747}$$

If we assume that the LDOS is given by Wigner Lorentzian then:

$$P(t) \quad = \quad \Big|\mathrm{FT}\left[2\pi\rho(E)\right]\Big|^2 \quad = \quad \mathrm{e}^{-\Gamma t} \tag{748}$$

Below we remind ourselves of the customary way to perform the Fourier transform in this course:

$$\begin{aligned} F(\omega) &= \int f(t)\mathrm{e}^{i\omega t}dt \\ f(t) &= \int \frac{d\omega}{2\pi} F(\omega)\mathrm{e}^{-i\omega t} \end{aligned} \tag{749}$$

The Wigner decay appears when we "break" first-order perturbation theory. The perturbation should be strong enough to create transitions to other levels. Else the system stays essentially at the same level all the time ($P(t) \approx 1$). Note the analogy with the analysis of the dynamics in a two level system. Also there in order to have for $P(t)$ large amplitude oscillations, the hopping amplitude should be significantly larger compared with the on site energy difference.

Dynamics and Driven Systems

[28] Probabilities and rates of transitions

[28.1] Time dependent Hamiltonians

To find the evolution which is generated by a time independent Hamiltonian is relatively easy. Such a Hamiltonian has eigenstates $|n\rangle$ which are the "stationary" states of the system. The evolution in time of an arbitrary state is:

$$|\Psi(t)\rangle = \sum_n \mathrm{e}^{-iE_n t}\psi_n|n\rangle \tag{750}$$

But in general the Hamiltonian can be time-dependent $[\mathcal{H}(t_1),\mathcal{H}(t_2)] \neq 0$. In such case the strategy that was described above for finding the evolution in time loses its significance. In this case, there is no simple expression for the evolution operator:

$$\hat{U}(t) \;=\; (1-idt_n\mathcal{H}(t_n))\cdots(1-idt_2\mathcal{H}(t_2))(1-idt_1\mathcal{H}(t_1)) \;\neq\; \mathrm{e}^{-i\int_0^t \mathcal{H}(t')dt'} \tag{751}$$

We are therefore motivated to develop different methods to deal with driven systems. Below we assume that the Hamiltonian can be written as a sum of a time independent part $\mathcal{H}_0$ and a time dependent perturbation. Namely,

$$\mathcal{H} \;=\; \mathcal{H}_0 + V \;=\; \mathcal{H}_0 + f(t)W \tag{752}$$

[28.2] The interaction picture

We would like to work in a basis such that $\mathcal{H}_0$ is diagonal:

$$\begin{aligned} \mathcal{H}_0|n\rangle &= E_n|n\rangle \\ |\Psi(t)\rangle &= \sum_n \Psi_n(t)|n\rangle \end{aligned} \tag{753}$$

The evolution is determined by the Schrödinger's equation:

$$i\frac{d\psi_n}{dt} = E_n\psi_n + \sum_{n'} V_{nn'}\Psi_{n'} \tag{754}$$

which can be written in a matrix style as follows:

$$i\frac{d}{dt}\begin{pmatrix}\Psi_1\\ \Psi_2\\ \vdots\end{pmatrix} = \begin{pmatrix}E_1\Psi_1\\ E_2\Psi_2\\ \vdots\end{pmatrix} + \begin{pmatrix}V_{11} & V_{12} & \cdots\\ V_{21} & V_{22} & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\\ \vdots\end{pmatrix} \tag{755}$$

Without the perturbation we would get $\psi_n(t) = C_n\mathrm{e}^{-iE_n t}$, where C_n are constants. It is therefore natural to use the variation of parameters method, and to write

$$\Psi_n(t) = C_n(t)\mathrm{e}^{-iE_n t} \tag{756}$$

In other words, we represent the "wave function" by the amplitudes $C_n(t) = \psi_n(t)e^{iE_n t}$ rather than by the amplitudes $\Psi_n(t)$. The Schrödinger's equation in the new representation takes the form

$$i\frac{dC_n}{dt} = \sum_{n'} e^{i(E_n - E_{n'})t} V_{nn'} C_{n'}(t) \tag{757}$$

This is called the Schrödinger's equation in the "interaction picture". It is a convenient equation because the term on the right is assumed to be "small". Therefore, the amplitudes $C_n(t)$ change slowly. This equation can be solved using an iterative scheme which leads naturally to a perturbative expansion. The iteration are done with the integral version of the above equation:

$$C_n(t) \;=\; C_n(0) - i\sum_{n'} \int_0^t e^{iE_{nn'}t} V_{n,n'} C_{n'}(t')dt' \tag{758}$$

where $E_{nn'} = E_n - E_{n'}$. In each iteration we get the next order. Let us assume that the system has been prepared in level n_0. This means that the zero order solution is

$$C_n^{[0]}(t) \;=\; C_n(0) \;=\; \delta_{n,n_0} \tag{759}$$

We iterate once and get the first-order solution:

$$C_n(t) = \delta_{n,n_o} - i\int_0^t e^{iE_{nn_0}t'} V_{n,n_0} dt' \tag{760}$$

So that the leading order is:

$$\begin{aligned} &C_n(t) \approx 1 \quad \text{for } n = n_0 \\ &C_n(t) = -iW_{n,n_0} \int_0^t f(t) e^{iE_{nn_0}t'} dt' \quad \text{otherwise} \end{aligned} \tag{761}$$

We notice that for very short times $t \ll 1/(E_n - E_{n'})$ we get $C_n(t) \approx -iV_{n,n_0}t$ which reflects the definition of the matrix elements of the Hamiltonian as a "hopping" amplitude per unit of time. For longer times the hopping amplitude is multiplied by a factor that oscillates at a frequency $E_n - E_{n'}$. This factor makes it "harder" for the particle to move between energy levels, since it does not allow the particle to "accumulate" amplitude.

In order to illustrate the effect of the oscillating factor, consider a problem in which the unperturbed Hamiltonian is "to be in some site". We consider the possibility to move from site to site as a perturbation. The energy differences in the site problem are the "potential differences". Let us assume we have a step potential. Even though the hopping amplitude is the same in each "hop" (even if the hop is through a wall), the probability amplitude does not "accumulate". What stops the particle from crossing the step is the potential difference between the sites.

═══ [28.3] The transition probability formula

The expression we found for the transition amplitude using first-order perturbation theory can be written as:

$$C_n(t) \;\approx\; -iW_{n,n_o} \mathrm{FT}\left[f(t)\right] \tag{762}$$

Therefore, the transition probability is:

$$P_t(n|m) \;\approx\; |W_{n,m}|^2 \;\left|\mathrm{FT}\left[f(t)\right]\right|^2 \tag{763}$$

Where the Fourier transform is defined by:

$$\mathrm{FT}\left[f(t)\right] = \int_{-\infty}^{\infty} f(t')\mathrm{e}^{iE_{nm}t'}dt' \tag{764}$$

And we use the convention that $f(t) = 0$ before and after the pulse. For example, if we turn on a constant perturbation for a certain amount of time, then $f(t)$ is a rectangle function.

[28.4] The effect of a constant perturbation

We consider the following scenario: A particle is prepared in the state n_0, and then a constant perturbation is turned on for a time t. We want to know what is the probability of finding the particle at some later time in the state n. Using the transition probability formula we get

$$C_n(t) \;=\; W_{nn_0}\left(1 - \frac{\mathrm{e}^{i(E_n - E_{n_0})t}}{E_n - E_{n_0}}\right) \tag{765}$$

We notice that the transition amplitude is larger to closer levels and smaller for distant levels.

$$P_t(n|n_0) \;=\; |C_n(t)|^2 \;=\; |W_{nn_0}|^2 \left|\frac{1 - \mathrm{e}^{i(E_n - E_{n_0})t}}{E_n - E_{n_0}}\right|^2 \tag{766}$$

In the next section we shall see that this expression can be regarded as a special case of a more general result.

[28.5] The effect of periodic driving

We will now discuss a more general case:

$$f(t') = \mathrm{e}^{-i\Omega t'} \quad \text{for } \; t' \in [0,t] \tag{767}$$

We notice that the Hamiltonian should be hermitian. Therefore this perturbation has a physical meaning only if it appears together with a conjugate term $\mathrm{e}^{+i\Omega t'}$. In other words, the driving is done by a real field $\cos(\Omega t')$ that changes periodically. Below we will treat only "half" of the perturbation. We can get the effect of the second half by making the swap $\Omega \mapsto -\Omega$. The calculation is done the same way as in the case of a constant perturbation. Using the transition probability formula we get

$$P_t(n|n_0) \;=\; |W_{nn_0}|^2 \left|\frac{1 - \mathrm{e}^{i(E_n - E_{n_0} - \Omega)t}}{E_n - E_{n_0} - \Omega}\right|^2 \tag{768}$$

A more convenient way of writing this expression is:

$$P_t(n|n_0) \;=\; |W_{n,n_0}|^2 \frac{2[1 - \cos(E_n - E_{n_0} - \Omega)t)]}{(E_n - E_{n_0} - \Omega)^2} \;=\; |W_{n,n_0}|^2 \frac{4\sin^2((E_n - E_{n_0}) - \Omega)t/2)}{(E_n - E_{n_0} - \Omega)^2} \tag{769}$$

And another optional notation is:

$$P_t(n|n_0) \;=\; |W_{n,n_0}|^2\, t^2\, \mathrm{sinc}^2((E_n - E_{n_0} - \Omega)t/2) \;=\; 2\pi t\, |W_{n,n_0}|^2\, \delta_{2\pi/t}(E_n - E_{n_0} - \Omega) \tag{770}$$

Where:

$$\begin{aligned} &\mathrm{sinc}(\nu) \equiv \frac{\sin(\nu)}{\nu} \\ &\int_{-\infty}^{\infty} \frac{d\nu}{2\pi}\mathrm{sinc}^2\left(\frac{\nu}{2}\right) \;=\; 1 \end{aligned} \tag{771}$$

We have used the notation $\delta_\epsilon(\omega)$ for a narrow function with width ϵ.

======= [28.6] The Fermi golden rule (FGR)

The main transitions according to what we have found above is to energy levels that obey the "resonance condition":

$$(E_n - E_{n_0}) \sim \hbar\omega \tag{772}$$

From the expression we found, we see that the probability of transition to levels that obey $|E_n - (E_{n_0} + \omega)| < 2\pi\hbar/t$ is proportional to t^2. That is what we would expect to get by the definition of the Hamiltonian as the probability amplitude for transitions per unit time. But the "width" of the area that includes these levels is proportional to $2\pi\hbar/t$. From this we conclude that the probability of transition to other levels grows linearly. We will call the rate of transition to other levels Γ.

$$\Gamma \;=\; \frac{2\pi}{\Delta}\,|W_{n,n_0}|^2 \;=\; 2\pi g(E)\,|W_{n,n_0}|^2 \tag{773}$$

The formula can be proved by calculating the probability to stay in level n_0:

$$P(t) = 1 - \sum_{n(\neq n_0)} P_t(n|n_0) = 1 - \int \frac{dE}{\Delta} P_t(E|E_0) = 1 - \frac{2\pi t}{\Delta}|W_{n,n_0}|^2 = 1 - \Gamma t \tag{774}$$

It is implicit in the above derivation that we assume a dense spectrum with well defined density of states. We also assume that the relevant matrix elements are all of the same order of magnitude.

Let us discuss the conditions for the validity of the Fermi golden rule picture. First-order perturbation theory is valid while $P(t) \approx 1$, or equivalently $\Gamma t \ll 1$. An important time scale that gets into the game is the Heisenberg time which is defined as:

$$t_H = \frac{2\pi\hbar}{\Delta} \tag{775}$$

We will distinguish below between the case of weak perturbation ($|W| \ll \Delta$) from the case of strong perturbation ($|W| > \Delta$).

In the case $|W| \ll \Delta$ perturbation theory is still valid when $t = t_H$. If perturbation theory is valid up to this time then it is valid at any time, since after the Heisenberg time the (small) probability that has moved from the initial state to other energy levels oscillates, and does not grow further. This argument is based on the assumption that the difference $(E_n - (E_{n_0} + \omega))$ is of the order Δ, even for levels in the middle of the resonance. If there is an "exact" resonance, it is possible to show that the probability will oscillate between the two energy levels, as in the "two-site" problem, and there is no "cumulative" leakage of the probability to other levels.

We will now discuss the case $\Delta < |W|$. In this case, first-order perturbation theory breaks down before the Heisenberg time. Then we must go to higher orders of perturbation theory. With some limitation we find the result:

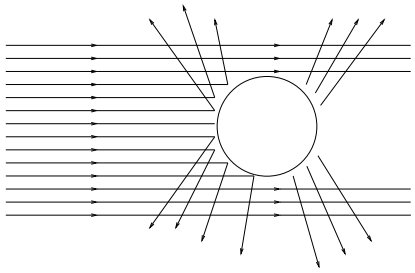
$$P(t) \;=\; \mathrm{e}^{-\Gamma t} \tag{776}$$

This means that there is a decay. In another lecture we analyze a simple model where we can get this result exactly. In the general case, this is an approximate result that is valid (if we are lucky) for times that are neither too long nor too short.

[29] The cross section in the Born approximation

[29.1] Cross Section

In both classical mechanics and quantum mechanics there are two types of problems: closed systems and open systems. We will discuss an open system. The dynamical problem that we will analyze is called a "scattering problem". For example, a wave that is scattered on a sphere. In a problem of this type the energy is given. We assume that there is an "incident particle flux" and we ask what is the "scattered flux".



We notice that the sphere "hides" a certain area of the beam. The total hidden area is called the "total cross section" σ_{total}. Let us assume that we have a beam of particles with energy E and velocity v_E, so that the current density is:

$$J[\text{particles/time/area}] \;=\; \rho_0 v_E \tag{777}$$

Where ρ_0 is the particle density. We write the scattered current as:

$$i_{\text{scattered}} \;=\; [\sigma_{\text{total}}] \times J \tag{778}$$

Where the cross section σ_{total} is defined as the ratio of the scattered current $i_{\text{scattered}}$ to the incident particle flux density J. We notice that each area element of the sphere scatters to a different direction. Therefore, it is more interesting to talk about the differential cross section $\sigma(\Omega)$. In full analogy $\sigma(\Omega)d\Omega$ is defined by the formula:

$$i_{\text{scattered}} \;=\; [\sigma(\Omega)d\Omega] \times J \tag{779}$$

Where $i_{\text{scattered}}$ is the current that is scattered into the angular element $d\Omega$.

[29.2] Cross section and rate of transition

For the theoretical discussion that will follow, it is convenient to think of the space as if it has a finite volume $L^3 = L_x L_y L_z$ with periodic boundary conditions. In addition we assume that the "incident" beam takes up the whole volume. If we normalize the particle density according to the volume then $\rho_0 = 1/L^3$. With this normalization, the flux J (particles per unit time) is actually the "probability current" (probability per unit time), and the current $i_{\text{scattered}}$ is in fact the scattering rate. Therefore an equivalent definition of the cross section is:

$$\Gamma(k \in d\Omega | k_0) \;=\; [\sigma(\Omega)d\Omega] \times \frac{1}{L^3} v_E \tag{780}$$

Below we will see that from the Fermi golden rule we can get a formula for the differential cross section called the "Born approximation":

$$\sigma(\Omega) \;=\; \left(\frac{\mathsf{m}}{2\pi}\right)^2 \left|\tilde{U}(\vec{k}_\Omega - \vec{k}_0)\right|^2 \tag{781}$$

where $\tilde{U}(q)$ is the Fourier transform of the scattering potential $U(r)$.

$$\tilde{U}(q) \;=\; \mathrm{FT}[U(r)] \tag{782}$$

The Born approximation is a first-order perturbation theory approximation. It can be derived with higher order corrections within the framework of scattering theory.

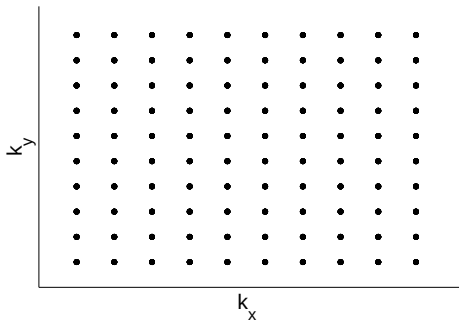
═══ [29.3] The DOS for a free particle

In order to use the Fermi golden rule we need an expression for the density of states of a free particle. In the past we defined $\mathrm{g}(E)dE$ as the number of states with energy $E < E_k < E + dE$. But in order to calculate the differential cross section we need a refined definition:

$$\mathrm{g}(E,\Omega)dEd\Omega \;=\; \text{Number of states with } E < E_k < E + dE \text{ and } \vec{k} \in d\Omega \tag{783}$$

If we have a three-dimensional space with volume $L^3 = L_x L_y L_z$ and periodic boundary conditions, then the momentum states are:

$$k_{n_x,n_y,n_z} \;=\; \left(\frac{2\pi}{L_x}n_x, \frac{2\pi}{L_y}n_y, \frac{2\pi}{L_z}n_z\right) \tag{784}$$



The number of states with a momentum that in a specified region of k space is:

$$\frac{dk_x\,dk_y\,dk_z}{\frac{2\pi}{L_x}n_x\,\frac{2\pi}{L_y}n_y\,\frac{2\pi}{L_z}n_z} \;=\; \frac{L^3}{(2\pi)^2}d^3k \;=\; \frac{L^3}{(2\pi)^3}k^2dkd\Omega \;=\; \frac{L^3}{(2\pi)^3}k_E^2\frac{dE}{v_E}d\Omega \tag{785}$$

Where we have moved to spherical coordinates and used the relation $dE = v_E dk$. Therefore, we find the result:

$$\mathrm{g}(E,\Omega)dEd\Omega \;=\; \frac{L^3}{(2\pi)^3}\frac{k_E^2}{v_E}dEd\Omega \tag{786}$$

═══ [29.4] Derivation of the Born formula

Let us assume that we have a flux of particles that are moving in a box with periodic boundary conditions in the z direction. They are described by the normalized wave equation:

$$\Psi(x) \;=\; \frac{1}{\sqrt{L^3}}\,\mathrm{e}^{ik_E z} \tag{787}$$

As a result of the presence of the scatterer there are transitions to other momentum states (i.e. to other directions of motion). According to the Fermi golden rule the transition rate is:

$$\Gamma(k \in d\Omega|k_0) \;=\; 2\pi\,[g(E,\Omega)d\Omega]\,|U_{k,k_0}|^2 \tag{788}$$

By comparing with the definition of a cross section we get the formula:

$$\sigma(\Omega) \;=\; \frac{2\pi}{v_E}\,L^3\,g(E,\Omega)\,|U_{k,k_0}|^2 \tag{789}$$

We notice that the matrix elements of the scattering potential are:

$$\langle\vec{k}|U(r)|\vec{k_0}\rangle \;=\; \int \frac{d^3x}{L^3}\,\mathrm{e}^{-ikx}U(r)\,\mathrm{e}^{ik_0x}d^3x \;=\; \frac{1}{L^3}\int U(r)\,\mathrm{e}^{-i(k-k_0)x}dx^3 = \frac{1}{L^3}\tilde{U}(k-k_0) \tag{790}$$

By substituting this expression and using the result for the density of states we get:

$$\sigma(\Omega) \;=\; \frac{1}{(2\pi)^2}\left(\frac{k_E}{v_E}\right)^2\,|\tilde{U}(k-k_0)|^2 \tag{791}$$

For a non-relativistic dispersion relation $v_E = k_E/\mathsf{m}$ we get the Born formula in the form that was mentioned previously.

[29.5] Scattering by a spherically symmetric potential

In order to use the Born formula in practice we define our system of coordinates as follows: the incident wave propagates in the z direction, and the scattering direction is $\Omega = (\theta_\Omega, \varphi_\Omega)$. The difference between the k of the scattered wave and the k_0 of the incident wave is $q = k - k_0$. Thus we have to calculate:

$$\tilde{U}(q) \;=\; \int\int\int U(r)\mathrm{e}^{-i\vec{q}\cdot\vec{r}}d^3r \tag{792}$$

If $U(r)$ is spherically symmetric we can use a rotated coordinate system for the calculation of this integral. Namely, we use spherical coordinates such that $\theta = 0$ is the direction of $\vec{q}$. Hence the integral can be written as:

$$\tilde{U}(q) \;=\; \int\int\int U(r)\mathrm{e}^{-iqr\,\cos(\theta)}d\phi d\cos(\theta)r^2dr \tag{793}$$

The angular integration can be done quite easily using:

$$\int_{-1}^{1}\mathrm{e}^{-i\lambda s}ds = \left[\frac{\mathrm{e}^{-i\lambda s}}{-i\lambda}\right]_{-1}^{1} = \frac{\mathrm{e}^{i\lambda}-\mathrm{e}^{-i\lambda}}{i\lambda} = \frac{2\sin(\lambda)}{\lambda} = 2\mathrm{sinc}(\lambda) \tag{794}$$

Leading to:

$$\tilde{U}(q) \;=\; 4\pi\int_0^\infty U(r)\,\mathrm{sinc}(qr)\,r^2dr \tag{795}$$

[29.6] Calculation of the total cross section

The total cross section is:

$$\sigma_{\text{total}} \;=\; \int\int \sigma(\Omega) d\Omega \;=\; \frac{1}{(2\pi)^2}\left(\frac{k_E}{v_E}\right)^2 2\pi \int_{-1}^{1} |\tilde{U}(q)|^2 d\cos\theta_\Omega \tag{796}$$

We note that by simple trigonometry:

$$q \;=\; 2k_E \sin\left(\frac{\theta_\Omega}{2}\right) \tag{797}$$

If we want to change the integration variable then it is useful to use the fact that:

$$dq \;=\; k_E \cos\left(\frac{\theta_{(\Omega)}}{2}\right) d\theta_\Omega \;=\; k_E^2 \frac{\sin(\theta_\Omega)}{q} d\theta_\Omega \;=\; -\frac{k_E^2}{q} d\cos(\theta) \tag{798}$$

Hence we can write the integral of the cross section as:

$$\sigma_{\text{total}} \;=\; \frac{1}{2\pi v_E^2} \int_0^{2k_E} |\tilde{U}(q)|^2 q dq \tag{799}$$

[30] Dynamics in the adiabatic picture

[30.1] The notion of adiabaticity

Consider a particle in a one dimensional box with infinite walls. We now move the wall. What happens to the particle? Let us assume that the particle has been prepared in a certain level. It turns out that if the wall is displaced slowly, then the particle will stay in the same level. This is called the "adiabatic approximation". We notice that staying in the same energy level means that the state of the particle changes! If the wall is moved very fast then the state of the particle does not have time to change. This is called the "sudden approximation". In the latter case the final state (after the displacement of the wall) is not an eigenstate of the (new) Hamiltonian. After a sudden displacement of the wall, the particle will have to "ergodize" it state inside the box.

The fact that the energy of the particle decreases when we move the wall outwards, means that the particle is doing work. If the wall is displaced adiabatically and then displaced back to its original location, then there is no net work done. In such case we say that the process is reversible. But if the displacement of the wall is not slow then the particle makes transitions to other energy levels. The scattering to other energy levels is in general irreversible.

In the problem that we have considered above, the parameter X that we change is the length L of the box. Therefore $V = \dot{X}$ is the velocity at which the wall (or the "piston") is displaced. In other problems X could be any field. An important example is a particle in a ring where $X = \Phi$ is the magnetic flux through the ring, and EMF $= -\dot{X}$ is the electro motive force (by Faraday law). In problems of this type, the change in the parameter X can be very large, so we cannot use standard perturbation theory to analyze the evolution in time. Therefore, we would like to find another way to write Schrödinger's equation, so that $\dot{X}$ is the small parameter.

[30.2] The Schrödinger equation in the adiabatic basis

We assume that we have Hamiltonian $\mathcal{H}(\hat{Q}, \hat{P}; X)$ that depends on a parameter X. The adiabatic states are the eigenstates of the instantaneous Hamiltonian:

$$\mathcal{H}(X)\ |n(X)\rangle \quad = \quad E_n(X)\ |n(X)\rangle \tag{800}$$

It is natural in such problems to work with the adiabatic basis and not with a fixed basis. We will write the state of the system as:

$$|\Psi\rangle = \sum_n a_n(t)|n(X(t))\rangle \tag{801}$$

which means

$$a_n(t) \ \equiv \ \langle n(X(t))|\Psi(t)\rangle \tag{802}$$

If we prepare the particle in the energy level n_0 and change X in an adiabatic way, then we expect $|a_n(t)|^2 \approx \delta_{n,n_0}$. In a later stage we shall find a slowness condition for the validity of this approximation.

The Schrödinger's equation is

$$\frac{d\Psi}{dt} = -i\mathcal{H}(x, p; X(t))\Psi \tag{803}$$

from here we get:

$$\frac{da_n}{dt} = \langle n|\frac{d}{dt}\Psi\rangle + \langle\frac{d}{dt}n|\Psi\rangle = -i\langle n|\mathcal{H}\psi\rangle + \sum_m \langle\frac{d}{dt}n|m\rangle\langle m|\Psi\rangle \tag{804}$$

and hence

$$\frac{da_n}{dt} = -iE_n a_n + \dot{X}\sum_m \langle \frac{\partial}{\partial X} n|m\rangle a_m \tag{805}$$

Using the notation

$$A_{nm} = -i\langle \frac{\partial}{\partial X} n|m\rangle \tag{806}$$

we get

$$\frac{da_n}{dt} = -iE_n a_n + i\dot{X}\sum_m A_{nm} a_m \tag{807}$$

For sake of analysis it is convenient to separate the diagonal part of the perturbation. So we define $A_n = A_{nn}$. We pack the off diagonal part into a matrix which is defined as $W_{nm} = -\dot{X}A_{nm}$ for $n \neq m$ and zero otherwise. With these notations the Schrödinger's equation in the adiabatic representation takes the form

$$\frac{da_n}{dt} = -i(E_n - \dot{X}A_n)a_n - i\sum_m W_{nm} a_m \tag{808}$$

It should be notices that the strength of the perturbation in this representation is determined by the rate $\dot{X}$ and not by the amplitude of the driving.

[30.3] The calculation of A_{nm}

Before we make further progress we would like do dwell on the calculation of the perturbation matrix A_{nm}. First of all we notice that

$$A_{nm} \;=\; -i\langle \frac{\partial}{\partial X} n|m\rangle \;=\; i\langle n|\frac{\partial}{\partial X} m\rangle \tag{809}$$

This is true because for any X

$$\begin{aligned} & \langle n|m\rangle = \delta_{nm} \\ \Rightarrow \quad & \frac{\partial}{\partial X}\langle n|m\rangle = 0 \\ \Rightarrow \quad & \langle \frac{\partial}{\partial X} n|m\rangle + \langle n|\frac{\partial}{\partial X} m\rangle = 0 \end{aligned} \tag{810}$$

In other words $\langle \frac{\partial}{\partial X} n|m\rangle$ is anti-Hermitian, and therefore $-i\langle \frac{\partial}{\partial X} n|m\rangle$ is Hermitian. We define more notations:

$$\begin{aligned} & A_n(X) \;=\; A_{nn} \;=\; i\langle n|\frac{\partial}{\partial X} n\rangle \\ & V_{nm} = \left(\frac{\partial \mathcal{H}}{\partial X}\right)_{nm} \end{aligned} \tag{811}$$

We want to prove that for $n \neq m$:

$$A_{nm} = \frac{iV_{nm}}{E_m - E_n} \tag{812}$$

This is a very practical formula. Its proof is as follows:

$$\begin{aligned} & \langle n|\mathcal{H}|m\rangle = 0 \quad \text{for } n \neq m \\ \Rightarrow \quad & \frac{\partial}{\partial X}\langle n|\mathcal{H}|m\rangle = 0 \\ \Rightarrow \quad & \langle \frac{\partial}{\partial X} n|\mathcal{H}|m\rangle + \langle n|\frac{\partial}{\partial X}\mathcal{H}|m\rangle + \langle n|\mathcal{H}|\frac{\partial}{\partial X} m\rangle = E_m\langle \frac{\partial}{\partial X} n|m\rangle + V_{nm} + E_n\langle n|\frac{\partial}{\partial X} m\rangle = 0 \end{aligned} \tag{813}$$

From the latter equality we get the required identity.

======= [30.4] The adiabatic approximation

If $\dot{X}$ is small enough the perturbation matrix W will not be able to induce transitions between levels, and then we get the adiabatic approximation $|a_n(t)|^2 \approx \text{const}$. This means that the probability distribution does not change with time. In particular, if the particle is prepared in level n, then is stays in this level all the time.

From the discussion of first-order perturbation theory we know that we can neglect the coupling between two different energy levels if the absolute value of the matrix element is smaller compared with the energy difference between the levels. Assuming that all the matrix elements are comparable the main danger to the adiabaticity are transitions to neighboring levels. Therefore the adiabatic condition is $|W| \ll \Delta$ or

$$\dot{X} \ll \frac{\Delta^2}{\hbar\sigma} \tag{814}$$

where σ is the estimate for the matrix element V_{nm} that couples neighboring levels.

An example is in order. Consider a particle in a box of length L. The wall is displaced at a velocity $\dot{X}$. Given that the energy of the particle is E we recall that the energy level spacing is $\Delta = (\pi/L)v_E$, while the coupling of neighboring levels, based on a formula that we have derived in a previous section, is

$$\sigma = \frac{1}{\mathsf{m}L}k_n^2 = \frac{1}{\mathsf{m}L}(\mathsf{m}v_E)^2 = \frac{1}{L}\mathsf{m}v_E^2 \tag{815}$$

It follows that the adiabatic condition is

$$\dot{X} \ll \frac{\hbar}{\mathsf{m}L} \tag{816}$$

Note that the result does not depend on E. This is not the typical case. In typical cases the density of states increases with energy, and consequently it becomes more difficult to satisfy the adiabatic condition.

Assuming we can ignore the coupling between different levels, the adiabatic equation becomes

$$\frac{da_n}{dt} = -i(E_n - \dot{X}A_n)a_n \tag{817}$$

And its solution is:

$$a_n(t) \;=\; \mathrm{e}^{-i\int_0^t (E_n - \dot{X}A_n)dt'} a_n(0) \tag{818}$$

As already observed the probability $|a_n(t)|^2$ to be in a specific energy level does not change in time. That is the adiabatic approximation. But it is interesting to look also at the phase that the particle accumulates. Apart from the dynamical phase, the particle also accumulates a geometrical phase

$$\text{phase} \;=\; \int_0^t (E_n - \dot{X}A_n)dt' \;=\; -\int_0^t E_n dt' \;+\; \int_{X(0)}^{X(t)} A_n(X')dX' \tag{819}$$

An interesting case is when we change more than one parameter. In this case, just as in the Aharonov-Bohm effect, the particle accumulates a "topological" phase that is called the "Berry phase".

$$\text{Berry phase} \equiv \oint A_n(X)dX \tag{820}$$

In fact, the Aharonov-Bohm effect can be viewed as a specific case of the topological effect that was explained above. In order to discuss further topological effects we have to generalize the derivation of the Adiabatic equation. This will be done in the next section.

[31] The Berry phase and adiabatic transport

[31.1] Definitions of A and B

The adiabatic equation is conventionally obtained from the Schrödinger equation by expanding the wavefunction in the x-dependent adiabatic basis:

$$\begin{aligned} \frac{d}{dt}|\psi\rangle &= -\frac{i}{\hbar}\mathcal{H}(x(t))\ |\psi\rangle \\ |\psi\rangle &= \sum_n a_n(t)\ |n(x(t))\rangle \\ \frac{da_n}{dt} &= -\frac{i}{\hbar}E_n a_n + \frac{i}{\hbar}\sum_m \sum_j \dot{x}_j A^j_{nm} a_m \end{aligned} \tag{821}$$

where we define

$$A^j_{nm}(x) = i\hbar \left\langle n(x)\middle|\frac{\partial}{\partial x_j} m(x)\right\rangle \tag{822}$$

Differentiation by parts of $\partial_j\langle n(x)|m(x)\rangle = 0$ leads to the conclusion that A^j_{nm} is a Hermitian matrix. Note that the effect of gauge transformation is

$$\begin{aligned} |n(x)\rangle &\mapsto \mathrm{e}^{-i\frac{\Lambda_n(x)}{\hbar}}\ |n(x)\rangle \\ A^j_{nm} &\mapsto \mathrm{e}^{i\frac{\Lambda_n-\Lambda_m}{\hbar}} A^j_{nm} + (\partial_j\Lambda_n)\delta_{nm} \end{aligned} \tag{823}$$

Note that the diagonal elements $A^j_n \equiv A^j_{nn}$ are real, and transform as $A^j_n \mapsto A^j_n + \partial_j\Lambda_n$.

Associated with $A_n(x)$ is the gauge invariant 2-form, which is defined as:

$$B^{kj}_n = \partial_k A^j_n - \partial_j A^k_n = -2\hbar \mathrm{Im}\langle\partial_k n|\partial_j n\rangle = -\frac{2}{\hbar}\mathrm{Im}\sum_m A^k_{nm}A^j_{mn} \tag{824}$$

This can be written in abstract notation as $B = \nabla \wedge A$.

Using standard manipulations, namely via differentiation by parts of $\partial_j\langle n(x)|\mathcal{H}|m(x)\rangle = 0$, we get for $n \neq m$ the expressions:

$$A^j_{nm}(x) = \frac{i\hbar}{E_m - E_n}\left\langle n\middle|\frac{\partial\mathcal{H}}{\partial x_j}\middle| m\right\rangle \equiv -\frac{i\hbar\mathcal{F}^j_{nm}}{E_m - E_n} \tag{825}$$

and hence

$$B^{kj}_n = 2\hbar \sum_{m(\neq n)} \frac{\mathrm{Im}\left[\mathcal{F}^k_{nm}\mathcal{F}^j_{mn}\right]}{(E_m - E_n)^2} \tag{826}$$

[31.2] Vector Analysis and "Geometrical Forms"

The following mathematical digression is useful in order to better understand topological effects that are associated with adiabatic processes.

Geometrical forms are the "vector analysis" generalization of the length, area and volume concepts to any dimension. In Euclidean geometry with three dimensions the basis for the usual vector space is $\hat{e}_1, \hat{e}_2, \hat{e}_3$. These are called 1-forms. We can also define a basis for surface elements:

$$\begin{aligned} \hat{e}_{12} &= \hat{e}_1 \wedge \hat{e}_2 \\ \hat{e}_{23} &= \hat{e}_2 \wedge \hat{e}_3 \\ \hat{e}_{31} &= \hat{e}_3 \wedge \hat{e}_1 \end{aligned} \tag{827}$$

These are called 2-forms. We also have the volume element $\hat{e}_1 \wedge \hat{e}_2 \wedge \hat{e}_3$ which is called 3-form. There is a natural duality between 2-forms and 1-forms, namely $\hat{e}_{12} \mapsto \hat{e}_3$ and $\hat{e}_{23} \mapsto \hat{e}_1$ and $\hat{e}_{31} \mapsto \hat{e}_2$. Note that $\hat{e}_{21} = -\hat{e}_{12} \mapsto -\hat{e}_3$, and $\hat{e}_1 \wedge \hat{e}_2 \wedge \hat{e}_3 = -\hat{e}_2 \wedge \hat{e}_1 \wedge \hat{e}_3$ etc.

The duality between surface elements and 1-forms does not hold in Euclidean geometry of higher dimension. For example in 4 dimensions the surface elements (2-forms) constitute $C_4^2 = 6$ dimensional space. In the latter case we have duality between the hyper-surface elements (3-forms) and the 1-forms, which are both 4 dimensional spaces. There is of course the simplest example of Euclidean geometry in 2 diemnsional space where 2-forms are regarded as either area or as volume and not as 1-form vectors. In general for N dimensional Euclidean geometry the k forms constitute a C_N^k dimensional vector space, and they are dual to the $(N-k)$ forms.

We can take two 1-forms (vectors) so as to create a surface element:

$$\sum A_i \hat{e_i} \wedge \sum B_i \hat{e_j} = \sum_{i,j} A_i A_j \hat{e_i} \wedge \hat{e_j} \ = \sum_{i<j} (A_i A_j - A_j A_i) \hat{e_i} \wedge \hat{e_j} \tag{828}$$

Note that $\hat{e_i} \wedge \hat{e_i} = \text{Null}$. This leads to the practical formula for a wedge product

$$(A \wedge B)_{ij} = A_i B_j - A_j B_i \tag{829}$$

We can also define the notation

$$(\partial \wedge A)_{ij} = \partial_i A_j - \partial_j A_i \tag{830}$$

Note that in 3 dimensional Euclidean geometry we have the duality

$$\begin{aligned} \partial \wedge A &\mapsto \ \nabla \times A \qquad \text{if } A \text{ is a 1-forms} \\ \partial \wedge B &\mapsto \ \nabla \cdot B \qquad \text{if } B \text{ is a 2-forms} \end{aligned} \tag{831}$$

The above identifications are implied by the following:

$$\begin{aligned} \partial &= \partial_1 \hat{e}_1 + \partial_1 \hat{e}_2 + \partial_1 \hat{e}_3 \\ A &= A_1 \hat{e}_1 + A_2 \hat{e}_2 + A_3 \hat{e}_3 \\ B &= B_{12} \cdot \hat{e}_{12} + B_{23} \cdot \hat{e}_{23} + B_{31} \cdot \hat{e}_{31} \end{aligned} \tag{832}$$

hence

$$(\partial \wedge A)_{12} = \partial_1 A_2 - \partial_2 A_1 = (\nabla \times A)_3 \qquad \text{etc} \tag{833}$$

and

$$\partial \wedge B = (\partial_1 \hat{e}_1 + \partial_2 \hat{e}_2 + \partial_3 \hat{e}_3) \wedge (B_{12} \hat{e}_{12} + B_{23} \hat{e}_{23} + B_{31} \hat{e}_{31}) = (\partial_1 B_{23} + \partial_2 B_{31} + \partial_3 B_{12}) \hat{e}_{123} \mapsto \nabla \cdot B \tag{834}$$

The generalized Stokes theorem relates the closed boundary integral over k-form to an integral over $(k+1)$ form within the interior.

$$\oint A \cdot dl = \int\int \partial \wedge A \cdot ds \tag{835}$$

In 3 dimensional Euclidean geometry this is the Stokes Integral Theorem if A is a 1-form, and the Divergence Integral Theorem if A is a 2-form.

[31.3] The Berry phase

We define the perturbation matrix as

$$W_{nm} = -\sum_j \dot{x}_j A^j_{nm} \qquad \text{for } n \neq m \tag{836}$$

and $W^j_{nm} = 0$ for $n = m$. Then the adiabatic equation can be re-written as follows:

$$\frac{da_n}{dt} = -\frac{i}{\hbar}(E_n - \dot{x}A_n)a_n - \frac{i}{\hbar}\sum_m W_{nm}a_m \tag{837}$$

If we neglect the perturbation W, then we get the strict adiabatic solution:

$$|\psi(t)\rangle \;=\; \mathrm{e}^{-\frac{i}{\hbar}\left(\int_0^t E_n(x(t'))dt' - \int_{x(0)}^{x(t)} A_n(x)\cdot dx\right)}\; |n(x(t))\rangle \tag{838}$$

The time dependence of this solution is exclusively via the x dependence of the basis states. On top, due to $A_n(x)$ we have the so called geometric phase. This can be gauged away unless we consider a closed cycle. For a closed cycle, the gauge invariant phase $\frac{1}{\hbar}\oint \vec{A}\cdot\vec{dx}$ is called the Berry phase.

With the above zero-order solution we can obtain the following result:

$$\langle \mathcal{F}^k \rangle \;=\; \left\langle \psi(t) \left| -\frac{\partial \mathcal{H}}{\partial x_k} \right| \psi(t) \right\rangle \;=\; -\frac{\partial}{\partial x_k}\,\langle n(x)|\; \mathcal{H}(x)\; |n(x)\rangle \tag{839}$$

In the case of the standard examples that were mentioned previously this corresponds to a conservative force or to a persistent current. From now on we ignore this trivial contribution to $\langle \mathcal{F}^k \rangle$, and look for the a first order contribution.

[31.4] Adiabatic Transport

For linear driving (unlike the case of a cycle) the $A_n(x)$ field can be gauged away. Assuming further that the adiabatic equation can be treated as parameter independent (that means disregarding the dependence of E_n and W on x) one realizes that the Schrödinger equation in the adiabatic basis possesses stationary solutions. To first order these are:

$$|\psi(t)\rangle \;=\; |n\rangle + \sum_{m(\neq n)} \frac{W_{mn}}{E_n - E_m}|m\rangle \tag{840}$$

Note that in a *fixed-basis representation* the above stationary solution is in fact time-dependent. Hence the explicit notations $|n(x(t))\rangle$ and $|m(x(t))\rangle$ are possibly more appropriate.

With the above solution we can write $\langle \mathcal{F}^k \rangle$ as a sum of zero order and first order contributions. From now on we ignore the zero order contribution, but keep the first order contribution:

$$\langle \mathcal{F}^k \rangle \;=\; -\sum_{m(\neq n)} \frac{W_{mn}}{E_n - E_m} \left\langle n \left| \frac{\partial \mathcal{H}}{\partial x_k} \right| m \right\rangle + \mathrm{CC} \;=\; \sum_j \left(i \sum_m A^k_{nm} A^j_{mn} + \mathrm{CC} \right) \dot{x}_j \;=\; -\sum_j B^{kj}_n\; \dot{x}_j \tag{841}$$

For a general *stationary* preparation, either pure or mixed, one obtains

$$\langle \mathcal{F}^k \rangle = -\sum_j G^{kj}\ \dot{x}_j \tag{842}$$

with

$$G^{kj}\ =\ \sum_n f(E_n)\ B_n^{kj} \tag{843}$$

Where $f(E_n)$ are weighting factors, with the normalization $\sum_n f(E_n) = 1$. For a pure state preparation $f(E_n)$ distinguishes only one state n, while for a canonical preparation $f(E_n) \propto \mathrm{e}^{-E_n/T}$, where T is the temperature. For a many-body system of non-interacting particles $f(E_n)$ is re-interpreted as the occupation function, so that $\sum_n f(E_n) = N$ is the total number of particles.

Thus we see that the assumption of a stationary first-order solution leads to a non-dissipative (antisymmetric) conductance matrix. This is known as either "adiabatic transport" or "geometric magnetism". In the next sections we are going to see that "adiabatic transport" is in fact a special limit of Kubo formula.

[31.5] Beyond the strict adiabatic limit

If the driving is not strictly adiabatic the validity of the stationary adiabatic solution becomes questionable. In general we have to take non-adiabatic transitions between levels into account. This leads to the Kubo formula for the response which we discuss in the next section. The Kubo formula has many type of derivations. One possibility is to use the same procedure as in the previous section starting with

$$|\psi(t)\rangle\ =\ \mathrm{e}^{-iE_n t}|n\rangle\ +\ \sum_{m(\neq n)} \left[-i\boldsymbol{W}_{mn}\int_0^t \mathrm{e}^{i(E_n-E_m)t'}dt'\right]\mathrm{e}^{-iE_m t}|m\rangle \tag{844}$$

We shall not expand further on this way of derivation, which becomes quite subtle once we go beyond the stationary adiabatic approximation. The standard textbook derivation is presented in the next section.

[32] Linear response theory and the Kubo formula

[32.1] Linear Response Theory

We assume that the Hamiltonian depends on several parameters, say three parameters:

$$\mathcal{H} \;=\; \mathcal{H}(\vec{r},\vec{p};\; x_1(t), x_2(t), x_3(t)) \tag{845}$$

and we define generalized forces

$$\mathcal{F}^k \;=\; -\frac{\partial \mathcal{H}}{\partial x_k} \tag{846}$$

Linear response means that

$$\langle \mathcal{F}^k \rangle_t \;=\; \sum_j \int_{-\infty}^{\infty} \alpha^{kj}(t-t')\; \delta x_j(t') dt' \tag{847}$$

Where $\alpha^{kj}(\tau) = 0$ for $\tau < 0$. The expression for the response Kernel is known as the Kubo formula:

$$\alpha^{kj}(\tau) = \Theta(\tau)\, \frac{i}{\hbar} \langle [\mathcal{F}^k(\tau), \mathcal{F}^j(0)] \rangle_0 \tag{848}$$

Where the average is taken with the assumed zero order stationary solution. Before we present the standard derivation of this result we would like to illuminate the *DC limit* of this formula, and to further explain the *adiabatic limit* that was discussed in the previous section.

[32.2] Susceptibility and DC Conductance

The Fourier transform of $\alpha^{kj}(\tau)$ is the generalized susceptibility $\chi^{kj}(\omega)$. Hence

$$[\langle \mathcal{F}^k \rangle]_\omega \;=\; \sum_j \chi_0^{kj}(\omega)[x_j]_\omega - \sum_j \mu^{kj}(\omega)[\dot{x}_j]_\omega \tag{849}$$

where the dissipation coefficient is defined as

$$\mu^{kj}(\omega) = \frac{\mathrm{Im}[\chi^{kj}(\omega)]}{\omega} = \int_0^{\infty} \alpha^{kj}(\tau) \frac{\sin(\omega\tau)}{\omega} d\tau \tag{850}$$

In the "DC limit" ($\omega \to 0$) it is natural to define the generalized conductance matrix:

$$G^{kj} \;=\; \mu^{kj}(\omega \sim 0) \;=\; \lim_{\omega\to 0} \frac{\mathrm{Im}[\chi^{kj}(\omega)]}{\omega} \;=\; \int_0^{\infty} \alpha^{kj}(\tau)\tau d\tau \tag{851}$$

Consequently the non-conservative part of the response can be written as a generalized Ohm law.

$$\langle \mathcal{F}^k \rangle = -\sum_j G^{kj}\; \dot{x}_j \tag{852}$$

It is convenient to write the conductance matrix as

$$G^{kj} \equiv\; \eta^{kj} + B^{kj} \tag{853}$$

where $\eta^{kj} = \eta^{jk}$ is the symmetric part of the conductance matrix, while $B^{kj} = -B^{jk}$ is the antisymmetric part. In our case there are three parameters so we can arrange the elements of the antisymmetric part as a vector $\vec{B} = (B^{23}, B^{31}, B^{12})$. Consequently the generalized Ohm law can be written in abstract notation as

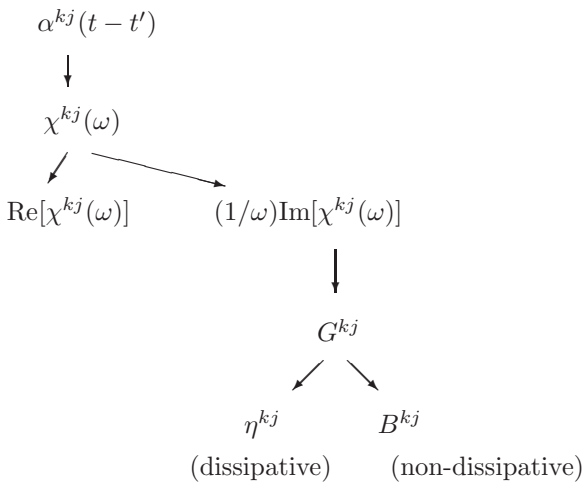
$$\langle \mathcal{F} \rangle \;=\; -\eta \cdot \dot{x} \;-\; B \wedge \dot{x} \tag{854}$$

where the dot product should be interpreted as matrix-vector multiplication, which involves summation over the index j. The wedge-product can also be regarded as a matrix-vector multiplication. It reduces to the more familiar cross-product in the case we have been considering - 3 parameters. The dissipation, which is defined as the rate at which energy is absorbed into the system, is given by

$$\dot{W} \;=\; -\langle \mathcal{F} \rangle \cdot \dot{x} \;=\; \sum_{kj} \eta^{kj}\; \dot{x}_k \dot{x}_j \tag{855}$$

which is a generalization of Joule's law. Only the symmetric part contributes to the the dissipation. The contribution of the antisymmetric part is identically zero.

The conductance matrix is essentially a synonym for the term "dissipation coefficient". However, "conductance" is a better (less misleading) terminology: it does not have the (wrong) connotation of being specifically associated with dissipation, and consequently it is less confusing to say that it contains a non-dissipative component. We summarize the various definitions by the following diagram:



[32.3] Derivation of the Kubo formula

In what follows we bring the standard textbook derivation of the Kubo formula. We note that there are more elaborated derivations that highlight the its limitations and attempt in improving over it. For notational simplicity we write the Hamiltonian as

$$\mathcal{H} \;=\; \mathcal{H}_0 \;- f(t) V \tag{856}$$

and use units with $\hbar = 1$. We assume that the system, in the absence of driving, is prepared in a stationary state ρ_0. In the presence of driving we look for a first order solution $\rho(t) = \rho_0 + \tilde{\rho}(t)$. The equation for $\tilde{\rho}(t)$ is:

$$\frac{\partial \tilde{\rho}(t)}{\partial t} \;\approx\; -i[\mathcal{H}_0, \tilde{\rho}(t)] + i f(t) [V, \rho_0] \tag{857}$$

Next we use the substitution $\tilde{\rho}(t) = U_0(t)\tilde{\tilde{\rho}}(t)U_0(t)^{-1}$, where $U_0(t)$ is the evolution operator which is generated by $\mathcal{H}_0$. Thus we eliminate from the equation the zero order term:

$$\frac{\partial\tilde{\tilde{\rho}}(t)}{\partial t} \;\approx\; if(t)[U_0(t)^{-1}VU_0(t),\rho_0] \tag{858}$$

The solution of the latter equation is straightforward and leads to

$$\rho(t) \;\approx\; \rho_0 + \int^t i\;[V(-(t-t')),\rho_0]\;f(t')dt' \tag{859}$$

where we use the common notation $V(\tau) = U_0(\tau)^{-1}VU_0(\tau)$.

Consider now the time dependence of the expectation value $\langle\mathcal{F}\rangle_t = \mathrm{trace}(\mathcal{F}\rho(t))$ of an observable. Disregarding the zero order contribution, the first order expression is

$$\langle\mathcal{F}\rangle_t \;\approx\; \int^t i\;\mathrm{trace}\,(\mathcal{F}[V(-(t-t')),\rho_0])\;\;f(t')dt' \;\;=\;\; \int^t \alpha(t-t')\;f(t')dt'$$

where the response kernel $\alpha(\tau)$ is defined for $\tau > 0$ as

$$\alpha(\tau) = i\;\mathrm{trace}\,(\mathcal{F}[V(-\tau),\rho_0]) \;= i\;\mathrm{trace}\,([\mathcal{F},V(-\tau)]\rho_0) \;= i\langle[\mathcal{F},V(-\tau)]\rangle \;= i\langle[\mathcal{F}(\tau),V]\rangle \tag{860}$$

Where we have used the cyclic property of the trace operation; the stationarity $U_0\rho_0U_0^{-1} = \rho_0$ of the unperturbed state; and the notation $\mathcal{F}(\tau) = U_0(\tau)^{-1}\mathcal{F}U_0(\tau)$.

[33] The Born-Oppenheimer Picture

We now consider a more complicated problem, where x becomes a dynamical variable. The standard basis for the representation of the composite system is $|x, Q\rangle = |x\rangle \otimes |Q\rangle$. We assume a total Hamiltonian of the form

$$\mathcal{H}_{\text{total}} \;=\; \frac{1}{2\mathsf{m}} \sum_j p_j^2 + \mathcal{H}(Q, P; x) - f(t)V(Q) \tag{861}$$

Rather than using the standard basis, we can use the Born-Oppenheimer basis $|x, n(x)\rangle = |x\rangle \otimes |n(x)\rangle$. Accordingly the state of the combined system is represented by the wavefunction $\Psi_n(x)$, namely

$$|\Psi\rangle \;=\; \sum_{n,x} \Psi_n(x)\; |x, n(x)\rangle \tag{862}$$

The matrix elements of $\mathcal{H}$ are

$$\langle x, n(x)|\mathcal{H}|x_0, m(x_0)\rangle \;=\; \delta(x - x_0) \times \delta_{nm} E_n(x) \tag{863}$$

The matrix elements of $V(Q)$ are

$$\langle x, n(x)|V(Q)|x_0, m(x_0)\rangle \;=\; \delta(x - x_0) \times V_{nm}(x) \tag{864}$$

The matrix elements of p are

$$\langle x, n(x)|p_j|x_0, m(x_0)\rangle \;=\; (-i\partial_j \delta(x - x_0)) \times \langle n(x)|m(x_0)\rangle$$

The latter can be manipulated "by parts" leading to

$$\langle x, n(x)|p_j|x_0, m(x_0)\rangle \;=\; -i\partial_j \delta(x - x_0)\delta_{nm} - \delta(x - x_0) A^j_{nm}(x) \tag{865}$$

This can be summarized by saying that the operation of p_j on a wavefunction is like the differential operator $-i\partial_j - A^j_{nm}(x)$. Thus in the Born-Oppenheimer basis the total Hamiltonian takes the form

$$\mathcal{H}_{\text{total}} \;=\; \frac{1}{2\mathsf{m}} \sum_j (p_j - A^j_{nm}(x))^2 + \delta_{nm} E_n(x) - f(t) V_{nm}(x) \tag{866}$$

Assuming that the system is prepared in energy level n, and disregarding the effect of A and V, the adiabatic motion of x is determined by the effective potential $E_n(x)$. This is the standard approximation in studies of diatomic molecules, where x is the the distance between the nuclei. If we treat the slow motion as classical, then the interaction with A can be written as

$$\mathcal{H}^{(1)}_{\text{interaction}} \;=\; -\sum_j \dot{x}_j A^j_{nm}(x) \tag{867}$$

This brings us back to the theory of driven systems as discussed in previous sections. The other interaction that can induce transitions between levels is

$$\mathcal{H}^{(2)}_{\text{interaction}} \;=\; -f(t) V_{nm}(x) \tag{868}$$

The analysis of molecular "wavepacket dynamics" is based on this picture.

The Green function approach

[34] The propagator and Feynman path integral

═══ [34.1] The propgator

The evolution of a quantum mechanical system is described by a unitary operator

$$|\Psi(t)\rangle \;=\; U(t,t_0)\;|\Psi(t_0)\rangle \tag{869}$$

The Hamiltonian is defined by writing the infinitesimal evolution as

$$U(t+dt,t) = 1 - idt\mathcal{H}(t) \tag{870}$$

This expression has an imaginary i in order to make $\mathcal{H}$ a Hermitian matrix. If we want to describe continuous evolution we can "break" the time interval into N infinitesimal steps:

$$U(t,t_0) \;=\; (1-idt_N\mathcal{H})\ldots(1-idt_2\mathcal{H})(1-idt_1\mathcal{H}) \;\equiv\; \mathcal{T}\mathrm{e}^{-i\int_{t_0}^{t}\mathcal{H}(t')dt'} \tag{871}$$

For a time independent Hamiltonian we get simply $U(t)=\mathrm{e}^{-it\mathcal{H}}$ because of the identity $\mathrm{e}^A\mathrm{e}^B=\mathrm{e}^{A+B}$ if $[A,B]=0$.

If we consider a particle and use the standard position representation then the unitary operator is represented by a matrix $U(x|x_0)$. The time interval $[t_0,t]$ is implicit. We alway assume that $t>t_0$. Later it would be convenient to define the propagator as $U(x|x_0)$ for $t>t_0$ and as zero otherwise. The reason for this convention is related to the formalism that we are going to introduce later on.

═══ [34.2] The Propagator for a free particle

Consider a free particle in one dimension. Let us find the propagator using a direct calculation. The hamiltonian is:

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} \tag{872}$$

As long as the Hamiltonian has a quadratic form, the answer will be a Gaussian kernel:

$$U(x|x_0) = \left\langle x\left|\mathrm{e}^{-i\frac{t}{2\mathsf{m}}p^2}\right|x_0\right\rangle = (\frac{\mathsf{m}}{2\pi it})^{\frac{1}{2}}\mathrm{e}^{i\frac{\mathsf{m}}{2t}(x-x_0)^2} \tag{873}$$

We note that in the case of a harmonic oscillator

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} + \frac{1}{2}\mathsf{m}\Omega^2x^2 \tag{874}$$

The propagator is

$$U(x|x_0) = \left(\frac{\mathsf{m}\Omega}{2\pi i\sin\Omega t}\right)^{\frac{1}{2}}\mathrm{e}^{i\frac{\mathsf{m}\Omega}{2\sin\Omega t}[\cos\Omega t(x^2+x_0^2)-2xx_0]} \tag{875}$$

If we take $t\to 0$ then $U\to\hat{1}$, and therefore $U(x|x_0)\to\delta(x-x_0)$.

The derivation of the expression for the propagator in the case of a free particle goes as follows. We use the notation $\tau = \frac{t}{\mathsf{m}}$:

$$\langle x|\mathrm{e}^{-\imath\frac{1}{2}\tau p^2}|x_0\rangle = \sum_k \langle x|k\rangle \mathrm{e}^{-\imath\frac{1}{2}\tau k^2}\langle k|x_0\rangle = \int \frac{dk}{2\pi}\mathrm{e}^{-\imath\frac{1}{2}\tau k^2 + ik(x-x_0)} \tag{876}$$

This is formally the FT of a Gaussian with $\sigma = i\tau$, which gives the desired result. We note that we can write the result in the form

$$\langle x|\mathrm{e}^{-\imath\frac{1}{2}\tau p^2}|x_0\rangle = \frac{1}{\sqrt{2\pi\imath\tau}}\mathrm{e}^{\frac{\imath(x-x_0)^2}{2\tau}} = \frac{1}{\sqrt{2\pi\imath\tau}}\left[\cos\frac{1}{2\tau}(x-x_0)^2 + \imath\sin\frac{1}{2\tau}(x-x_0)^2\right] \tag{877}$$

If $\tau \to 0$ we should get a delta function. This is implied by the FT, but it would be nice to verify this statement directly. Namely we have to show that in this limit we get a narrow function whose "area" is unity. For this purpose we use identity

$$\int \cos r^2 \ldots dr \;=\; \int \frac{\cos u}{2\sqrt{u}}\ldots du \tag{878}$$

and a similar expression in case of sin function. Then we recall the elementary integrals

$$\int_0^\infty \frac{\sin u}{\sqrt{u}}du = \int_0^\infty \frac{\cos u}{\sqrt{u}}du = \sqrt{\frac{\pi}{2}} \tag{879}$$

Thus the "area" of the two terms in the square brackets is proportional to $(1+i)/\sqrt{2}$ which cancels the $\sqrt{i}$ of the prefactor.

═══ [34.3] Feynman Path Integrals

How can we find the propagator $U(x|x_0)$ for the general Hamiltonian $\mathcal{H} = \frac{p^2}{2\mathsf{m}} + V(x)$? The idea is to write $\langle x|\mathrm{e}^{-\imath t\mathcal{H}}|x_0\rangle$ as a convolution of small time steps:

$$\langle x|\mathrm{e}^{-\imath t\mathcal{H}}|x_0\rangle = \sum_{x_1,x_2,\ldots x_{N-1}} \langle x|\mathrm{e}^{-\imath\delta t_N\mathcal{H}}|x_{N-1}\rangle \ldots \langle x_2|\mathrm{e}^{-\imath\delta t_2\mathcal{H}}|x_1\rangle\langle x_1|\mathrm{e}^{-\imath\delta t_1\mathcal{H}}|x_0\rangle \tag{880}$$

Now we have to find the propagator for each infinitesimal step. At first sight it looks as if we just complicated the calculation. But then we recall that for infinitesimal operations we have:

$$\mathrm{e}^{\varepsilon A+\varepsilon B} \approx \mathrm{e}^{\varepsilon A}\mathrm{e}^{\varepsilon B} \approx \mathrm{e}^{\varepsilon B}\mathrm{e}^{\varepsilon A} \qquad \text{for any } A \text{ and } B \tag{881}$$

This is because the higher order correction can be made as small as we want. So we write

$$\langle x_j|\mathrm{e}^{-\imath\delta t(\frac{p^2}{2\mathsf{m}}+V(x))}|x_{j-1}\rangle \approx \langle x_j|\mathrm{e}^{-\imath\delta tV(x))}\mathrm{e}^{-\imath\delta t\frac{p^2}{2\mathsf{m}}}|x_{j-1}\rangle \approx (\frac{\mathsf{m}}{2\pi\imath dt_j})^{\frac{1}{2}}\mathrm{e}^{\imath\frac{\mathsf{m}}{2dt_j}(x_j-x_{j-1})^2 - dt_jV(x_j)} \tag{882}$$

and get:

$$U(x|x_0) = \int dx_1dx_2\ldots dx_{N-1}(\frac{\mathsf{m}}{2\pi\imath dt})^{\frac{N}{2}}\mathrm{e}^{i\mathcal{A}[x]} \;\equiv\; \int d[x]\;\mathrm{e}^{i\mathcal{A}[x]} \tag{883}$$

where $\mathcal{A}[x]$ is called the **action**.

$$\mathcal{A}[x] = \sum_{j=1}^{N-1} \Big[\frac{\mathsf{m}}{2dt}(x_j - x_{j-1})^2 - dtV(x) \Big] = \int (\frac{1}{2}\mathsf{m}\dot{x}^2 - V(x))dt = \int \mathcal{L}(x,\dot{x})dt \tag{884}$$

More generally, if we include the vector potential in the Hamiltonian, then we get the Lagrangian

$$\mathcal{L}(x,\dot{x}) \;\; = \;\; \frac{1}{2}\mathsf{m}\dot{x}^2 - V(x) + A(x)\dot{x} \tag{885}$$

leading to:

$$\mathcal{A}[x] = \int (\frac{1}{2}\mathsf{m}\dot{x}^2 - V(x))dt + \int A(x)\cdot dx \tag{886}$$

═══ [34.4] Stationary Point Approximation

This method helps us to solve integrals of the form $\int \mathrm{e}^{\imath S(x)}dx$. The main contribution to the integral comes from the point $x = x_0$, called a **s**tationary point, where $S'(x) = 0$. We expand the function $S(x)$ near the stationary point:

$$S(x) = S(x_0) + \frac{1}{2}S''(x_0)(x - x_0)^2 + \ldots \tag{887}$$

Leading to

$$\int \mathrm{e}^{\imath S(x)}dx \approx \mathrm{e}^{\imath S(x_0)} \int \mathrm{e}^{\imath \frac{1}{2} S^{"}(x_0)(x-x_0)^2} = \sqrt{\frac{i2\pi}{S^{"}(x_0)}}\mathrm{e}^{\imath S(x_0)} \tag{888}$$

Where the exponential term is a leading order term, and the prefactor is an "algebraic decoration".

The generalization of this method to multi-dimensional integration over $d[x]$ is immediate. The stationary point is in fact the trajectory for which the first order variation is zero ($\delta\mathcal{A} = 0$). This leads to Lagrange equation, which implies that the "stationary point" is in fact the classical trajectory. Consequently we get the so called semiclassical (Van-Vleck) approximation:

$$U(x|x_0) \;\; = \;\; \int d[x]\; \mathrm{e}^{\mathcal{A}[x]} \;\; \approx \;\; \sum_{cl} \left(\frac{1}{i2\pi\hbar}\right)^{d/2} \sqrt{\det\left(-\frac{\partial^2 \mathcal{A}_{cl}}{\partial x \partial x_0}\right)}\; \mathrm{e}^{i\mathcal{A}_{cl}(x,x_0) - i(\pi/2)\nu_{cl}} \tag{889}$$

Where d is the number of degrees of freedom, and

$$\mathcal{A}_{cl}(x,x_0) \equiv \mathcal{A}[x_{cl}] \tag{890}$$

is the action of the classical trajectory as a function of the two end points. In d dimensions the associated determinant is $d \times d$. The Morse-Maslov index ν_{cl} counts the number of conjugate points along the classical trajectory. The recipe for its determination is as follows: The linearized equation of motion for $x(t) = x_{cl}(t) + \delta x(t)$ is

$$\mathsf{m}\delta\ddot{x} + V''(x_{cl})\delta x = 0 \tag{891}$$

A conjugate point (in time) is defined as the time when the linearized equation has a non-trivial solution. With this rule we expect that in case of a reflection from a wall, the Morse index is $\mathbf{+1}$ for each collision. This is correct

for "soft" wall. In case of "hard" wall the standard semiclassical result for ν_{cl} breaks down, and the correct result turns out to be **+2** for each collision. The latter rule is implied by the **Dirichlet** boundary conditions. Note, that it would be **+0** in the case of **Neumann** boundary conditions. The Van-Vleck semiclassical approximation is exact for quadratic Hamiltonians because the "stationary phase integral" is exact if there are no higher order terms in the Taylor expansion.

Let us compute again $U(x|x_0)$ for a free particle, this time using the Van-Vleck expression: The action $\mathcal{A}[x]$ for the free particle is

$$\mathcal{A}[x] = \int_0^t \frac{1}{2}\mathsf{m}\dot{x}^2 dt'. \tag{892}$$

Given the end points we find the classical path

$$x_{cl} = x_0 + \frac{x - x_0}{t}t' \tag{893}$$

and hence

$$\mathcal{A}_{cl}(x, x_0) = \int_0^t \frac{1}{2}\mathsf{m}(\frac{x - x_0}{t})^2 dt' = \frac{\mathsf{m}}{2t}(x - x_0)^2. \tag{894}$$

We also observe that

$$-\frac{\partial^2 \mathcal{A}_{cl}}{\partial x \partial x_0} \quad = \quad \frac{\mathsf{m}}{t} \tag{895}$$

which leads to the exact result. The big advantage of this procedure emerges clearly once we try to derive the more general expression in case of a harmonic oscillator.

[35] The resolvent and the Green Function

[35.1] The resolvent

The resolvent is defined in the complex plane as

$$G(z) = \frac{1}{z - \mathcal{H}} \tag{896}$$

In case of a bounded system it has poles at the eigenvalues. We postpone for later the discussion of unbounded systems. It is possibly more illuminating to look on the matrix elements of the resolvent

$$G(x|x_0) \;=\; \langle x|G(z)|x_0\rangle \;=\; \sum_n \frac{\psi^n(x)\psi^n(x_0)^*}{z - E_n} \;\equiv\; \sum_n \frac{q_n}{z - E_n} \tag{897}$$

where $\psi^n(x) = \langle x|n\rangle$ are the eigenstates of the Hamiltonian. If we fix x and x_0 and regard this expression as a function of z this is formally the complex representation of an electric field in a two dimensional electrostatic problem.

We can look on $G(x|x_0)$, with fixed $z = E$ and x_0, as a wavefunction in the variable x. We see that $G(x|x_0)$ is a superposition of eigenstates. If we operate on it with $(E - \mathcal{H})$ the coefficients of this superposition are multiplied by $(E - E_k)$, and because of the completeness of the basis we get $\delta(x - x_0)$. This means that $G(x|x_0)$ satisfies the Schrodinger equation with the complex energy E and with an added source at $x = x_0$. Namely,

$$(E - \mathcal{H})G(x|x_0) = \delta(x - x_0) \tag{898}$$

This is simply the standard representation of the equation $(z - \mathcal{H})G = \hat{1}$ which defines the matrix inversion $G = 1/(z - \mathcal{H})$. The wavefunction $G(x|x_0)$ should satisfy that appropriate boundary conditions. If we deal with a prticle in a box this means Dirichlet boundary conditions. In case of an unbounded system the issue of boundary conditions deserves further discussion (see later).

The importance of the Green functions comes from its Fourier transform relation to the propagator. Namely,

$$FT\Big[\ \Theta(t)\mathrm{e}^{-\eta t}\ U(t)\Big] \;\;=\;\; iG(\omega + i\eta) \tag{899}$$

Where $\Theta(t)$ is the step function, $\Theta(t)U(t)$ is the "propagator", and $\mathrm{e}^{-\eta t}$ is an envelope function that guarantees convergence of the FT integral. Later we discuss the limit $\eta \to 0$.

We note that we can extract from the resolvent useful information. For example, we can get the energy eigenfunction by calculation the residues of $G(z)$. The Green functions, which we discuss in the next section are obtained (defined) as follows:

$$G^{\pm}(\omega) \;=\; G(z = \omega \pm i0) \;=\; \frac{1}{\omega - \mathcal{H} \pm i0} \tag{900}$$

From this definition follows that

$$\mathrm{Im}[G^+] \equiv -\frac{i}{2}(G^+ - G^-) = -\pi\delta(E - \mathcal{H}) \tag{901}$$

From here we get expression for the density of states $g(E)$ and for the local density of states $\rho(E)$, where the latter is with respect to an arbitrary reference state Ψ

$$\begin{aligned} g(E) \;&=\; -\frac{1}{\pi}\mathrm{trace}\Big(\ \mathrm{Im}[G^+(E)]\ \Big) \\ \rho(E) \;&=\; -\frac{1}{\pi}\Big\langle \Psi\Big|\ \mathrm{Im}[G^+(E)]\ \Big|\Psi\Big\rangle \end{aligned} \tag{902}$$

Further applications of the Green functions will be discussed later on.

Concluding this section we note that from the above it should become clear that there are three methods of calculating the matrix elements of the resolvent:

- Summing as expansion in the energy basis
- Solving an equation (Helmholtz for a free particle)
- Finding the Fourier transform of the propagator

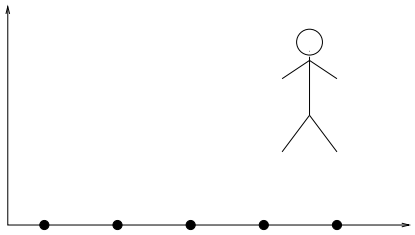
Possibly the second method is the simplest, while the third one is useful in semiclassical schemes.

[35.2] Analytic continuation

The resolvent is well defined for any z away from the real axis. We define $G^+(z) = G(z)$ in the upper half of the complex plane. As long as we discuss bounded systems this "definition" looks like a duplication. The mathematics becomes more interesting once we consider unbounded systems with a continuous energy spectrum. In the latter case there are circumstances that allow analytic continuation of $G^+(z)$ into the lower half of the complex plane. This analytical continuation, if exists, would not coincide with $G^-(z)$.

In order to make the discussion of analytical continuation transparent let us assume, without loss of generality, that we are interested in the following object:

$$f(z) \;=\; \langle\Psi|G(z)|\Psi\rangle \;=\; \sum_n \frac{q_n}{z-E_n} \tag{903}$$

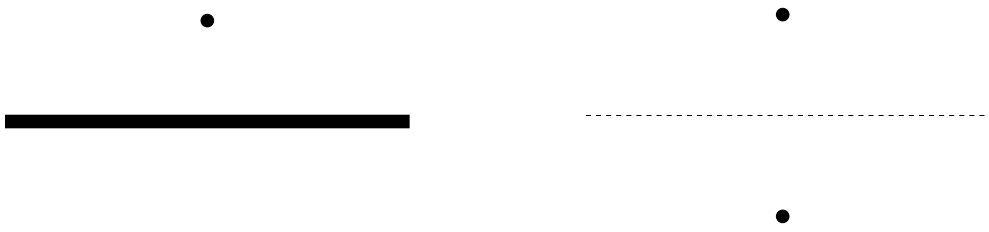


The function $f(z)$ with $z = x + iy$ can be regarded as describing the electric field in a two dimensional electrostatic problem. The field is created by charges that are placed along the real axis. As the system grows larger and larger the charges become more and more dense, and therefore in the "far field" the discrete sum $\sum_n$ can be replaced by an integral $\int g(E)dE$ where $g(E)$ is the smoothed density of states. By "far field" we mean that $\mathrm{Im}[z]$ is much larger compared with the mean level spacing and therefore we cannot resolve the finite distance between the charges. In the limit of an infinite system this becomes exact for any finite (non-zero) distance from the real axis.

In order to motivate the discussion of analytical continuation let us consider a typical problem. Consider a system built of two weakly coupled 1D regions. One is a small "box" and the other is a very large "surrounding". The barrier between the two regions is a large delta function. According to perturbation theory the zero order states of the "surrounding" are mixed with the zero order bound states of the "box". The mixing is strong if the energy difference of the zero order states is small. Thus we have mixing mainly in the vicinity of the energies E_r where we formerly we had bound states of the isolated "box". Let us assume that Ψ describes the initial preparation of the particle inside the "box". Consequently we have large q_n only for states with $E_n \approx E_r$. This means that we have an increased "charge density" in the vicinity of energies E_r. It is the LDOS rather than the DOS which is responsible for this increased charge density. Now we want to calculate $f(z)$. What would be the implication of the increased charge density on the calculation?

In order to understand the implication of the increased charge density on the calculation we recall a familiar problem from electrostatics. Assume that we have a conducting metal plate and a positive electric charge. Obviously there will be an induced negative charge distribution on the metal plate. We can follow the electric field lines through the

plate, from above the plate to the other side. We realize that we can replace all the charge distribution on the plate by a single negative electric charge (this is the so called "image charge").



Returning to the resolvent, we realize that we can represent the effect of the increased "charge density" using an "image charge" which we call a "resonance pole". The location of the "resonance pole" is written as $E_r - i(\Gamma_r/2)$. Formally we say that the resonance poles are obtained by the analytic continuation of $G(z)$ from the upper half plane into the lower half plane. In practice we can find these poles by looking for complex energies for which the Schrodinger equation has solutions with "outgoing" boundary conditions. In another section we give an explicit solution for the above problem. Assume that this way or another we find an approximation for $f(z)$ using such "image charges":

$$f(E) \;=\; \langle\Psi|G^{+}(E)|\Psi\rangle \;=\; \sum_n \frac{q_n}{E-(E_n-i0)} \;=\; \sum_r \frac{Q_r}{E-(E_r-i(\Gamma_r/2))} + \text{smooth background} \tag{904}$$

We observe that the sum over n is in fact an integral, while the sum over r is a discrete sum. So the analytic continuation provides a simple expression for $G(z)$. Now we can use this expression in order to deduce physical information. We immediately find the the LDOS can be written as as sum over Lorentzians. The Fourier transform of the LDOS is the survival amplitude, which comes out a sum over exponentials. In fact we can get the result for the survival amplitude directly by recalling that $\Theta(t)U(t)$ is the FT of $iG^{+}(\omega)$. Hence

$$\langle x|U(t)|x_0\rangle \;=\; \sum_r Q_r \mathrm{e}^{-iE_rt-(\Gamma_r/2)t} + \text{short time corrections} \tag{905}$$

If Ψ involves contribution form only one resonance, then the probability to stay inside the "box" decreases exponentially with time. This is the type of result that we would expect form either Wigner theory or from the Fermi Golden rule. Indeed we are going later to develop a perturbation theory for the resolvent, and to show that the expression for Γ in leading order is as expected.

[35.3] The Green function of a bounded particle

In order to get insight into the mathematics o f $G^{+}(z)$ we first consider how $G(z)$ looks like for a particle in a very large box. To be more specific we can consider a particle in a potential well or on a ring. In the latter case it means periodic boundary conditions rather than Dirichlet boundary conditions. Later we would like to take the length L of the box to be infinite so as to have a "free particle". Expanding $\psi(x) = \langle x|G(z)|x_0\rangle$ in the energy basis we get the following expressions:

$$\begin{aligned}
\langle x|G_{\text{well}}(z)|x_0\rangle \;&=\; \frac{2}{L}\sum_n \frac{\sin(k_nx)\sin(k_nx_0)}{z-E_n} \\
\langle x|G_{\text{ring}}(z)|x_0\rangle \;&=\; \frac{1}{L}\sum_n \frac{\mathrm{e}^{ik_n(x-x_0)}}{z-E_n}
\end{aligned} \tag{906}$$

where the real k_n correspond to a box of length L. As discussed in the previous lecture, this sum can be visualized as the field which is created by a string of charges along the real axis. If we are far enough from the real axis we get a field which is the same as that of a smooth distribution of "charge". Let us call it the "far field" region. As we take the volume of the box to infinity the "near field" region, whose width is determined by the level spacing, shrinks

and disappears. Then we are left with the "far field" which is the resolvent of a free particle. The result should not depend on whether we consider Dirichlet of periodic boundary conditions.

The summation of the above sums is technically too difficult. In order to get an explicit expression for the resolvent we recall that $\psi(x) = \langle x|G(z)|x_0\rangle$ is the solution of a Schrodinger equation with complex energy z and a source at $x = x_0$. The solution of this equation is

$$\langle x|G(z)|x_0\rangle = -i\frac{\mathsf{m}}{k}\mathrm{e}^{ik|x-x_0|} + A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx} \tag{907}$$

where $k = (2\mathsf{m}z)^{1/2}$ corresponds to the complex energy z. The first term satisfies the matching condition at the source, while the other two terms are "free waves" that solve the associated homogeneous equation. The coefficients A and B should be adjusted such that the boundary conditions are satisfied. For the "well" we should ensure the Dirichlet boundary conditions $\psi(x) = 0$ for $x = 0, L$, while for the "ring" we should ensure the periodic boundary conditions $\psi(0) = \psi(L)$ and $\psi'(0) = \psi'(L)$.

Let us try to gain some insight for the solution. If z is in the upper half plane then we can write $k = k_E + i\alpha$ where both k_E and α are positive(!) real numbers. This means that a propagating wave (either right going or left going) exponentially decays to zero in the propagation direction, and exponentially explodes in the opposite direction. It is not difficult to conclude that in the limit of a very large L the coefficients A and B become exponentially small. In the strict $L \to \infty$ limit we may say that $\psi(x)$ should satisfy "outgoing boundary conditions". If we want to make analytical continuation of $G(z)$ to the lower half plane, we should stick to these "outgoing boundary conditions". The implication is that $\psi(x)$ in the lower half plane exponentially explodes at infinity.

An optional argument that establishes the application of the outgoing boundary conditions is based on the observation that the FT of the retarded $G^+(\omega)$ gives the propagator. The propagator is identically zero for negative times. If we use the propagator to propagate a wavepacket, we should get a non-zero result for positive times and a zero result for negative times. In case of an unbounded particle only outgoing waves are consistent with this description.

======= [35.4] The Green function of a free particle

For a free particle the eigenstates are known and we can calculate the expression by inserting a complete set and integrating. From now on we set $\mathsf{m} = 1$ in calculations, but we restore it in the final result.

$$\begin{aligned} G^+(x|x_0) &= \sum_k \langle x|k\rangle \frac{1}{E - \frac{1}{2}k^2 + i0}\langle k|x_0\rangle \\ &= \int \frac{d\mathbf{k}}{(2\pi)^d}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\frac{1}{E - \frac{1}{2}k^2 + i0} \end{aligned} \tag{908}$$

where d is the dimension of the space. In order to compute this expression we define $\vec{r} = \vec{x} - \vec{x_0}$ and choose our coordinate system in such a way that the $\hat{z}$ direction will coincide with the direction of $\mathbf{r}$.

$$G^+(x|x_0) = \int \frac{2\mathrm{e}^{ikr\cos\theta}}{{k_E}^2 - k^2 + i0}\frac{d\Omega k^{d-1}dk}{(2\pi)^d} \tag{909}$$

where $k_E = \sqrt{2\mathsf{m}E}$ is the wavenumber for a particle with energy E. The integral is a d-dimensional spherical integral. The solutions of $|\mathbf{k}| = k$ in 1D give two k's, while in 2D and 3D the k's lie on a circle and on a sphere respectively. We recall that Ω_d is $2, 2\pi, 4\pi$ in 1D, 2D and 3D respectively, and define averaging over all directions for a function $f(\theta)$ as follows:

$$\langle f(\theta)\rangle_d = \frac{1}{\Omega_d}\int f(\theta)d\Omega \tag{910}$$

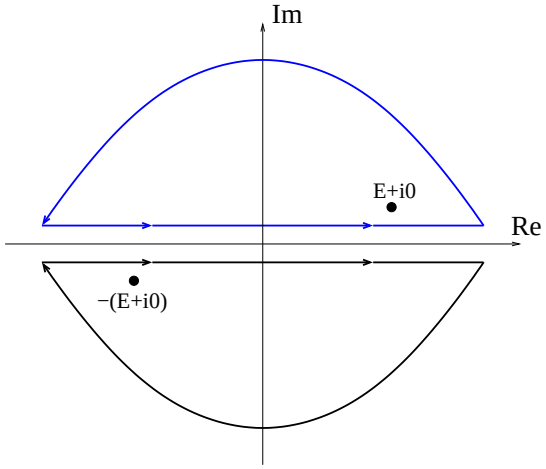
With this definition we get

$$\langle \mathrm{e}^{ikr\cos\theta}\rangle_d = \begin{cases} \cos(kr), & \mathrm{d}=1; \\ \mathrm{J}_0(kr), & \mathrm{d}=2; \\ \mathrm{sinc}(kr), & \mathrm{d}=3. \end{cases} \tag{911}$$

where $\mathrm{J}_0(x)$ is the zero order *Bessel function of the first kind*. Substituting these results and using the notation $z = kr$ we get in the 3D case:

$$\begin{aligned} G^+(\mathbf{r}) &= \frac{1}{\pi^2 r}\frac{1}{2}\int_{-\infty}^{\infty}\frac{z\sin z}{{z_E}^2 - z^2 + i0}dz = \frac{1}{\pi^2 r}\frac{1}{4i}\int_{-\infty}^{\infty}\frac{z(\mathrm{e}^{iz} - \mathrm{e}^{-iz})}{{z_E}^2 - z^2 + i0}dz \\ &= \frac{1}{\pi^2 r}\frac{1}{4i}\left[-\int\frac{z\mathrm{e}^{iz}}{(z-(z_E+i0))(z+(z_E+i0))}dz + \int\frac{z\mathrm{e}^{-iz}}{(z-(z_E+i0))(z+(z_E+i0))}dz\right] \\ &= \frac{1}{2\pi r}\sum_{\text{poles}}\mathrm{Res}[f(z)] = \frac{1}{2\pi r}\left[-\frac{1}{2}\mathrm{e}^{iz_E} - \frac{1}{2}\mathrm{e}^{-i(-z_E)}\right] = -\frac{\mathsf{m}}{2\pi}\frac{\mathrm{e}^{ik_E r}}{r} \end{aligned} \tag{912}$$

The integral just solved is a complex integral where the poles are at $\pm(z_E + i0)$ and the path chosen is the upper half of the plane for the part containing e^{-iz} and the lower half for the part with e^{iz}. See figure. We see that the solution is a modification or modulation of the regular Coulomb law.



The other method to find the Green function is by solving the Schrodinger equation with a source and appropriate boundary conditions. In case of a free particle we get the Helmholtz equation which is a generalization of the Poisson equation of electrostatic problems:

$$(\nabla^2 + {k_E}^2)G(\mathbf{r}|\mathbf{r}_0) = -q\delta(\mathbf{r} - \mathbf{r}_0) \tag{913}$$

where the "charge" in our case is $q = -2\mathsf{m}/\hbar^2$. For $k_E = 0$ this is the Poisson equation and the solution is the Coulomb law. For $k_E \neq 0$ the solution is a modulated Coulomb law. We shall explore below the results in case of a particle in 3D, and then also for 1D and 2D.

The 3D case:

In the 3D case the "Coulomb law" is:

$$G(\mathbf{r}|\mathbf{r}_0) = \frac{q}{4\pi|\mathbf{r} - \mathbf{r}_0|}\cos(k_E|\mathbf{r} - \mathbf{r}_0|) \tag{914}$$

This solution still has a gauge freedom, just as in electrostatics where we have a "free constant". We can add to this solution any "constant", which in our case means an arbitrary (so called "free wave") solution of the homogeneous equation. Note that any "free wave" can be constructed from a superpostion of planar waves. In particular the "spherical" free wave is obtained by averaging $e^{i\mathbf{k}\cdot\mathbf{r}}$ over all directions. If we want to satisfy the "outgoing wave" boundary conditions we get:

$$G(r) = \frac{q}{4\pi r}\cos(k_E r) + i\frac{q}{4\pi r}\sin(k_E r) = \frac{q}{4\pi r}e^{ik_E r} = -\frac{\mathsf{m}}{2\pi r}e^{ik_E r} \tag{915}$$

The solutions for 1D and 2D can be derived in the same way.

The 1D case:

In one dimension the equation is

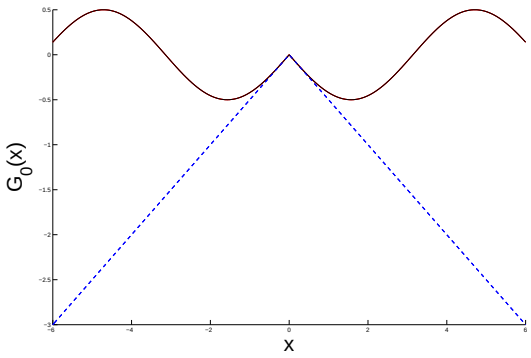
$$\left(\frac{\partial^2}{\partial x^2} + k_E^2\right) G(x) = -q\delta(x) \tag{916}$$

where for simplicity we set $x_0 = 0$. Because of the delta function, our boundary conditions require that: $G'(+0) - G'(-0) = -q$, in other words in order for the second derivative to be a delta function the first derivative must have a step function. Thus, when $k_E = 0$ we get the 1D Coulomb law $G(x) = -(q/2)|x|$, but for $k_E \neq 0$ we have the modulated Coulomb law

$$G(x) = -\frac{q}{2k_E}\sin(k_E|x|) \tag{917}$$

(see figure). To this we can add any 1D free wave. In order to satisfy the "outgoing waves" boundary conditions we add $\cos(kx) = \cos(k|x|)$ to this expression, hence we get the retarded Green's function in 1D

$$G(x) = i\frac{q}{2k_E}e^{ik_E|x|} = -i\frac{\mathsf{m}}{k_E}e^{ik_E|x|} \tag{918}$$



The modulated Coulomb law in 1D (solid black line) and the regular Coulomb law when $k = 0$ (dashed blue line).

The 2D case:

In two dimensions for $k_E = 0$ we use Gauss' law to calculate the electrostatic field that goes like $1/r$, and hence the electrostatic potential is $G(r) = -(1/(2\pi))\ln r$. for $k_E \neq 0$ we get the modulated result

$$G(r) = -\frac{q}{4}\mathrm{Y}_0(k_E r) \tag{919}$$

where $\mathrm{Y}_0(x)$ is the Bessel function of the second kind

$$\begin{aligned} \mathrm{Y}_0{}'(x) &= -\mathrm{Y}_1(x) \\ \mathrm{Y}_0(x) &\sim \sqrt{\frac{2}{\pi x}}\sin(x-\frac{\pi}{4}) \quad , \text{ for large } x \end{aligned} \tag{920}$$

The second independent solution of the associated homogeneous equation is the Bessel function of the first kind $\mathrm{J}_0(x)$. Adding this "free wave" solution leads to a solution that satisfies the "outgoing wave" boundary conditions. Hence we get the retarded Green's function in 2D

$$G(r) = i\frac{q}{4}\mathrm{H}_0(k_E r) = -i\frac{\mathsf{m}}{2}\mathrm{H}_0(k_E r) \tag{921}$$

where $\mathrm{H}_0(x) = \mathrm{J}_0(x) + i\mathrm{Y}_0(x)$ is the Hankel function.

[35.5] Green's Theorem

The Schrödinger equation $\mathcal{H}\psi = E\psi_0$ can be written as $\mathcal{H}_E\psi = 0$ where $\mathcal{H}_E = -\nabla^2 + U_E(r)$ with $U_E(r) = U(r) - E$. Green's function solves the equation $\mathcal{H}_E G(r|r_0) = -q\delta(r-r_0)$ with $q = -2\mathsf{m}/\hbar^2$. In this section we follow the convention of electrostatics and set $q = 1$. Thus we have

$$\begin{aligned} &\mathcal{H}_E G(r|r_0) = \delta(r-r_0) \\ &\mathcal{H}_E\psi(r) = 0 \end{aligned} \tag{922}$$

Assume that $r = r(s)$ is the boundary of some domain, and define

$$\begin{aligned} &\psi(s) = \psi(r(s)) \\ &\partial\psi(s) = \vec{n}\cdot\nabla\psi(r(s)) \end{aligned} \tag{923}$$

where $\vec{n}$ is a normal unit vector that points outwards. Green's theorem allows us to express the wavefunction $\psi(r)$ at an arbitrary point inside the domain using a boundary integral over $\psi(s)$ and its normal derivative $\partial\psi(s)$.

The key idea of the Green theorem derivation is that $U_E(r)\psi(r) = \nabla^2\psi(r)$. This allows us to "get rid" of the potential and to end up with a boundary integral:

$$\begin{aligned} \psi(r_0) &= \int \psi(r)\delta(r-r_0)dr = \int \psi(r)\mathcal{H}_E G(r|r_0)dr \\ &= -\int \psi(r)\nabla^2 G(r|r_0)dr + \int \psi(r)U_E(r)G(r|r_0)dr \\ &= -\int \psi(r)\nabla^2 G(r|r_0)dr + \int (U_E(r)\psi(r))G(r|r_0)dr \\ &= -\int \psi(r)\nabla^2 G(r|r_0)dr + \int (\nabla^2\psi(r))G(r|r_0)dr \\ &= \int \nabla(-\psi(r)\nabla G(r|r_0) + G(r|r_0)\nabla\psi(r))dr = \oint [G(s|r_0)]\partial\psi(s) - [\partial G(s|r_0)]\psi(s))ds \end{aligned} \tag{924}$$

We see that by using integration by parts and Gauss's theorem we arrive at a boundary integral.

For the case where the wave function vanishes on the boundary $\psi(s) = 0$ the expression becomes very simple

$$\psi(r) = \oint G(s'|r)\varphi(s')ds' \tag{925}$$

where $\varphi(s) = \partial\psi(s)$, and in particular as we approach the boundary we should get:

$$\int G(s'|s)\varphi(s')ds' = 0 \tag{926}$$

An obvious application of this formula is as a powerful numerical method to find eigenfunctions. This is the so called *boundary integral method*. Let us consider the problem of a particle in a billiard potential. Our Green's function is (up to a constant)

$$G(s'|s) = \mathrm{Y}_0(k_E|r(s') - r(s)|) \tag{927}$$

If we divide the boundary line into N segments then for any point on the boundary the equality $\int G(s'|s)\varphi(s')ds' = 0$ should hold, so:

$$\sum_j A_{ij}\varphi_j = 0 \qquad \text{with} \quad A_{ij} = \mathrm{Y}_0(k_E|r(s_j) - r(s_i)|) \tag{928}$$

Every time the determinant $\det(A)$ vanishes we get a non trivial solution to the equation, and hence we can construct an eigenfunction. So all we have to do is plot the determinant $\det(A)$ as a function of k_E. The points where $\det(A)$ equals zero are the values of k_E for which the energy E is an eigenvalue of the Hamiltonian $\mathcal{H}$.

[36] Perturbation Theory

[36.1] Perturbation theory for the resolvent

If A and B are operators then

$$\begin{aligned}\frac{1}{(1-B)} &= (1-B)^{-1} = \sum_{n=0}^{\infty} B^n \\ \frac{1}{A-B} &= (A(1-A^{-1}B))^{-1} = (1-A^{-1}B)^{-1}A^{-1} = \sum_n (A^{-1}B)^n A^{-1} = \frac{1}{A} + \frac{1}{A}B\frac{1}{A} + \frac{1}{A}B\frac{1}{A}B\frac{1}{A} + \dots\end{aligned} \tag{929}$$

Consider

$$G(z) = \frac{1}{z-\mathcal{H}} = \frac{1}{z-(\mathcal{H}_0+V)} = \frac{1}{(z-\mathcal{H}_0)-V} \tag{930}$$

From the above it follows that

$$G(z) = G_0(z) + G_0(z)VG_0(z) + G_0(z)VG_0(z)VG_0(z) + \dots \tag{931}$$

Or, in matrix representation

$$G(x|x_0) = G_0(x|x_0) + \int G(x|x_2)dx_2\langle x_2|V|x_1\rangle dx_1 G(x_1|x_0) + \dots \tag{932}$$

Note that for the scalar potential $\hat{V} = u(\hat{x})$ we get

$$G(x|x_0) = G_0(x|x_0) + \int dx' G(x|x')u(x')G(x'|x_0) + \dots \tag{933}$$

[36.2] Perturbation Theory for the Propagator

For the Green function we get

$$G^+(\omega) = G_0^+(\omega) + G_0^+(\omega)VG_0^+(\omega) + G_0^+(\omega)VG_0^+(\omega)VG_0^+(\omega) + \dots \tag{934}$$

Recall that

$$G^+(\omega) \to FT \to -i\Theta(\tau)U(\tau) \tag{935}$$

Then from the convolution theorem it follows that

$$(-i)[\Theta(t)U(t)] = (-i)[\Theta U_0(t)] + (-i)^2 \int dt'[\Theta(t-t')U(t-t')]\,[V]\,[\Theta(t')U(t')] + \dots \tag{936}$$

which leads to

$$U(t) = U_0(t) + \sum_{n=1}^{\infty}(-i)^n \int_{0<t_1<t_2<\dots<t_n<t} dt_n \dots dt_2 dt_1\, U_0(t-t_n)V \dots U_0(t_2-t_1)VU_0(t_1) \tag{937}$$

for $t > 0$ and zero otherwise. This can be illustrated diagrammatically using Feynman diagrams.

Let us see how we use this expression in order to get the transition probability formula. The first order expression for the evolution operator is

$$U(t) = U_0 - i \int dt^{'} U_0(t - t^{'}) V U_0(t^{'}) \tag{938}$$

Assume that the system is prepared in an eigenstate m of the unperturbed Hamiltonian, we get the the amplitude to find it after time t in another eigenstate n is

$$\langle n|U(t)|m\rangle = \mathrm{e}^{-iE_n}\delta_{nm} - i \int dt^{'} \mathrm{e}^{-iE_n(t-t^{'})} \langle m|V|n\rangle \mathrm{e}^{-iE_n t^{'}} \tag{939}$$

If $n \neq m$ it follows that:

$$P_t(n|m) = |\langle n|U(t)|m\rangle|^2 = \left| \int_0^t dt' V_{nm} \mathrm{e}^{i(E_n - E_m)t'} \right|^2 \tag{940}$$

======= [36.3] Perturbation theory for the evolution

In this section we review the elementary approach to solve the evolution problem via an iterative scheme with the Schrodinger equation. Then we make the bridge to a more powerful procedure. Consider

$$|\Psi\rangle = \sum_n \Psi_n(t)|n\rangle \tag{941}$$

It follows that:

$$i\frac{\partial \Psi_n}{\partial t} = E_n \Psi_n + \sum_{n'} V_{nn'} \Psi_{n'} \tag{942}$$

We want to solve in the method which is called "variation of parameters", so we set:

$$\Psi_n(t) = C_n(t)\mathrm{e}^{-iE_n t} \tag{943}$$

Hence:

$$\frac{dC_n}{dt} \;=\; -i \sum_{n'} \mathrm{e}^{i(E_n - E_{n'})t} V_{nn'} C_{n'}(t) \tag{944}$$

From the zero order solution $C_n(t) = \delta_{nm}$ we get after one iteration:

$$C_n(t) = \delta_{nm} - i \int_0^t dt' \mathrm{e}^{i(E_n - E_m)t'} V_{nm} \tag{945}$$

In order to make the connection with the formal approach of the previous and of the next section we write

$$C_n = \mathrm{e}^{iE_n t}\Psi_n = \left\langle n|U_0^{-1}U(t)|m\right\rangle \equiv \langle n|U_I(t)|m\rangle \tag{946}$$

and note that

$$e^{i(E_n-E_m)t}V_{nm} \;=\; \big\langle n|U_0(t)^{-1}VU_0(t)|m\big\rangle \;\equiv\; \langle n|V_I(t)|m\rangle \tag{947}$$

Hence the above first order result can be written as

$$\langle n|U_I(t)|m\rangle = \delta_{nm} - i\int_0^t \langle n|V_I(t')|m\rangle\, dt' \tag{948}$$

In the next sections we generalize this result to all orders.

[36.4] The Interaction Picture

First we would like to recall the definition of time ordered exponentiation

$$U(t,t_0) = (1-idt_N\mathcal{H}(t_N))\dots(1-idt_2\mathcal{H}(t_2))(1-idt_1\mathcal{H}(t_1)) \equiv \mathcal{T}\,e^{-i\int_{t_0}^t \mathcal{H}(t')dt'} \tag{949}$$

Previously we have assumed that the Hamiltonian is not time dependent. But in general this is not the case, so we have to keep the time order. The parenthesis in the above definition can be "opened" and then we can assemble the terms of order of dt. Then we get the expansion

$$\begin{aligned} U(t,t_0) \;&=\; 1 - i(dt_N\mathcal{H}(t_N))\cdots - i(dt_1\mathcal{H}(t_1)) + (-i)^2(dt_N\mathcal{H}(t_N))(dt_{N-1}\mathcal{H}(t_{N-1})) + \dots \\ &=\; 1 - i\int_{0<t'<t}\mathcal{H}(t')dt' + (-i)^2\int_{t_0<t'<t''<t}\mathcal{H}(t'')\mathcal{H}(t')dt''dt' + \dots \\ &=\; \sum_{n=0}^{\infty}(-i)^n\int_{t_0<t_1<t_2\cdots<t_n<t} dt_n\dots dt_1\mathcal{H}(t_n)\dots\mathcal{H}(t_1) \end{aligned} \tag{950}$$

Note that if $\mathcal{H}(t') = \mathcal{H}$ is not time dependent then we simply get the usual Taylor expansion of the exponential function where the $1/n!$ prefactors would come from the time ordering limitation.

The above expansion is not very useful because the sum is likely to be divergent. What we would like to consider is the case $\mathcal{H} = \mathcal{H}_0 + V$, where V is a small perturbation. The perturbation V can be either time dependent or time independent. For simplicity we adopt from now on the convention $t_0 = 0$, and use the notation $U(t)$ instead of $U(t,t_0)$. By definition of $\mathcal{H}$ as the generator of the evolution we have:

$$\frac{d}{dt}U(t) = -i(\mathcal{H}_0 + V)U(t) \tag{951}$$

We define

$$\begin{aligned} U_I(t) \;&=\; U_0(t)^{-1}U(t) \\ V_I(t) \;&=\; U_0(t)^{-1}\;V\;U_0(t) \end{aligned} \tag{952}$$

With these notations the evolution equation takes the form

$$\frac{d}{dt}U_I(t) = -iV_I(t)U_I(t) \tag{953}$$

The solution is by time ordered exponentiation

$$U_I(t) = \mathcal{T}\exp\left(i\int_0^t V_I(t')dt'\right) = \sum_{n=0}^{\infty}(-i)^n\int_{0<t_1<t_2\cdots<t_n} dt_n\dots dt_1V_I(t_n)\dots V_I(t_1) \tag{954}$$

Which can be written as

$$U(t) = \sum_{n=0}^{\infty} (-i)^n \int_{0<t_1<t_2<\cdots<t_n<t} dt_n \ldots dt_2 dt_1 \, U_0(t-t_n) V \ldots U_0(t_2-t_1) V U_0(t_1) \tag{955}$$

The latter expression is more general than the one which we had obtained via FT of the resolvent expansion, because here V is allowed to be time dependent.

[37] Complex poles from perturbation theory

[37.1] Models of interest

In this section we solve the particle decay problem using perturbation theory for the resolvent. We are going to show that for this Hamiltonian the analytical continuation of the resolvent has a pole in the lower part of the complex z-plane. The imaginary part ("decay rate") of the pole that we find is the same as we found by either the Fermi golden rule or by the exact solution of the Schrödinger equation.

We imagine that we have an "unperturbed problem" with one energy level $|0\rangle$ of energy E_0 and a continuum of levels $|k\rangle$ with energies E_k. A model of this kind may be used for describing tunneling from a metastable state. Another application is the decay of an excited atomic state due to emission of photons. In the latter case the initial state would be the excited atomic state without photons, while the continuum are states such that the atom is in its ground state and there is a photon. Schematically we have

$$\mathcal{H} = \mathcal{H}_0 + V \tag{956}$$

where we assume

$$\begin{aligned} &\langle k|V|0\rangle = \sigma_k \qquad \text{(coupling to the continuum)} \\ &\langle k'|V|k\rangle = 0 \qquad \text{(no transitions within the continuum)} \end{aligned} \tag{957}$$

Due to gauge freedom we can assume that the coupling coefficients are real numbers without loss of generality. The Hamiltonian matrix can be illustrated as follows:

$$\mathcal{H} = \begin{pmatrix} E_0 & \sigma_1 & \sigma_2 & \sigma_3 & . & . & . & \sigma_k & . \\ \sigma_1 & E_1 & 0 & 0 & . & . & . & 0 & . \\ \sigma_2 & 0 & E_2 & 0 & . & . & . & 0 & . \\ \sigma_3 & 0 & 0 & E_3 & . & . & . & 0 & . \\ . & . & . & . & . & . & . & 0 & . \\ . & . & . & . & . & . & . & 0 & . \\ . & . & . & . & . & . & . & 0 & . \\ \sigma_k & 0 & 0 & 0 & 0 & 0 & 0 & E_k & . \\ . & . & . & . & . & . & . & . & . \end{pmatrix} \tag{958}$$

We later assume that the system under study is prepared in state $|0\rangle$ at an initial time ($t = 0$), and we want to obtain the probability amplitude to stay in the initial state at a later times.

It is important to notice the following (a) we take one state and neglect other states in the well. (b) we assume that V allows transitions from this particular state in the well (zero state $|0\rangle$) into the $|k\rangle$ states in the continuum, while we do not have transitions in the continuum itself. These assumptions allow us to make exact calculation using perturbation theory to infinite order. The advantage of the perturbation theory formalism is that it allows the treatment of more complicated problems for which exact solutions cannot be found.

[37.2] The $P + Q$ formalism

The Hamiltonian of the previous section is of the form

$$\mathcal{H} = \mathcal{H}_0 + V = \begin{pmatrix} \mathcal{H}_0^P & 0 \\ 0 & \mathcal{H}_0^Q \end{pmatrix} + \begin{pmatrix} 0 & V^{PQ} \\ V^{QP} & 0 \end{pmatrix} \tag{959}$$

where $\mathcal{H}_0^p$ is a 1×1 matrix, and $\mathcal{H}_0^Q$ is an $\infty \times \infty$ matrix. The perturbation allows transitions between P and Q

states. In the literature it is customary to define projectors $\mathcal{P}$ and $\mathcal{Q}$ on the respective sub-spaces.

$$P + Q \;=\; \hat{1} \tag{960}$$

We want to calculate the resolvent. But we are interested only in the single matrix element $(0,0)$ because we want to know the probability to stay in the $|0\rangle$ state:

$$\text{survival probability} \;=\; \Big|\text{FT}\Big[\; \langle 0|G(\omega)|0\rangle \;\Big]\Big|^2 \tag{961}$$

Here $G(\omega)$ is the retarded Green function. More generally we may have several states in the well. In such a case instead of $P = |0\rangle\langle 0|$ we have

$$P = \sum_{n\in \text{well}} |n\rangle\langle n| \tag{962}$$

If we prepare the particle in an arbitrary state Ψ inside the well, then the probability to survive in the same state is

$$\text{survival probability} \;=\; \Big|\text{FT}\Big[\; \langle \Psi|G(\omega)|\Psi\rangle \;\Big]\Big|^2 \;=\; \Big|\text{FT}\Big[\; \langle \Psi|G^P(\omega)|\Psi\rangle \;\Big]\Big|^2 \tag{963}$$

Namely, we are interested only in one block of the resolvent which we call

$$G^P(z) = \mathcal{P}G(z)\mathcal{P} \tag{964}$$

Using the usual expansion we can write

$$\begin{aligned} G^P \;&=\; PGP = P\frac{1}{z-(\mathcal{H}_0+V)}P = P(G_0 + G_0VG_0 + \dots)P \\ &=\; PG_0P + PG_0(P+Q)V(P+Q)G_0P + PG_0(P+Q)V(P+Q)G_0(P+Q)V(P+Q)G_0P + \dots \\ &=\; G_0^P + G_0^P\Sigma^P G_0^P + G_0^P\Sigma^P G_0^P\Sigma^P G_0^P + \dots \\ &=\; \frac{1}{z-(\mathcal{H}_0^P + \Sigma^P)} \end{aligned} \tag{965}$$

where the "self energy" term

$$\Sigma^P = V^{PQ}G_0^Q V^{QP} \tag{966}$$

represents the possibility of making a round trip out of the well. Note that only even order terms contribute to this perturbative expansion because we made the simplifying assumption that the perturbation does not have "diagonal blocks". In our problem Σ^P is a 1×1 matrix that we can calculate as follows:

$$\begin{aligned} \Sigma^P \;&=\; \sum_k \langle 0|V|k\rangle\langle k|G_0|k\rangle\langle k|V|0\rangle = \sum_k \frac{|V_k|^2}{E - E_k + i0} \\ &=\; \sum_k \frac{|V_k|^2}{E-E_k} - i\pi\sum_k |V_k|^2\delta(E-E_k) \;\equiv\; \delta E_0 - i(\Gamma_0/2) \end{aligned} \tag{967}$$

where

$$\Gamma_0 = 2\pi\sum_k |V_k|^2\delta(E-E_k) \;\equiv\; 2\pi|V|^2 g(E) \tag{968}$$

which is in agreement with the Fermi golden rule. Thus, the resolvent is the 1×1 matrix.

$$G^P(z) = \frac{1}{z - (\mathcal{H}_0^P + \Sigma^P)} = \frac{1}{z - (\varepsilon_0 + \delta E_0) + i(\Gamma_0/2)} \tag{969}$$

We see that due to the truncation of the Q states we get a complex Hamiltonian, and hence the resolvent has a pole in the lower plane. The Fourier transform of this expression is the survival amplitude. After squaring it gives a simple exponential decay $\mathrm{e}^{-\Gamma t}$.

Scattering Theory

[38] The plane wave basis

There are several different conventions for the normalization of plane waves:
- Box normalized plane waves $|n\rangle$
- Density normalized plane waves $k\rangle$
- Energy shell normalized plane waves $E, \Omega\rangle$

We are going to be very strict in our notations, else errors are likely. We clarify the three conventions in the following first in the 1D case, and later in the 3D case.

[38.1] Plane waves in 1D

The most intuitive basis set originates from quantization in a box with periodic boundary conditions (a torus):

$$|n\rangle \longrightarrow \frac{1}{\sqrt{L}} \mathrm{e}^{ik_n x} \tag{970}$$

where

$$k_n = \frac{2\pi}{L} n \tag{971}$$

Orthonormality:

$$\langle n|m\rangle = \delta_{nm} \tag{972}$$

Completeness:

$$\sum_n |n\rangle\langle n| = \hat{1} \tag{973}$$

The second convention is to have the density normalized to unity:

$$|k\rangle \longrightarrow \mathrm{e}^{ikx} \tag{974}$$

Orthonormality:

$$\langle k|k'\rangle = 2\pi\delta(k-k') \tag{975}$$

Completeness:

$$\int |k\rangle \frac{dk}{2\pi} \langle k| = \hat{1} \tag{976}$$

Yet there is a third convention which assumes that the states are labeled by their energy, and by another index that indicate the direction.

$$|E,\Omega\rangle = \frac{1}{\sqrt{v_E}} |k_\Omega\rangle \longrightarrow \frac{1}{\sqrt{v_E}} \mathrm{e}^{ik_\Omega x} \tag{977}$$

where $0 < E < \infty$ and $\Omega = \pm 1$ and

$$k_\Omega = \Omega k_E = \pm\sqrt{2mE} \tag{978}$$

Orthonormality:

$$\langle E, \Omega | E', \Omega' \rangle = 2\pi\delta(E - E')\delta_{\Omega\Omega'} \tag{979}$$

Completeness:

$$\int \frac{dE}{2\pi} \sum_\Omega |E, \Omega\rangle\langle E, \Omega| \;=\; \hat{1} \tag{980}$$

In order to prove the orthonormality we note that $dE = v_E dk$ and therefore

$$\delta(E - E') = \frac{1}{v_E}\delta(k - k') \tag{981}$$

The energy shell normalization of plane waves in 1D is very convenient also for another reason. We see that the probability flux of the plane waves is normalized to unity. We note that this does not hold in more than 1D. Still also in more than 1D in the S matrix formalism reduces the scattering problem to 1D channels, and therefore this property is very important in general.

═══ [38.2] Plane waves in 3D

The generalization of the box normalization convention to the 3D case is immediate. The same applied to the density normalized plane waves:

$$|\vec{k}\rangle \longrightarrow \mathrm{e}^{i\vec{k}\vec{x}} \tag{982}$$

Orthonormality:

$$\langle \vec{k} | \vec{k}' \rangle = (2\pi)^3 \delta^3(\vec{k} - \vec{k}') \tag{983}$$

Completeness:

$$\int |\vec{k}\rangle \frac{d^3k}{(2\pi)^3} \langle \vec{k}| = \hat{1} \tag{984}$$

The generalization of the energy shell normalization convention is less trivial:

$$|E, \Omega\rangle = \frac{1}{2\pi}\frac{k_E}{\sqrt{v_E}}|\vec{k}_\Omega\rangle \longrightarrow \frac{1}{2\pi}\frac{k_E}{\sqrt{v_E}}\mathrm{e}^{i\vec{k}_\Omega\cdot\vec{x}} \tag{985}$$

where we define the direction by $\Omega = (\theta, \varphi)$, with an associated unit vector $\vec{n}_\Omega$ and a wavenumber

$$\vec{k}_\Omega = k_E \vec{n}_\Omega \tag{986}$$

Orthonormality:

$$\langle E, \Omega | E', \Omega' \rangle = 2\pi\delta(E - E')\delta(\Omega - \Omega') \tag{987}$$

Completeness:

$$\int \frac{dE}{2\pi} \int |E,\Omega\rangle d\Omega \langle E,\Omega| = \hat{1} \tag{988}$$

To prove the identities above we note that

$$d^3k = k^2 dk d\Omega \;=\; k_E^2 \frac{dE}{v_E} d\Omega \;=\; k_E^2 \frac{dE}{v_E} d\varphi d\cos\theta \tag{989}$$

and

$$\delta^3(\vec{k}-\vec{k}') \;=\; \frac{v_E}{k_E^2}\delta(E-E')\delta(\Omega-\Omega') \;=\; \frac{v_E}{k_E^2}\delta(E-E')\delta(\varphi-\varphi')\delta(\cos\theta-\cos\theta') \tag{990}$$

In general we have to remember that any change of the "measure" is associated with a compensating change in the normalization of the delta functions.

[39] Scattering in the T Matrix Formalism

[39.1] The Scattering States

Our purpose is to solve the Schrödinger's equation for a given energy E.

$$(\mathcal{H}_0 + V)\Psi = E\Psi \tag{991}$$

If we rearrange the terms, we get:

$$(E - \mathcal{H}_0 - V)\Psi = 0 \tag{992}$$

In fact we want to find scattering solutions. These are determined uniquely if we define what is the "incident wave" and require outgoing boundary conditions for the scattered component. Thus we write Ψ as a superposition of a free wave and a scattered wave,

$$\Psi = \phi + \Psi^{scatt} \tag{993}$$

The scattered wave Ψ^{scatt} is required to satisfy outgoing boundary conditions. The free wave ϕ is any solution of:

$$\mathcal{H}_0\phi = E\phi \tag{994}$$

Substituting, we obtain:

$$(E - \mathcal{H}_0 - V)\Psi^{scatt} = V\phi \tag{995}$$

with the solution

$$\Psi^{scatt} = G^+V\phi \tag{996}$$

leading to:

$$\Psi = (1 + G^+V)\phi \tag{997}$$

[39.2] The Lippman Schwinger equation

The explicit solution for Ψ that was found in the previous section is in typically useless, because it is difficult to get G. A more powerful approach is to write an integral equation for Ψ. For this purpose we re-arrange the differential equation as

$$(E - \mathcal{H}_0)\Psi = V\Psi \tag{998}$$

Using exactly the same procedure as in the previous section we get

$$\Psi = \phi + G_0^+V\Psi \tag{999}$$

This Lippman Schwinger equation can be solved for Ψ using standard techniques. One option is of course to solve it iteratively. This leads to a perturbative expansion for Ψ which we are going to derive in the next section using a simpler approach.

[39.3] Perturbation Theory for the Scattering State

Going back to the formal solution for Ψ we can substitute there the perturbative expansion of G

$$G = G_0 + G_0VG_0 + G_0VG_0VG_0 + \dots \tag{1000}$$

leading to

$$\Psi = (1 + G^+V)\phi = \phi + G_0V\phi + G_0VG_0V\phi + \dots \tag{1001}$$

As an example consider the typical case of scattering by a potential $V(x)$. In this case the above expansion to leading order in space representation is:

$$\Psi(x) = \phi(x) + \int G_0(x,x')V(x')\phi(x')\,dx' \tag{1002}$$

[39.4] The T matrix

It is customary to define the T matrix as follows

$$T = V + VG_0V + \dots \tag{1003}$$

The T matrix can be regarded as a "corrected" version of the potential V, so as to make the following first order look-alike expression exact:

$$G = G_0 + G_0TG_0 \tag{1004}$$

Or the equivalent expression for the wavefunction:

$$\Psi = \phi + G_0^+T\phi \tag{1005}$$

Later it is convenient to take matrix elements in the unperturbed basis of free waves:

$$\begin{aligned} V_{\alpha\beta} &= \left\langle \phi^\alpha \left| V \right| \phi^\beta \right\rangle \\ T_{\alpha\beta}(E) &= \left\langle \phi^\alpha \left| T(E) \right| \phi^\beta \right\rangle \end{aligned} \tag{1006}$$

In principle we can take the matrix elements between any states. But in practice our interest is in states that have the same energy, namely $E_\alpha = E_\beta = E$. Therefore it is convenient to use two indexes (E,a), where the index a distinguishes different free waves that have the same energy. In particular a may stand for the "direction" (Ω) of the plane wave. Thus in practice we are interested only in matrix elements "on the energy shell":

$$T_{ab}(E) = \left\langle \phi^{E,a} \left| T(E) \right| \phi^{E,b} \right\rangle \tag{1007}$$

One should be very careful with the re-scaling of the matrix elements which is implied if by the change of measure that is associated with different type of indexes. In particular note that in 3D we have:

$$T_{\Omega,\Omega_0} = \frac{1}{v_E}\left(\frac{k_E}{2\pi}\right)^2 T_{k_\Omega,k_{\Omega_0}} \tag{1008}$$

[39.5] Scattering state for an incident plane wave

In this section we look for a scattering solution that originates from the free wave $|k_0\rangle$. Using the result of a previous section we write $\Psi = \phi^{k_0} + G_0^+ T \phi^{k_0}$ with

$$\phi^{k_0}(r) = \mathrm{e}^{i\vec{k_0}\cdot\vec{r}} \qquad \text{[density normalized]} \tag{1009}$$

In Dirac notations:

$$|\Psi\rangle = |\phi^{k_0}\rangle + G_0^+ T |\phi^{k_0}\rangle \tag{1010}$$

In space representation:

$$\langle r|\Psi\rangle = \langle r|\phi^{k_0}\rangle + \langle r|G_0^+ T|\phi^{k_0}\rangle \tag{1011}$$

or in "old style" notation:

$$\Psi(r) = \phi^{k_0}(r) + \langle r|G_0^+ T|\phi_0^k\rangle = \phi^{k_0}(r) + \int G_0^+(r|r_0) dr_0 \langle r_0|T|k_0\rangle \tag{1012}$$

where

$$G_0^+(r|r_0) = \langle r|G_0^+|r_0\rangle = -\frac{\mathsf{m}}{2\pi}\cdot\frac{\mathrm{e}^{ik_E|r-r_0|}}{|r-r_0|} \tag{1013}$$

Thus we get

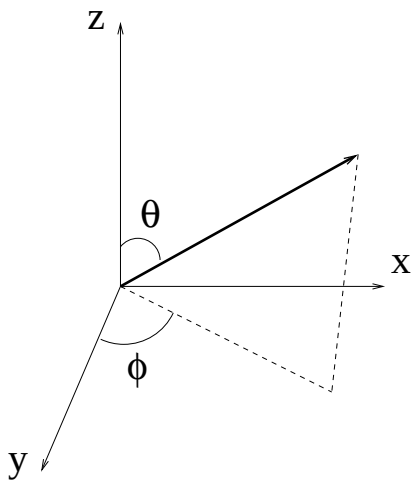
$$\Psi(r) = \phi^{k_0}(r) - \frac{\mathsf{m}}{2\pi}\int \frac{\mathrm{e}^{ik_E|r-r_0|}}{|r-r_0|}\langle r_0|T|k_0\rangle\, dr_0 \tag{1014}$$

So far everything is exact. Now we want to get a simpler expression for the asymptotic form of the wavefunction. Note that from the experimental point of view only the "far field" region (far away from the target) is of interest. The major observation is that the dr_0 integration is effectively bounded to the scattering region $|r| < r_0$ where the matrix elements of V and hence of T are non-zero. Therefore for $|r| \gg |r_0|$ we can use the approximation

$$|\vec{r}-\vec{r}_0| = \sqrt{(\vec{r}-\vec{r}_0)^2} = \sqrt{|r|^2 - 2\vec{r}\cdot\vec{r}_0 + \mathcal{O}(|r_0|^2)} \approx |r|\left[1 - \vec{n}_\Omega\cdot\frac{\vec{r_0}}{|r|}\right] = |r| - \vec{n}_\Omega\cdot\vec{r}_0 \tag{1015}$$

Here and below we use the following notations:

$$\begin{aligned} \vec{r} &\equiv |r|\vec{n}_\Omega \\ \Omega &= (\theta,\varphi) = \text{spherical coordinates} \\ \vec{n}_\Omega &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \\ \vec{k}_\Omega &= k_E\vec{n}_\Omega \end{aligned} \tag{1016}$$



With the approximation above we get:

$$\Psi(r) \approx \mathrm{e}^{i\vec{k}_0\cdot\vec{r}} - \frac{\mathsf{m}}{2\pi}\frac{\mathrm{e}^{ik_E|r|}}{r}\int \mathrm{e}^{-i\vec{k}_\Omega\cdot\vec{r}_0}\langle r_0|T|k_0\rangle\, dr_0 \tag{1017}$$

which can be written as

$$\Psi(r) \approx \mathrm{e}^{i\vec{k}_0\cdot\vec{r}} + f(\Omega)\frac{\mathrm{e}^{ik_E|r|}}{|r|} \tag{1018}$$

where

$$f(\Omega) = -\frac{\mathsf{m}}{2\pi}\langle\vec{k}_\Omega|T(E)|\vec{k}_0\rangle \tag{1019}$$

It follows that the differential cross section is

$$\frac{d\sigma}{d\Omega} \;=\; |f(\Omega)|^2 \;=\; \Big(\frac{\mathsf{m}}{2\pi\hbar}\Big)^2\,\Big|\frac{1}{\hbar}T_{k_\Omega,k_0}\Big|^2 \tag{1020}$$

This formula assumes density normalized plane waves. It relates the scattering which is described by $f(\Omega)$ to the T matrix. It is in fact a special case of a more general relation between the S matrix and the T matrix. The S matrix, which we define later, is a unitary matrix. The unitarity condition can be "translated" either to the T matrix language, or to the $f(\Omega)$ language. The result, which is know as the "optical theorem", relates the total cross section to the forward scattering amplitude $f(0)$.

═══ [39.6] Born approximation and beyond

For potential scattering the first order approximation $T \approx V$ leads to the Born approximation:

$$f(\Omega) = -\frac{\mathsf{m}}{2\pi}\langle\vec{k}_\Omega|T(E)|\vec{k}_0\rangle \approx -\frac{\mathsf{m}}{2\pi}\tilde{V}(q) \tag{1021}$$

where $\vec{q} = \vec{k}_\Omega - \vec{k}_0$ and $\tilde{V}(\vec{q})$ is the Fourier transform of $V(\vec{r})$. The corresponding formula for the cross section is consistent with the Fermi golden rule.

It is customary in high energy physics to take into account higher orders. The various terms in the expansion are illustrated using Feynman diagrams. However, there are circumstance where we can gain better insight by considering

the analytical properties of the Green function. In particular we can ask what happens if G has a pole at some complex energy $z = E_r - i(\Gamma_r/2)$. Assuming the the scattering is dominated by that resonance we get that the cross section has a Lorentzian line shape. More generally, If there is an interference between the resonance and the non-resonant terms then we get a Fano line shape. We shall discuss further resonances later on within the framework of the S matrix formalism.

[40] Scattering in the S-matrix formalism

[40.1] Channel Representation

Before we define the S matrix, Let us review some of the underlying assumptions of the S matrix formalism. Define

$$\rho(x) = |\psi(x)|^2 \tag{1022}$$

The continuity equation is

$$\frac{\partial \rho}{\partial t} = \nabla \cdot J \tag{1023}$$

We are working with a time-independent Hamiltonian and looking for stationary solutions, hence:

$$\nabla \cdot J = 0 \tag{1024}$$

The standard basis for representation is $|x\rangle$. We assume that the wave function is separable outside of the scattering region. Accordingly we arrange the basis as follows:

$$\begin{aligned} &|x \in \text{inside}\rangle = \text{the particle is located inside the scattering region} \\ &|a, r\rangle = \text{the particle is located along one of the outside channels} \end{aligned} \tag{1025}$$

and write the quantum state in this representation as

$$|\psi\rangle \;\; = \;\; \sum_{x \in \text{inside}} \varphi(x) \; |x\rangle \;\; + \;\; \sum_{a,r} R_a(r) \; |a, r\rangle \tag{1026}$$

The simplest example for a system that has (naturally) this type of structure is a set of 1D wires connected together to some "dot". In such geometry the index a distinguishes the different wires. Another, less trivial example, is a lead connected to a "dot". Assuming for simplicity 2D geometry, the wavefunction in the lead can be expanded as

$$\psi(x) \;\; = \;\; \psi(r, s) \;\; = \;\; \sum_a R_a(r) \chi^a(s) \tag{1027}$$

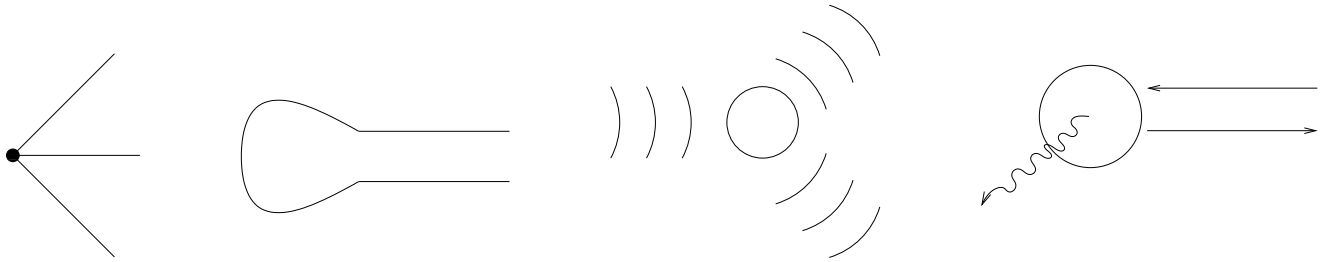
where the channel functions (waveguide modes) are:

$$\chi^a(s) \;\; = \;\; \sqrt{\frac{2}{\ell}} \sin\left(\left(\frac{\pi}{\ell} a\right) s\right) \qquad \text{with } a = 1, 2, 3 \ldots \text{ and } 0 < s < \ell \tag{1028}$$

In short, we can say that the wavefunction outside of the scattering region is represented by a set of radial functions:

$$\psi(x) \;\; \mapsto \;\; R_a(r) \qquad \text{where } a = 1, 2, 3 \ldots \text{ and } 0 < r < \infty \tag{1029}$$

The following figures illustrate several examples for scattering problems (from left to right): three connected wires, dot-waveguide system, scattering in spherical geometry, and inelastic scattering. The last two systems will be discussed below and in the exercises.



[40.2] The Definition of the S Matrix

Our Hamiltonian is time-independent, so the energy E is a good quantum number, and therefore the Hamiltonian $\mathcal{H}$ is block diagonal if we take E as one index of the representation. For a given energy E the Hamiltonian has an infinite number of eigenstates which form the so called "energy shell". For example in 3D for a given energy E we have all the plane waves with momentum $|\vec{k}| = k_E$, and all the possible superpositions of these waves. Once we are on the energy shell, it is clear that the radial functions should be of the form

$$R_a(r) = A_a R^{E,a,-}(r) - B_a R^{E,a,+}(r) \tag{1030}$$

For example, in case of a waveguide

$$R^{E,a,\pm}(r) = \frac{1}{\sqrt{v_a}}\, \mathrm{e}^{\pm i k_a r} \qquad \text{[flux normalized]} \tag{1031}$$

where the radial momentum in channel a corresponds to the assumed energy E,

$$k_a = \sqrt{2\mathsf{m}\left(E - \frac{1}{2\mathsf{m}}\left(\frac{\pi}{\ell}a\right)^2\right)} \tag{1032}$$

and the velocity $v_a = k_a/\mathsf{m}$ in channel a is determined by the dispersion relation. Thus on the energy shell the wavefunctions can be represented by a set of ingoing and outgoing amplitudes:

$$\psi(x) \;\mapsto\; (A_a, B_a) \qquad \text{with } a = 1, 2, 3 \ldots \tag{1033}$$

But we should remember that not all sets of amplitudes define a stationary energy state. In order to have a valid energy eigenstate we have to match the ingoing and outgoing amplitudes on the boundary of the scattering region. The matching condition is summarized by the S matrix.

$$B_b = \sum_a S_{ba} A_a \tag{1034}$$

By convention the basis radial functions are "flux normalized". Consequently the current in channel a is $i_a = |B_a|^2 - |A_a|^2$ and from the continuity equation it follows that

$$\sum_a |B_a|^2 = \sum_a |A_a|^2 \tag{1035}$$

From here follows that the S matrix is unitary.

In order to practice the definition of the S matrix consider a system with a single 2D lead. Let us assume that the lead has 3 open channels. That means that k_a is a real number for $a = 1, 2, 3$, and becomes imaginary for $a > 3$. The

$a > 3$ channels are called "closed channels" or "evanescent modes". They should not be included in the S matrix because if we go far enough they contribute nothing to the wavefunction (their contribution decays exponentially). Thus we have a system with 3 open channels, and we can write

$$\begin{aligned} R_1(r) &= \frac{1}{\sqrt{v_1}}(A_1 \mathrm{e}^{-ik_1 r} - B_1 \mathrm{e}^{+k_1 r}) \\ R_2(r) &= \frac{1}{\sqrt{v_2}}(A_2 \mathrm{e}^{-ik_2 r} - B_2 \mathrm{e}^{+k_2 r}) \\ R_3(r) &= \frac{1}{\sqrt{v_3}}(A_3 \mathrm{e}^{-ik_3 r} - B_3 \mathrm{e}^{+k_3 r}) \end{aligned} \tag{1036}$$

and

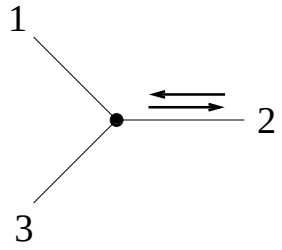
$$\begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix} = \mathbf{S} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} \tag{1037}$$

═══ [40.3] Scattering states

Let us define the unperturbed Hamiltonian $\mathcal{H}_0$ as that for which the particle cannot make transitions between channels. Furthermore without loss of generality the phases of $R^{a\pm}(r)$ is chosen such that $S_{ab} = \delta_{ab}$, or equivalently $B_a = A_a$, should give the "free wave" solutions. We label the "free" energy states that correspond to the Hamiltonian $\mathcal{H}_0$ as $|\phi\rangle$. In particular we define a complete set $|\phi^\alpha\rangle$, that are indexed by $\alpha = (E, a)$, Namely, we define

$$|\phi^\alpha\rangle = |\phi^{E_\alpha a_\alpha}\rangle \to \delta_{a,a_\alpha}(R^{a-}(r) - R^{a+}(r)) \tag{1038}$$

The following figure illustrates how the "free wave" $|\phi^{E,2}\rangle$ l of a three wire system looks like.



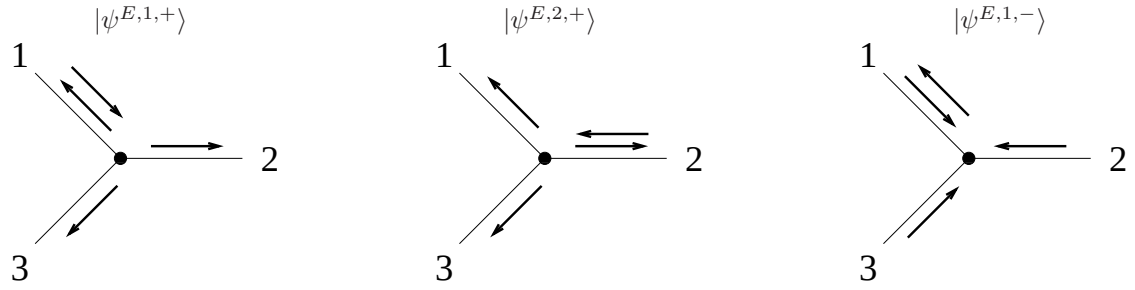
It is clear that the states $|\phi^{E,a}\rangle$ form a complete basis. Now we take the actual Hamiltonian $\mathcal{H}$ that permits transitions between channels. The general solution is written as

$$|\psi^\alpha\rangle \to A_a R^{a-}(r) - B_a R^{a+}(r) \tag{1039}$$

where $B_a = S_{ab}A_b$ or the equivalent relation $A_a = (S^{-1})_{ab}B_b$. In particular we can define the following sets of solutions:

$$\begin{aligned} |\psi^{\alpha+}\rangle &= |\psi^{E_\alpha a_\alpha +}\rangle \to \delta_{a,a_\alpha} R^{a-}(r) - S_{a,a_\alpha} R^{a+}(r) \\ |\psi^{\alpha-}\rangle &= |\psi^{E_\alpha a_\alpha -}\rangle \to -(S^{-1})_{a,a_\alpha} R^{a-}(r) + \delta_{a,a_\alpha} R^{a+}(r) \end{aligned} \tag{1040}$$

The set of (+) states describes an incident wave in the a_α channel ($A_a = \delta_{a,a_\alpha}$) and a scattered wave that satisfies "outgoing" boundary conditions. We illustrate some of these states in the case of a three wire system.



[40.4] Time reversal in scattering theory

It is tempting to identify $(-)$ scattering as the time reversed version of the $(+)$ scattering states. This is indeed correct in the absence of a magnetic field, when we have time reversal symmetry. Otherwise it is wrong. We shall clarify this point below.

Assuming that we have the solution

$$|\psi^{E,a_0,+}\rangle \longrightarrow \delta_{a,a_0}\mathrm{e}^{-ikx} - S_{a,a_0}\mathrm{e}^{+ikx} \tag{1041}$$

then the time reversed state is

$$\mathcal{T}|\psi^{E,a_0,+}\rangle \longrightarrow \delta_{a,a_0}\mathrm{e}^{ikx} - (S^*)_{a,a_0}\mathrm{e}^{-ikx} \tag{1042}$$

This should be contrasted with

$$|\psi^{E,a_0,-}\rangle \longrightarrow -(S^{-1})_{a,a_0}\mathrm{e}^{-ikx} + \delta_{a,a_0}\mathrm{e}^{ikx} \tag{1043}$$

We see that the two coincide only if

$$S^* = S^{-1} \tag{1044}$$

which means that the S matrix should be symmetric ($S^{\mathrm{T}} = S$). This is the condition for having time reversal symmetry in the language of scattering theory.

[40.5] Orthonormality of the scattering states

The $(+)$ states form a complete orthonormal basis. Also the $(-)$ states form a complete orthonormal basis. The orthonormality relation and the transformation that relates the two basis sets are

$$\begin{aligned}
\langle E,a,+|E',b,+\rangle &= 2\pi\delta(E-E')\delta_{ab} \\
\langle E,a,-|E',b,-\rangle &= 2\pi\delta(E-E')\delta_{ab} \\
\langle E,a,-|E',b,+\rangle &= 2\pi\delta(E-E')S_{ab}
\end{aligned} \tag{1045}$$

The last equality follows directly from the definition of the S matrix. Without loss of generality we prove this lemma for the 3 wire system. For example let us explain why we have

$$\langle\psi^{E,1,-}|\psi^{E_0,2,+}\rangle = -2\pi\delta(E-E_0)S_{12} \tag{1046}$$

By inspection of the figure in a previous section we see that the singular overlaps come only from the first and the second channels. Disregarding the "flux" normalization factor the overlap integral is

$$\int_0^\infty (-(S^{-1})_{11}\mathrm{e}^{-ikr} + \mathrm{e}^{ikr})^*(-S_{12}\mathrm{e}^{+ik_0r})dr + \int_0^\infty (-(S^{-1})_{21}\mathrm{e}^{-ikr})^*(\mathrm{e}^{-ik_0r} - S_{22}\mathrm{e}^{+ik_0r})dr \tag{1047}$$

keeping only the singular overlaps, changing the dummy integration variable in the second integral from r to $-r$, and using $(S^{-1})^*_{21} = S_{12}$ we get

$$\int_0^\infty S_{12}\mathrm{e}^{-i(k-k_0)r}dr + \int_{-\infty}^0 S_{12}\mathrm{e}^{-i(k-k_0)r}dr = -2\pi\delta(k-k_0)S_{12} \tag{1048}$$

If we restore the "flux normalization" factor we get the desired result. One can wonder what about the non-singular contributions to the overlaps. These may give, and indeed give, an overlap that goes like $1/(E \pm E_0)$. But on the other hand we know that for $E \neq E_0$ the overlap should be exactly zero due to the orthogonality of states with different energy (the Hamiltonian is Hermitian). If we check whether all the non-singular overlaps cancel, we find that this is not the case. What is wrong? The answer is simple. In the above calculation we disregarded a non-singular overlap which is contributed by the scattering region. This must cancel the non-singular overlap in the outside region because as we said, the Hamiltonian is Hermitian.

[40.6] Getting the S matrix from the T matrix

The derivation of the relation between the S matrix and the T matrix goes as follows: On the one hand we express the overlap of the ingoing and outgoing scattering states using the S matrix. On the other hand we express it using the T matrix. Namely,

$$\begin{aligned}\langle\psi^{E_\alpha,a_\alpha,-}|\psi^{E_\beta,a_\beta,+}\rangle &= -2\pi\delta(E_\alpha - E_\beta)\, S_{a_\alpha a_\beta} \\ \langle\psi^{E_\alpha,a_\alpha,-}|\psi^{E_\beta,a_\beta,+}\rangle &= -2\pi\delta(E_\alpha - E_\beta)\,(\delta_{a_\alpha a_\beta} - iT_{a_\alpha a_\beta})\end{aligned} \tag{1049}$$

By comparing the two expressions we derive a relation between the S matrix and the T matrix.

$$S_{a_\alpha a_\beta} = \delta_{a_\alpha a_\beta} - iT_{a_\alpha a_\beta} \tag{1050}$$

or in abstract notation $S = 1 - iT$. The rest of this section is dedicated to the derivation of T matrix expression. For notational simplicity we write it as

$$\langle\Psi^{E_2,a_2,-}|\Psi^{E_1,a_1,+}\rangle = -2\pi\delta(E_2 - E_1)\,(\delta_{a_2,a_1} - iT_{a_2,a_1}) \tag{1051}$$

We recall that the scattering state $\Psi^{E,a,+}$ is defined as the solution of $\mathcal{H}\Psi = E\Psi$ that has the form

$$\Psi = \phi^{E,a} + \Psi^{scatt} \tag{1052}$$

with outgoing boundary conditions on the scattered component. The states $\Psi^{E,a,-}$ are defined in the same way but with ingoing boundary conditions. We note that each set of states is a complete orthonormal basis. For example:

$$\langle\Psi^{E_2,a_2,+}|\Psi^{E_1,a_1,+}\rangle = 2\pi\delta(E_2 - E_1)\delta_{a_2,a_1} \tag{1053}$$

Our proof is based on the following identities:

$$\begin{aligned}\Psi^{E_1,a_1,+} &= (1 + G^+(E_1)V)\phi^{E_1,a_1} = \left(1 + \frac{1}{E_1 - \mathcal{H} + i0}V\right)\phi^{E_1,a_1} \\ \Psi^{E_2,a_2,-} &= (1 + G_0^-(E_2)T(E_2)^\dagger)\phi^{E_2.a_2} = \left(1 + \frac{1}{E_2 - \mathcal{H}_0 - i0}T(E_2)^\dagger\right)\phi^{E_2.a_2}\end{aligned} \tag{1054}$$

We use the first identity for the "ket", and after that the second identity for the "bra". Namely:

$$\begin{aligned}
\langle\Psi^{E_2,a_2^-}|\Psi^{E_1,a_1^+}\rangle &= \langle\Psi^{E_2,a_2^-}\left|1+\frac{1}{E_1-\mathcal{H}+i0}V\right|\phi^{E_1,a_1}\rangle \\
&= \langle\Psi^{E_2,a_2^-}\left|1+\frac{1}{E_1-E_2+i0}V\right|\phi^{E_1,a_1}\rangle \\
&= \langle\phi^{E_2,a_2}\left|\left[1+T(E_2)\frac{1}{E_2-\mathcal{H}_0+i0}\right]\left[1+\frac{V}{E_1-E_2+i0}\right]\right|\phi^{E_1,a_1}\rangle \\
&= \langle\phi^{E_2,a_2}\left|\left[1+\frac{T(E_2)}{E_2-E_1+i0}\right]\right|\phi^{E_1,a_1}\rangle + \langle\phi^{E_2,a_2}\left|\frac{V+T(E_2)G_0^+(E_2)V}{E_1-E_2+i0}\right|\phi^{E_1,a_2}\rangle \\
&= \langle\phi^{E_2,a_2}\left|1+\frac{T(E_2)}{E_2-E_1+i0}\right|\phi^{E_1,a_1}\rangle + \langle\phi^{E_2,a_2}\left|\frac{T(E_2)}{E_1-E_2+i0}\right|\phi^{E_1,a_1}\rangle
\end{aligned} \tag{1055}$$

where in the last step we have used the relation $V+TG_0V=T$. From the last expression we get the desired result.

[40.7] The Optical Theorem

We have argued that there is a connection between the S matrix and the T matrix:

$$S_{ab}=\delta_{ab}-iT_{ab}=\delta_{ab}-i\langle\phi^a|T|\phi^b\rangle \tag{1056}$$

The equation above can be written as $S=1-iT$. But we should remember that S is not an operator, and that S_{ab} were not defined as matrix elements of an operator. In contrast to that T_{ab} are matrix elements of an operator in the free wave basis.

Now we remember that S is unitary, so $S^\dagger S=1$. Therefore we conclude that the T matrix should satisfy the following equality:

$$(T-T^\dagger)=-iTT^\dagger \tag{1057}$$

In particular we can write:

$$\langle a_0|T-T^\dagger|a_0\rangle=-i\sum_a\langle a_0|T|a\rangle\langle a|T^\dagger|a_0\rangle \tag{1058}$$

and we get:

$$\sum_a|T_{aa_0}|^2=-2\mathrm{Im}[T_{a_0a_0}] \tag{1059}$$

This establishes a connection between the "cross section" and the forward scattering amplitude $T_{a_0a_0}$.

We can write the optical theorem in various levels of abstraction:

$$\begin{aligned}
\sum_a|\langle\phi^a|T|\phi^{a_0}\rangle|^2 &= -2\mathrm{Im}[\langle\phi^{a_0}|T|\phi^{a_0}\rangle] \\
\sum_{\ell,m}|\langle\phi^{E,\ell,m}|T|\phi^{E,\ell_0,m_0}\rangle|^2 &= -2\mathrm{Im}[\langle\phi^{E,l_0,m_0}|T|\phi^{E,l_0,m_0}\rangle] \\
\sum_\Omega|\langle\phi^{E,\Omega}|T|\phi^{E,\Omega_0}\rangle|^2 &= -2\mathrm{Im}[\langle\phi^{E,\Omega_0}|T|\phi^{E,\Omega_0}\rangle]
\end{aligned} \tag{1060}$$

Using the relations

$$|E,\Omega\rangle = \frac{1}{\sqrt{v_E}}\frac{k_E}{2\pi}|k_\Omega\rangle \tag{1061}$$
$$f(\Omega) = -\frac{\mathsf{m}}{2\pi}\langle\vec{k}_\Omega|T(E)|\vec{k}_0\rangle$$

we get the familiar versions of this theorem:

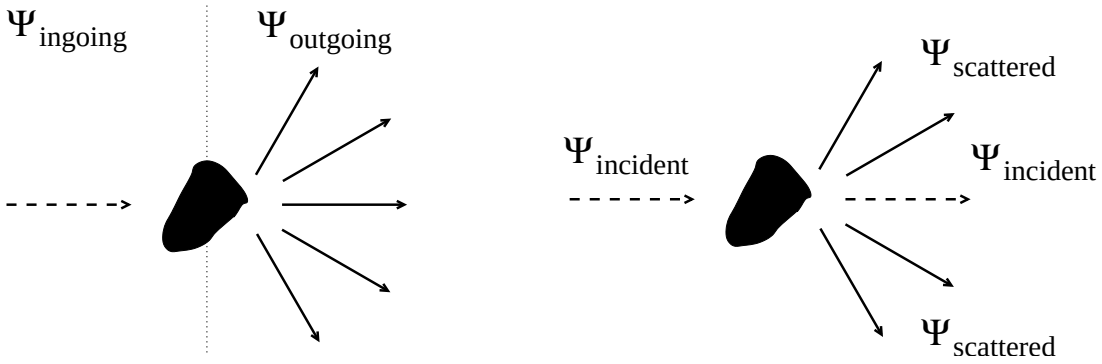
$$\int |\langle\vec{k}_\Omega|T|\vec{k}_0\rangle|^2 d\Omega = -2v_E\left(\frac{2\pi}{k_E}\right)^2 \mathrm{Im}[\langle\vec{k}_0|T|\vec{k}_0\rangle] \tag{1062}$$
$$\sigma_{\text{total}} = \int |f(\Omega)|^2 d\Omega = \frac{4\pi}{k_E}\mathrm{Im}[f(0)]$$

[40.8] The generalized notion of cross section

Assume that we have a scattering state Ψ. We can write it as a sum of "ingoing" and "outgoing" waves or as a sum of "incident" and "scattered" waves. This is not the same thing!

$$\Psi = \Psi_{ingoing} + \Psi_{outgoing} \tag{1063}$$
$$\Psi = \Psi_{incident} + \Psi_{scattered}$$

The "incident wave" is a "free wave" that contains the "ingoing" wave with its associated "outgoing" component. It corresponds to the $\mathcal{H}_0$ Hamiltonian. The "scattered wave" is what we have to add in order to get a solution to the scattering problem with the Hamiltonian $\mathcal{H}$. In the case of the usual boundary conditions it contains only an "outgoing" component.



Below is an illustration of the 1D case where we have just two directions of propagation (forwards and backwards):

The S matrix gives the amplitudes of the outgoing wave, while the $T = i(\hat{1} - S)$ matrix gives the amplitudes of the scattered component (up to a phase factor). Let us consider extreme case in order to clarify this terminology. If we

have in the above 1D geometry a very high barrier, then the outgoing wave on the right will have zero amplitude. This means that the scattered wave must have the same amplitude as the incident wave but with the opposite sign.

In order to define the "cross section" we assume that the incident wave is a density normalized ($\rho = 1$) plane wave. This is like having a current density $J = \rho v_E$. If we regard the target as having some "area" σ then the scattered current is

$$i_{scattered} \;=\; (\rho v_E) \times \sigma \tag{1064}$$

It is clear from this definition that the units of the cross section are $[\sigma] = L^{d-1}$. In particular in 1D geometry the "differential cross section" into channel a, assuming an incident wave in channel a_0 is simply

$$\sigma_a \;=\; |T_{a,a_0}|^2 \tag{1065}$$

and by the "optical theorem" the total cross section is

$$\sigma_{\rm total} \;=\; -2{\rm Im}[T_{a_0,a_0}] \tag{1066}$$

The notion of "cross section" is problematic conceptually because it implies that it is possible for the scattered flux to be larger than the incident flux. This is most evident in the 1D example that we have discussed above. We see that the scattered wave is twice the incident wave, whereas in fact the forward scattering cancels the outgoing component of the incident wave. Later we calculate the cross section of a sphere in 3D and get twice the classical cross section ($2\pi a^2$). The explanation is the same - there must be forward scattering that is equal in magnitude (but opposite in sign) to the outgoing component of the incident wave in order to create a "shadow region" behind the sphere.

[41] Scattering in quasi 1D geometry

[41.1] Elastic scattering by a delta junction

The $\boldsymbol{S}$ matrix for a delta function scatterer $V(r) = u\delta(r)$ in one dimension is

$$\boldsymbol{S} = \begin{pmatrix} r & t \\ t & r \end{pmatrix} = \mathrm{e}^{i\gamma} \begin{pmatrix} -i\sqrt{1-g}\mathrm{e}^{i\alpha} & \sqrt{g}\mathrm{e}^{-i\phi} \\ \sqrt{g}\mathrm{e}^{i\phi} & -i\sqrt{1-g}\mathrm{e}^{-i\alpha} \end{pmatrix} \tag{1067}$$

with

$$\begin{aligned} v_E &\equiv (2E/\mathsf{m})^{1/2} && (1068)\\ t &= \frac{1}{1+i(u/v_E)} && (1069)\\ r &= t-1 && (1070)\\ \gamma &= \arg(t) = -\arctan(u/v_E) \qquad \mathrm{mod}\ (\pi) && (1071)\\ g &= \frac{1}{1+(u/v_E)^2} = (\cos(\gamma))^2 && (1072)\\ \alpha &= 0 && (1073)\\ \phi &= 0 && (1074) \end{aligned}$$

Note that we use the common ad-hoc convention of writing the channel functions as $\psi(r) = A\exp(-ikr) + B\exp(-ikr)$ where $r = |x|$. In the alternate convention, which is used for s-scattering, $B \mapsto -B$, so as to have $\boldsymbol{S} = \mathbf{1}$ in the limit of zero coupling ($u = \infty$).

If we have $\mathcal{M}$ wires connected at one point we can define a generalized "delta junction" as follows:

$$\boldsymbol{S}_{ab} = -\delta_{ab} + \frac{2}{\mathcal{M}}\left(\frac{1}{1+i(u/v_E)}\right) \tag{1075}$$

For $u = 0$ we get zero reflection for $\mathcal{M} = 2$, while for $\mathcal{M} = 3$

$$\boldsymbol{S} = \begin{pmatrix} -1/3 & 2/3 & 2/3 \\ 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \end{pmatrix} \tag{1076}$$

In the limit $\mathcal{M} \to \infty$ we get total reflection.

[41.2] Elastic scattering by a regularized delta function

It is instructive to consider the scattering by a regularized delta function. The systematic procedure below can be generalized to more than one dimension in order to analyze s-scattering. In particular it illuminates how a divergent series for T can give a finite result, and why in the absence of regularization a delta function does not scatter in more than one dimension. By a regularized delta function we mean a potential $V(x)$ that has the matrix elements $V_{k,k'} = u$ for any k and k' within some finite momentum range. For example $|k| < \Lambda$, where Λ is a large momentum cutoff. Another possibility which is of relevance in the analysis of Kondo problem is $E_F < |k| < \Lambda$, where E_F is the Fermi energy.

First we make a note regarding a useful identity. Given a column vector a, one can form a matrix $A = aa^t$, such that $\mathrm{trace}[A] = aa^t$. From

$$\frac{1}{1-aa^t} = 1 + (aa^t) + (aa^t)^2 + (aa^t)^3 ... = 1 + a[1 + (a^t a) + (a^t a)^2 + ...]a^t = 1 + \frac{1}{1-a^t a}aa^t \tag{1077}$$

it follows that

$$\frac{1}{1-A} = 1 + \frac{1}{1-\mathrm{trace}[A]}A \tag{1078}$$

and more generally we get

$$\frac{1}{B-A} = \frac{1}{B} + \left(\frac{1}{1-\mathrm{trace}[A/B]}\right)\frac{1}{B}A\frac{1}{B} \tag{1079}$$

We use these formulas above in order to calculate the Green function G and the T matrix for a regularized delta scatterer. These formulas can be regarded as the sum of a zero order term and a renormalized first order term. The expression for the Green function is

$$G = \frac{1}{E-\mathcal{H}_0-V} = G_0 + \frac{1}{1-\nu_E u}G_0 V G_0 \tag{1080}$$

The expression for the T matrix is

$$T = G_0^{-1}GV = \frac{1}{1-\nu_E u}V \tag{1081}$$

where

$$\nu_E = \sum_k \frac{1}{E-E_k+i0} \tag{1082}$$

where $\sum_k$ should be treated with the appropriate integration measure. The $\sum_k$ integral equals $-i/v_E$ for a non-regularized Dirac delta function in one dimension. Hence from the expression for T we get easily the familiar result for the reflection of a non-regularized delta scatterer in one dimension. In higher dimensions ν_E has a real part that diverges, which implies that the scattering goes to zero. The regularization makes ν_E finite. In three dimensions we get $\nu_E = -(\mathsf{m}/\pi^2)\Lambda_E$ where

$$\Lambda_E = -2\pi^2\int_0^\Lambda \frac{d^3k}{(2\pi)^3}\frac{1}{k_E^2-k^2+i0} = \Lambda - \frac{1}{2}k_E\log\left(\frac{\Lambda+k_E}{\Lambda-k_E}\right) + i\frac{\pi}{2}k_E \tag{1083}$$

Still we may have divergence if E is very close to a threshold energy. Such threshold exits if, say, there exists a lower cutoff E_F. The divergence near a threshold is logarithmic. It is quite amusing that the second order as well as all the higher terms in perturbation theory are divergent, while their sum goes to zero...

[41.3] Digression: Kondo scattering

One can wonder whether the Fermi energy, due to the Pauli exclusion principle, is like a lower cutoff that "regularize" the scattering cross section of of electrons in a metal. We explain below that this is not the case unless the scattering involves a spin flip. The latter is known as the Kondo effect. The scattering is described by

$$V = \sum_{k',k} a^\dagger_{k'}V_{k',k}a_k \tag{1084}$$

hence

$$T^{[2]} = \left\langle k_2\left|V\frac{1}{E-\mathcal{H}}V\right|k_1\right\rangle = \sum_{k'_b,k_b}\sum_{k'_a,k_a}\left\langle k_2\left|a^\dagger_{k'_b}V_{k'_b,k_b}a_{k_b}\frac{1}{E-\mathcal{H}}a^\dagger_{k'_a}V_{k'_a,k_a}a_{k_a}\right|k_1\right\rangle \tag{1085}$$

where both the initial and the final states are zero temperature Fermi sea with one additional electron above the Fermi energy. The initial and final states have the same energy:

$$E \;=\; E_0 + \epsilon_{k_1} \;=\; E_0 + \epsilon_{k_2} \tag{1086}$$

where E_0 is the total energy of the zero temperature Fermi sea. The key observation is that all the intermediate states are with definite occupation. therefore we can pull out the resolvent:

$$T^{[2]} = \sum_{k'_b,k_b,k'_a,k_a} \frac{V_{k'_b,k_b}V_{k'_a,k_a}}{E - E_{k_a,k'_a}} \left\langle k_2 \left| a^\dagger_{k'_b} a_{k_b} a^\dagger_{k'_a} a_{k_a} \right| k_1 \right\rangle \tag{1087}$$

where

$$E_{k_a,k'_a} \;=\; E_0 + \epsilon_{k_1} - \epsilon_{k_a} + \epsilon_{k'_a} \tag{1088}$$

As in the calculation of "exchange" we have two non-zero contribution to the sum. Either (k'_b, k_b, k'_a, k_a) equals (k_2, k', k', k_1) with k' above the Fermi energy, or (k', k_1, k_2, k') with k' below the Fermi energy. Accordingly $E - E_{k_a,k'_a}$ equals either $(\epsilon_{k'} - \epsilon_{k_1})$ or $-(\epsilon_{k'} - \epsilon_{k_1})$. Hence we get

$$T^{[2]} = \sum_{k'} \left[\frac{V_{k_2,k'}V_{k',k_1}}{+(\epsilon_{k'} - \epsilon_{k_1})} \left\langle k_2 \left| a^\dagger_{k_2} a_{k'} a^\dagger_{k'} a_{k_1} \right| k_1 \right\rangle + \frac{V_{k',k_1}V_{k_2,k'}}{-(\epsilon_{k'} - \epsilon_{k_1})} \left\langle k_2 \left| a^\dagger_{k'} a_{k_1} a^\dagger_{k_2} a_{k'} \right| k_1 \right\rangle \right] = \sum_{k'} \frac{V_{k_2,k'}V_{k',k_1}}{\epsilon_{k'} - \epsilon_{k_1}} \tag{1089}$$

leading to a result which is not divergent at the Fermi energy, as if the Fermi energy does not exist at all:

$$T^{[2]} = \sum_{k'} \frac{V_{k_2,k'}V_{k',k_1}}{\epsilon_{k'} - \epsilon_{k_1}} \tag{1090}$$

we have used

$$\left\langle k_2 \left| a^\dagger_{k_2} a_{k'} a^\dagger_{k'} a_{k_1} \right| k_1 \right\rangle = \left\langle k_2 \left| a^\dagger_{k_2} (1 - n_{k'}) a_{k_1} \right| k_1 \right\rangle = +1 \times \left\langle k_2 \left| a^\dagger_{k_2} a_{k_1} \right| k_1 \right\rangle \tag{1091}$$

which holds if k' is above the Fermi energy (otherwise it is zero). And

$$\left\langle k_2 \left| a^\dagger_{k'} a_{k_1} a^\dagger_{k_2} a_{k'} \right| k_1 \right\rangle = \left\langle k_2 \left| a_{k_1} (n_{k'}) a^\dagger_{k_2} \right| k_1 \right\rangle = -1 \times \left\langle k_2 \left| a^\dagger_{k_2} a_{k_1} \right| k_1 \right\rangle \tag{1092}$$

which holds if k' is below the Fermi energy (otherwise it is zero). Note that irrespective of gauge

$$\left\langle k_2 \left| a^\dagger_{k_2} a_{k_1} \right| k_1 \right\rangle^2 = 1 \tag{1093}$$

If there is a spin flip, as in the Kondo problem, the divergence for E close to the Fermi energy is not avoided. Say that we want to calculate the scattering amplitude

$$\langle k_2 \uparrow, \Downarrow | T | k_1, \uparrow, \Downarrow \rangle \tag{1094}$$

where the double arrow stands for the spin of a magnetic impurity. It is clear that the only sequences that contribute are those that take place *above* the Fermi energy. The other set of sequences, that involve the creation of an electron-hole pair do not exist: Since we assume that the magnetic impurity is initially "down", it is not possible to generate a pair such that the electron spin is "up".

[41.4] Inelastic scattering by a delta scatterer (I)

We consider the following scattering problem in one dimensions:

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} + Q\delta(x) + \mathcal{H}_{\text{scatterer}} \tag{1095}$$

The scatterer is assumed to have energy levels n with eigenvalues E_n. It should be clear that inelastic scattering of a spinless particle by a multi level atom is mathematically equivalent to inelastic scattering of a multi level atom by some static potential. Outside of the scattering region the total energy of the system (particle plus scatterer) is

$$\mathcal{E} = \epsilon_k + E_n \tag{1096}$$

We look for scattering states that satisfy the equation

$$\mathcal{H}|\Psi\rangle = \mathcal{E}|\Psi\rangle \tag{1097}$$

The scattering channels are labeled as

$$\boldsymbol{n} = (n_0, n) \tag{1098}$$

where $n_0 =$ left,right. We define

$$k_{\boldsymbol{n}} = \sqrt{2m(\mathcal{E} - E_n)} \qquad \text{for } n \in \text{open} \tag{1099}$$
$$\alpha_{\boldsymbol{n}} = \sqrt{-2m(\mathcal{E} - E_n)} \qquad \text{for } n \in \text{closed} \tag{1100}$$

later we use the notations

$$v_{\boldsymbol{n}} = k_{\boldsymbol{n}}/\mathsf{m} \tag{1101}$$
$$u_{\boldsymbol{n}} = \alpha_{\boldsymbol{n}}/\mathsf{m} \tag{1102}$$

and define diagonal matrices $\boldsymbol{v} = \text{diag}\{v_n\}$ and $\boldsymbol{u} = \text{diag}\{u_n\}$. The channel radial functions are written as

$$R(r) = A_n \mathrm{e}^{-ik_n r} + B_n \mathrm{e}^{+ik_n r} \qquad \text{for } n \in \text{open} \tag{1103}$$
$$R(r) = C_n \mathrm{e}^{-\alpha_n r} \qquad \text{for } n \in \text{closed} \tag{1104}$$

where $r = |x|$. Next we derive expression for the $2N \times 2N$ matching matrix $\boldsymbol{M}$ and for the $2N \times 2N$ scattering matrix $\boldsymbol{S}$, where N is the number of open modes. The wavefunction can be written as

$$\Psi(r, n_0, Q) = \sum_n R_{n_0,n}(r)\chi^n(Q) \tag{1105}$$

The matching equations are

$$\Psi(0, \text{right}, Q) = \Psi(0, \text{left}, Q) \tag{1106}$$
$$\frac{2}{2\mathsf{m}}\left[\Psi'(0, \text{right}, Q) + \Psi'(0, \text{left}, Q)\right] = \hat{Q}\Psi(0, Q) \tag{1107}$$

The operator $\hat{Q}$ is represented by the matrix Q_{nm} that has the block structure

$$Q_{nm} = \begin{pmatrix} Q_{vv} & Q_{vu} \\ Q_{uv} & Q_{uu} \end{pmatrix} \tag{1108}$$

For sake of later use we define

$$M_{nm} = \begin{pmatrix} \frac{1}{\sqrt{v}} Q_{vv} \frac{1}{\sqrt{v}} & \frac{1}{\sqrt{v}} Q_{vu} \frac{1}{\sqrt{u}} \\ \frac{1}{\sqrt{u}} Q_{uv} \frac{1}{\sqrt{v}} & \frac{1}{\sqrt{u}} Q_{uu} \frac{1}{\sqrt{u}} \end{pmatrix} \tag{1109}$$

The matching conditions lead to the following set of matrix equations

$$\begin{aligned} A_R + B_R &= A_L + B_L && (1110)\\ C_R &= C_L && (1111)\\ -i\boldsymbol{v}(A_R - B_R + A_L - B_L) &= 2Q_{vv}(A_L + B_L) + 2Q_{vu}C_L && (1112)\\ -\boldsymbol{u}(C_R + C_L) &= 2Q_{uv}(A_L + B_L) + 2Q_{uu}C_L && (1113) \end{aligned}$$

from here we get

$$\begin{aligned} A_R + B_R &= A_L + B_L && (1114)\\ A_R - B_R + A_L - B_L &= i2(\boldsymbol{v})^{-1}\mathcal{Q}(A_L + B_L) && (1115) \end{aligned}$$

where

$$\mathcal{Q} = Q_{vv} - Q_{vu}\frac{1}{(\boldsymbol{u} + Q_{uu})}Q_{uv} \tag{1116}$$

The set of matching conditions can be written as

$$\begin{pmatrix} B_R \\ A_R \end{pmatrix} = \boldsymbol{M} \begin{pmatrix} A_L \\ B_L \end{pmatrix} \tag{1117}$$

with the matching matrix

$$\boldsymbol{M} = \begin{pmatrix} M_{++} & M_{+-} \\ M_{-+} & M_{--} \end{pmatrix} = \begin{pmatrix} 1 - i\mathcal{M} & -i\mathcal{M} \\ i\mathcal{M} & 1 + i\mathcal{M} \end{pmatrix} \tag{1118}$$

where $\mathcal{M} = (\boldsymbol{v})^{-1}\mathcal{Q}$.

═══ [41.5] Inelastic scattering by a delta scatterer (II)

We want to switch to flux normalization convention, so as to get a unitary $\boldsymbol{S}$ matrix. In this convention the proper definition of the amplitudes is $\tilde{A_n} = \sqrt{v_n}A_n$ and $\tilde{B_n} = \sqrt{v_n}B_n$. Therefore we redefine the $\mathcal{M}$ matrix using the prescription

$$\mathcal{M}_{nm} \mapsto \sqrt{v_n}\mathcal{M}_{nm}\frac{1}{\sqrt{v_m}} \tag{1119}$$

leading to

$$\mathcal{M} = \frac{1}{\sqrt{\boldsymbol{v}}}\mathcal{Q}\frac{1}{\sqrt{\boldsymbol{v}}} = M_{vv} - M_{vu}\frac{1}{1 + M_{uu}}M_{uv} \tag{1120}$$

The $\boldsymbol{S}$ matrix is defined via

$$\begin{pmatrix} \tilde{B}_L \\ \tilde{B}_R \end{pmatrix} = \boldsymbol{S} \begin{pmatrix} \tilde{A}_L \\ \tilde{A}_R \end{pmatrix} \tag{1121}$$

and can be written in block form as

$$\boldsymbol{S}_{\boldsymbol{n},\boldsymbol{m}} = \begin{pmatrix} \boldsymbol{S}_R & \boldsymbol{S}_T \\ \boldsymbol{S}_T & \boldsymbol{S}_R \end{pmatrix} \tag{1122}$$

A straightforward elimination gives

$$\boldsymbol{S} = \begin{pmatrix} -\boldsymbol{M}_{--}^{-1}\boldsymbol{M}_{-+} & \boldsymbol{M}_{--}^{-1} \\ \boldsymbol{M}_{++}-\boldsymbol{M}_{-+}\boldsymbol{M}_{--}^{-1}\boldsymbol{M}_{+-} & \boldsymbol{M}_{+-}\boldsymbol{M}_{--}^{-1} \end{pmatrix} = \begin{pmatrix} (1+i\mathcal{M})^{-1}-1 & (1+i\mathcal{M})^{-1} \\ (1+i\mathcal{M})^{-1} & (1+i\mathcal{M})^{-1}-1 \end{pmatrix} \tag{1123}$$

Now we can write expressions for $\boldsymbol{S}_R$ and for $\boldsymbol{S}_T$ using the $\mathcal{M}$ matrix.

$$\boldsymbol{S}_T = \frac{1}{1+i\mathcal{M}} = 1 - i\mathcal{M} - \mathcal{M}^2 + i\mathcal{M}^3 + ... \tag{1124}$$

$$\boldsymbol{S}_R = \boldsymbol{S}_T - \boldsymbol{1} \tag{1125}$$

======= [41.6] Elastic scattering by a delta in a waveguide

The *elastic* scattering of a spinless particle by a regularized delta scatterer in a waveguide is mathematically the same problem as that of the previous section. We have

$$Q = c\delta(y - y_0) \tag{1126}$$

for which

$$Q_{\rm nm} = c\int \chi_n \delta(y-y_0)\chi_m {\rm dy} = c\,\chi^n(y_0)\chi^m(y_0) \tag{1127}$$

Given the total energy we define

$$M_{nm} = \frac{1}{\sqrt{|v_n|}} Q_{nm} \frac{1}{\sqrt{|v_m|}} \equiv \begin{pmatrix} M_{vv} & M_{vu} \\ M_{uv} & M_{uu} \end{pmatrix} \tag{1128}$$

Regularization means that one impose a cutoff on the total number of coupled channels, hence M is a finite (truncated) matrix.

Using the formula for inverting a matrix of the type $1 - aa^{dag}$, we first obtain $\mathcal{M}$ and then obtain

$$\boldsymbol{S}_R = \frac{iM_{vv}}{1 + i\ {\rm trace}[M_{vv}] + {\rm trace}[M_{uu}]} \tag{1129}$$

Let us consider what happens as we change the total energy: Each time that a new channels is opened the scattering cross section becomes zero. Similarly, if we remove the regularization we get zero scattering for any energy because of the divergent contribution of the closed channels.

[41.7] Analysis of the cavity plus leads system

Consider a cavity to which a lead is attached. The Fisher-Lee relation established a connection between the $\boldsymbol{S} = 1 - iT$ matrix and the Green function G. It can be regarded as a special variant of $T = V + VGV$. The channels index is a and the cavity states are n. There is no direct coupling between the channels, but only lead-cavity couplings W_{an}. Consequently we expect an expression of the form

$$\boldsymbol{S} \;=\; \mathbf{1} - i\boldsymbol{T} \;=\; 1 - iWGW^\dagger \tag{1130}$$

From perturbation theory we further expect to get

$$G = \frac{1}{E - \mathcal{H}_{\text{in}} + i(W^\dagger W/2)} \tag{1131}$$

where $\mathcal{H}_{\text{in}}$ is the truncated Hamiltonian of the interior region. The latter is known as the Widenmiller formula, and can be regarded as the outcome of R matrix theory which we detail below.

The standard derivation of the Fisher-Lee relation goes as follows [Datta]: We place a source at the lead and use the S matrix to define the boundary conditions on the surface $x(s)$ of the scattering region. We solve for the outgoing amplitudes and find that

$$G(s|s_0) = i\sum_{ab} \frac{1}{\sqrt{v_a}}\chi^a(s)\ (\boldsymbol{S} - \mathbf{1})_{ab}\ \frac{1}{\sqrt{v_b}}\chi^b(s_0) \tag{1132}$$

This relation can be inverted:

$$\boldsymbol{S}_{ab} = \delta_{ab} - i\sqrt{v_a v_b}\int \chi^a(s)\ G(s|s_0)\ \chi^b(s_0)\ ds ds_0 \tag{1133}$$

The definition of W is implied by the above expression. In the next section we find it useful to define a complete set $\varphi^{(n)}(x)$ of cavity wavefunctions. Then the integral over s becomes a sum over n, and we get

$$W_{an} = \sqrt{v_a}\int \chi^a(s)\varphi^{(n)}(x(s))\ ds \tag{1134}$$

The $\boldsymbol{R}$ matrix formalism opens the way for a powerful numerical procedure for finding the $\boldsymbol{S}$ matrix of a cavity-lead system. The idea is to reduce the scattering problem to a bound state problem by chopping the leads. It can be regarded as a generalization of the one-dimensional phase shift method where the outer solution is matched to an interior solution. The latter is characterized by its log derivative on the boundary. In the same spirit the $\boldsymbol{R}$ matrix is defined through the relation

$$\psi(s) = \int \boldsymbol{R}(s,s')\partial\psi(s')\ ds' \tag{1135}$$

If we decompose this relation into channels we can rewrite it as

$$\psi_a = \sum_b \boldsymbol{R}_{ab}\partial\psi_b \tag{1136}$$

Expressing ψ_a and $\partial\psi_a$ as the sum and the difference of the the ingoing and the outgoing amplitudes A_a and B_a, one finds a simple relation between the $\boldsymbol{R}$ matrix and the $\boldsymbol{S}$ matrix:

$$\boldsymbol{R}_{ab} = i\frac{1}{\sqrt{k_a k_b}}\left(\frac{1-\boldsymbol{S}}{1+\boldsymbol{S}}\right)_{ab} \tag{1137}$$

The inverse relation is

$$\boldsymbol{S} = \frac{1 + i\sqrt{\boldsymbol{k}}\boldsymbol{R}\sqrt{\boldsymbol{k}}}{1 - i\sqrt{\boldsymbol{k}}\boldsymbol{R}\sqrt{\boldsymbol{k}}} \tag{1138}$$

From the Green theorem it follows that

$$\boldsymbol{R}(s, s') = -\frac{\hbar^2}{2\mathsf{m}} G^N(s'|s) \tag{1139}$$

where G^N is the Green function of the interior with Neumann boundary conditions on the surface of the scattering region. If we find a complete set of interior eigenfunctions then

$$G^N(s'|s) = \sum_n \frac{\varphi^{(n)}(s')\varphi^{(n)}(s)}{E - E_n} \tag{1140}$$

and consequently

$$\boldsymbol{R}_{ab} = -\frac{1}{2} \sum_n \left(\frac{W_{an}}{\sqrt{k_a}}\right) \frac{1}{E - E_n} \left(\frac{W_{bn}}{\sqrt{k_b}}\right) \tag{1141}$$

The corresponding result for the $\boldsymbol{S}$ matrix is obtained by expanding $(1 + x)/(1 - x) = 1 + 2(...)$ with the identification of $(...)$ as the diagrammatic expression of the resolvent. The result is known as the Weidenmiller formula:

$$\boldsymbol{S} = \mathbf{1} - iW \frac{1}{E - \mathcal{H}_{\text{in}} + i(W^\dagger W/2)} W^\dagger \tag{1142}$$

which agree with the Fisher Lee relation.

[42] Scattering in a spherical geometry

[42.1] The spherical Bessel functions

Of special interest is scattering in 3D geometry. The wavefunction is separable outside the scattering region in spherical coordinates. This means that we can expand any wavefunction as follows:

$$\psi(x) = \sum_{\ell,m} R_{\ell,m}(r) Y^{\ell m}(\theta,\varphi) \tag{1143}$$

The channel index is $a = (\ell, n)$ while $\Omega = (\theta, \varphi)$ is analogous to the s of the 2D lead system. The $Y^{\ell m}$ are the channel functions. In complete analogy with the case of 1D geometry we can define the following set of functions:

$$\begin{aligned} &h_\ell^+(k_E r) \leftrightarrow \mathrm{e}^{ik_E r} \\ &h_\ell^-(k_E r) \leftrightarrow \mathrm{e}^{-ik_E r} \\ &j_\ell(k_E r) \leftrightarrow \sin(k_E r) \\ &n_\ell(k_E r) \leftrightarrow \cos(k_E r) \end{aligned} \tag{1144}$$

Note that the right side equals the left side in the special case $\ell = 0$, provided we divide by r. This is because the semi-1D radial equation becomes literally the 1D Schrödinger equation only after the substitution $R(r) = u(r)/r$.

In what follows we use Messiah convention p.489. Note that other textbooks may use different sign convention. The relation between the functions above is defined as follows:

$$h_\ell^\pm \;=\; n_\ell(kr) \pm i j_\ell(kr) \tag{1145}$$

We note that the $j_n(r)$ are regular at the origin, while the $n_n(r)$ are singular at the origin. Therefore only the former qualify as global "free waves". The $l = 0$ functions are:

$$\begin{aligned} j_0(kr) \;&=\; \frac{\sin(kr)}{kr} \\ n_0(kr) \;&=\; \frac{\cos(kr)}{kr} \end{aligned} \tag{1146}$$

The asymptotic behavior for $kr \gg \ell$ is:

$$\begin{aligned} &h_\ell^\pm(kr) \sim (\mp i)^\ell \, \frac{\mathrm{e}^{\pm ikr}}{kr} \\ &n_\ell(kr) \sim \frac{\cos(kr - \frac{\pi}{2}\ell)}{kr} \\ &j_\ell(kr) \sim \frac{\sin(kr - \frac{\pi}{2}\ell)}{kr} \end{aligned} \tag{1147}$$

The short range $kr \ll \ell$ behavior is:

$$\begin{aligned} n_\ell(kr) \;&\approx\; (2l-1)!! \left(\frac{1}{kr}\right)^{\ell+1} \left[1 + \frac{1}{2(2l-1)}(kr)^2 + \dots\right] \\ j_\ell(kr) \;&\approx\; \frac{(kr)^\ell}{(2l+1)!!} \left[1 - \frac{1}{2(2l+3)}(kr)^2 + \dots\right] \end{aligned} \tag{1148}$$

[42.2] Free spherical waves

On the energy shell we write the radial wavefunctions as

$$R_{\ell m}(r) = A_{\ell m} R^{E,\ell m,-}(r) - B_{\ell m} R^{E,\ell,m,+}(r) \tag{1149}$$

where in complete analogy with the 1D case we define

$$R^{E,\ell m,\pm}(r) = \frac{k_E}{\sqrt{v_E}}\, h_\ell^{\pm}(k_E r) \tag{1150}$$

The asymptotic behavior of the spherical Hankel functions is $(\mp i)^\ell \mathrm{e}^{\pm i k_E r}/(k_E r)$. From this follows that the flux of the above radial functions is indeed normalized to unity as required. Also the sign convention that we use for $R^{E,\ell m,\pm}(r)$ is appropriate because the free waves are indeed given by

$$|\phi^{E,\ell m}\rangle \;=\; [R^{lm-}(r) - R^{lm+}(r)]\, Y^{\ell m}(\theta,\varphi) \;=\; -i\frac{k_E}{\sqrt{v_E}}\, 2 j_\ell(k_E r)\, Y^{\ell m}(\theta,\varphi) \tag{1151}$$

This spherical free wave solution is analogous to the planar free wave $|\phi^{E,\Omega}\rangle \mapsto \mathrm{e}^{i k_E \vec{n}_\Omega \cdot \vec{x}}$. If we decide (without loss of generality) that the planar wave is propagating in the z direction, then we can use the following expansion in order to express a planar wave as a superposition of spherical waves:

$$\mathrm{e}^{i k_E z} \;=\; \sum_\ell (2\ell+1)\,(i)^\ell\, P_\ell(\cos(\theta))\, j_\ell(k_E r) \tag{1152}$$

We note that we have only $m = 0$ basis functions because there is no dependence on the angle φ. In different phrasing one may say that a plane wave that propagates in the z direction has $L_z = 0$ angular momentum. Using the identity

$$Y_{\ell 0} = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos(\theta)) \tag{1153}$$

we can write

$$\mathrm{e}^{i k_E z} \;=\; \sum_{\ell,m=0} \sqrt{(2l+1)\pi}\,(i)^{\ell+1} \frac{\sqrt{v_E}}{k_E}\, \phi^{E,\ell,m}(r,\theta,\varphi) \tag{1154}$$

which makes it easy to identify the ingoing and the outgoing components:

$$\begin{aligned} (\mathrm{e}^{ikz})_{\text{ingoing}} &= \sum_{\ell m} A_{\ell m} Y^{\ell m}(\theta,\varphi) R^{\ell m-}(r) \\ (\mathrm{e}^{ikz})_{\text{outgoing}} &= -\sum_{\ell m} B_{\ell m} Y^{\ell m}(\theta,\varphi) R^{\ell m+}(r) \end{aligned} \tag{1155}$$

where

$$B_{\ell m} \;=\; A_{\ell m} \;=\; \delta_{m,0}\, \sqrt{(2l+1)\pi}\, (i)^{\ell+1}\, \frac{\sqrt{v_E}}{k_E} \tag{1156}$$

This means that the incident flux in channel $(\ell, 0)$ is simply

$$i_{\text{incident}} = \left[\frac{\pi}{k_E^2}(2\ell+1)\right] v_E \tag{1157}$$

The expression in the square brackets has units of area, and has the meaning of cross section. The actual across section would contain an additional factor that express how much of the incident wave is being scattered.

[42.3] The scattered wave, phase shifts, cross section

In the past we were looking for a solution which consists of incident planar wave plus scattered component. Namely,

$$\Psi(r) = \mathrm{e}^{ik_0 z} + f(\Omega)\frac{\mathrm{e}^{ik_E r}}{r} \tag{1158}$$

From the decomposition of the incident plane wave it is implied that the requested solution is

$$\begin{aligned} \Psi_{\text{ingoing}} &= \sum_{\ell m} A_{\ell m} Y^{\ell m}(\theta,\varphi) R^{\ell m -}(r) \\ \Psi_{\text{outgoing}} &= -\sum_{\ell m} B_{\ell m} Y^{\ell m}(\theta,\varphi) R^{\ell m +}(r) \end{aligned} \tag{1159}$$

where

$$\begin{aligned} A_{\ell m} &= \delta_{m,0}\ \sqrt{(2l+1)\pi}\ (i)^{\ell+1}\ \frac{\sqrt{v_E}}{k_E} \\ B_{\ell m} &= S_{\ell m,\ell' m'}\ A_{\ell' m'} \end{aligned} \tag{1160}$$

If we are interested in the scattered wave then we have to subtract from the outgoing wave the incident component. This means that in the expression above we should replace $S_{\ell m,\ell' m'}$ by $-iT_{\ell m,\ell' m'}$.

Of major interest is the case where the target has spherical symmetry. In such case the S matrix is diagonal:

$$\begin{aligned} S_{\ell m,\ell' m'}(E) &= \delta_{\ell\ell'}\delta_{mm'}\,\mathrm{e}^{2i\delta_\ell} \\ T_{\ell m,\ell' m'}(E) &= -\delta_{\ell\ell'}\delta_{mm'}\,\mathrm{e}^{i\delta_\ell}\,2\sin(\delta_\ell) \end{aligned} \tag{1161}$$

Consequently we get

$$\Psi_{\text{scattered}} \;=\; -\sum_{\ell m} T_{\ell\ell}\,\sqrt{(2\ell+1)\pi}\,(i)^\ell\,Y_{\ell 0}(\theta,\varphi) h^+_\ell(r) \;\sim\; f(\Omega)\frac{\mathrm{e}^{ikr}}{r} \tag{1162}$$

with

$$f(\Omega) = -\frac{1}{k_E}\sum_{\ell m}\sqrt{(2\ell+1)\pi}\,T_{\ell\ell}\,Y_{\ell 0}(\theta,\varphi) \tag{1163}$$

It follows that

$$\sigma_{\text{total}} \;=\; \int |f(\Omega)|^2 d\Omega \;=\; \frac{\pi}{k_E^2}\sum_\ell (2\ell+1)|T_{\ell\ell}|^2 \;=\; \frac{4\pi}{k_E^2}\sum_\ell (2\ell+1)|\sin(\delta_\ell)|^2 \tag{1164}$$

By inspection we see that this corresponds to the sum over the scattered flux in each of the $(\ell, m{=}0)$ channels:

$$i_\ell \;=\; |T_{\ell\ell}|^2 \times \left[\frac{\pi}{k_E^2}(2\ell+1)\right] v_E \;\equiv\; \sigma_\ell v_E \tag{1165}$$

It is also important to realize that the scattered flux i_ℓ can be as large as 4 times the corresponding incident flux. The maximum is attained if the scattering induces a $\pi/2$ phase shift which inverts the sign of the incident wave. In such case the scattered wave should be twice the incident wave with an opposite sign.

======= [42.4] The Born approximation for the phase shift

We can get expressions for $T_{\ell\ell}$ using the the Born expansion, and hence to get approximations for the phase shift δ_ℓ and for the partial cross section σ_ℓ.

$$T_{\ell\ell} \;=\; -\mathrm{e}^{i\delta_\ell} 2\sin(\delta_\ell) \;=\; V_{\ell\ell} + (VGV)_{\ell\ell} \tag{1166}$$

Let us consider two particular cases:

- First order non-resonant scattering by a weak potential V
- Resonant scattering which is dominated by a single pole of G

In the case of scattering by a weak potential we use the leading order Born approximation for the T matrix:

$$T_{\ell\ell} \;\approx\; V_{\ell\ell} \;=\; \langle \phi^{E\ell m} | V | \phi^{E\ell m} \rangle \tag{1167}$$

We recall that the flux normalized free waves are

$$|\phi^{E\ell m}\rangle = -i\frac{k_E}{\sqrt{v_E}} 2 j_\ell(k_E r) Y^{\ell m}(\theta,\varphi) \tag{1168}$$

The assumption of weak scattering implies that $\delta_\ell \ll 1$, leading to the first order Born approximation for the phase shift:

$$\delta_\ell^{\text{Born}} \approx -\frac{2}{\hbar v_E}\int_0^\infty V(r)\left(k_E r j_l(k_E r)\right)^2 dr \tag{1169}$$

where $v_E = \sqrt{2E/\mathsf{m}}$. This formula is similar to the WKB phase shift formula which we discuss in the next section. We note that we have manged above to avoid the standard lengthy derivation of this formula, which is based on the Wronskian theorem (Messiah p.404).

The analysis of resonant scattering is greatly simplified if we assume that the the cross section is dominate by a single pole of the resolvent:

$$T_{\ell\ell} \;\approx\; (VGV)_{\ell\ell} \;=\; \frac{|\langle r|V|\phi^{E\ell m}\rangle|^2}{E - E_r + i(\Gamma_r/2)} \tag{1170}$$

From the optical theorem $2\mathrm{Im}[T_{\ell\ell}] = -|T_{\ell\ell}|^2$ we can deduce that the numerator must be equal $Gamma_r/2$. Thus we can write this relations as

$$-\,\mathrm{e}^{i\delta_\ell} 2\sin(\delta_\ell) = \frac{(\Gamma_r/2)}{E - E_r + i(\Gamma_r/2)} \tag{1171}$$

The left hand side is "exact" and therefore satisfies automatically the optical theorem. If the optical theorem were not satisfied by the approximation in the right hand side, this equation would not have a real solution for the phase shift. We can re-write the above equation as

$$\tan(\delta_\ell) = -\frac{\Gamma_r/2}{E - E_r} \tag{1172}$$

[42.5] Digression: WKB approximation

The WKB (Wentzel, Kramers, Brillouin) approximation [**Messiah p.231**] is designed mainly to treat slowly varying potentials in 1D where the wavefunction looks locally like a plane wave (if $V(x) < E$) or as a decaying exponential (in regions where $V(x) > E$). A more refined version of WKB, called "uniform approximation" allows also to do the matching at the turning points (where $V(x) \sim E$). The generalization of the $d = 1$ WKB to $d > 1$ dimensions integrable systems is known as the EBK scheme. There is also a different type of generalization of WKB to $d > 1$ chaotic systems.

Assuming free wave propagation, hence neglecting back reflection, the WKB wavefunction is written as

$$\Psi(x) = \sqrt{\rho(x)}\mathrm{e}^{iS(x)} \tag{1173}$$

This expression is inserted into the 1D Schrödinger equation. In leading order in $\hbar$ we get a continuity equation for the probability density $\rho(x)$, while the local wavenumber should be as expected

$$\frac{dS(x)}{dx} = p(x) = \sqrt{2\mathsf{m}(E - V(x))} \tag{1174}$$

Hence (for a right moving wave) one obtains the WKB approximation

$$\psi(x) = \frac{1}{\sqrt{p(x)}}\mathrm{e}^{i\int^x p(x')dx'} \tag{1175}$$

In contrast to this in a "forbidden" region we have a decaying exponential (say to the right)

$$\psi(x) \sim \mathrm{e}^{-\int^x \alpha(x')dx'} \tag{1176}$$

where $\alpha(x) = (2\mathsf{m}(V(x) - E))^{1/2}$. If we have a particle in a well, then we have on both sides WKB decaying exponentials, while in the middle we have WKB standing wave. As mentioned above the WKB scheme can be extended so as to provide matching conditions at the two turning points. Both matching conditions can be satisfied simultaneously if the "Born Oppenheimer quantization condition" is satisfied:

$$\oint p(x)dx = (\frac{1}{2} + n)2\pi\hbar \tag{1177}$$

where $n = 0, 1, 2, \ldots$ is an integer. The integral is taken along the energy contour which is formed by the curves $p = \pm p(x)$. We note that the $d > 1$ generalization of this idea is the statement that the number of states up to energy E is equal to the phase space volume divided by $(2\pi\hbar)^d$. The latter statement is known as Weyl law, and best derived using the Wigner-Weyl formalism.

Finally we consider the 1D scattering problem in case of a "soft" barrier. As we already said, there is no back-reflection in the WKB approximation. But we can still calculate the phase shift for the forward scattering:

$$\begin{aligned} 2\delta^{\mathrm{WKB}} &= \int_{-\infty}^{\infty} p(x)dx - \int_{-\infty}^{\infty} p_E dx = \int_{-\infty}^{\infty} \left[\sqrt{2\mathsf{m}(E - V(x))} - \sqrt{2\mathsf{m}E}\right] dx \\ &= \sqrt{2\mathsf{m}E}\int_{-\infty}^{\infty} \left[\sqrt{1 - \frac{V(x)}{E}} - 1\right] dx \;\approx\; -\sqrt{\frac{\mathsf{m}}{2E}}\int_{-\infty}^{\infty} V(x)dx \end{aligned} \tag{1178}$$

Hence we get

$$\delta_{1D}^{\mathrm{WKB}} = -\frac{1}{2}\frac{1}{\hbar v_E}\int_{-\infty}^{\infty} V(x)dx \tag{1179}$$

It should be emphasized that $\delta_{1D}^{\rm WKB}$ is the phase shift in a 1D scattering geometry ($-\infty < x < \infty$), while $\delta_{\ell=0}^{\rm Born}$ can be regarded as a formula for the phase shift in a semi-1D geometry ($r > 0$).

[42.6] The cross section at resonances

We have found that a practical expression for the phase shift in the vicinity of a resonance is

$$\delta_\ell = \delta_\ell^\infty - \arctan\left(\frac{\Gamma_r/2}{E-E_r}\right) \tag{1180}$$

For sake of generality we have incorporated into this expression a slowly varying "background" phase that we call δ_ℓ^∞. There are two physical quantities which are of special interest and can be deduced from the phase shift. One is the time delay that we shall discuss in the next section, and the other is the cross section:

$$\sigma_\ell(E) = (2\ell+1)\frac{4\pi}{k_E^2}|\sin(\delta_\ell)|^2 \tag{1181}$$

As a function of energy the "line shape" of the cross section versus energy plot is typically Breit-Wigner and more generally of Fano type. The former is obtained if we neglect δ_ℓ^∞, leading to

$$\sigma_\ell = (2\ell+1)\frac{4\pi}{k_E^2}\frac{(\Gamma_r/2)^2}{(E-E_r)^2+(\Gamma_r/2)^2} \tag{1182}$$

We see that due to a resonance the partial cross section σ_ℓ can attain its maximum value (the so called "unitary limit"). If we take δ_ℓ^∞ into account we get a more general result which is known as Fano line shape:

$$\sigma_\ell = (2\ell+1)\frac{4\pi}{k_E^2}[\sin(\delta_\ell^\infty)]^2\frac{[\varepsilon+q]^2}{\varepsilon^2+1} \tag{1183}$$

where $\varepsilon = (E-E_r)/(\Gamma/2)$ is the scaled energy, and $q = -\cot(\delta_\ell^\infty)$ is the so called Fano asymmetry parameter. The Breit-Wigner peak is obtained in the limit $q \to \infty$, while a Breit-Wigner dip (also known as anti-resonance) is obtained for $q = 0$.

[42.7] The Wigner time delay

We turn now to discuss the so called Wigner time delay, which is defined as

$$\tau_\ell(E) = \hbar\frac{d\theta_\ell}{dE} \qquad [\text{where } \theta_\ell = 2\delta_\ell] \tag{1184}$$

Consider for example the time delay in the case of a scattering on a "hard" sphere of radius a. We shall see that in such case we have a smooth energy dependence $\delta_0 \sim -ka$ and consequently we get $\tau_0 \sim -2a/v_E$. On the other hand we shall consider the case of a scattering on a shielded well. If the energy is off resonance we would get the same result $\tau_0 \sim -2a/v_E$. But E is in the vicinity of a resonance, then we can get very large (positive) time delay $\tau_0 \sim \hbar/\Gamma_r$ which reflects "trapping". This time delay would be associated with an abrupt variation of the cross section as discussed in the previous section.

Let us explain further the reasoning that leads to the definition of the Wigner time delay. For this purpose we consider the propagation of a Gaussian wavepacket in one dimension:

$$\Psi(x) = \int dk\ \mathrm{e}^{-\sigma^2(k-k_0)^2}\exp\left[i\left(k(x-x_0)+\theta-Et\right)\right] \tag{1185}$$

where both θ and E are functions of k. In order to determine the position $\bar{x}$ of the wavepaket we use the stationary phase approximation. Disregarding the Gaussian envelope most of contribution to the dk integral comes from the k region where the phase is stationary. This leads to

$$x - x_0 + \frac{d\theta}{dk} - \frac{dE}{dk}t = 0 \tag{1186}$$

The position $\bar{x}$ of the wavepacket is determined by the requirement that the above equation should have a solution for $k \sim k_0$. Thus we get

$$\bar{x} = x_0 + v_{\text{group}} \times (t - \tau_{\text{delay}}) \tag{1187}$$

where $v_{\text{group}} = (dE/dk)$ is the group velocity for $k = k_0$ and τ_{delay} is the Wigner time delay as defined above.

How this is related to a scattering problem? Consider for example scattering on one dimensions where we have "left" and "right" channels. Assume that the wavepacket at $t = 0$ is an undistorted Gaussian with $\theta = 0$. The initial wavepacket is centered on the "left" around $\bar{x} = x_0$ with momentum $\bar{k} = k_0$. We would like to know how $\bar{x}$ evolves with time before and after the scattering. Say that we observe the transmitted part of the wavepacket that emerges in the "right" channel. Following the above analysis we conclude that the effect of introducing $\theta \neq 0$ is the Wigner time delay.

======= [42.8] Scattering by a spherical target

If the scattering potential $V(r)$ depends only on the distance from the origin we can perform separation of variables. The equation for the radial function $u(r) = rR(r)$ reduces to a one dimensional Schrödinger equation on the $0 < r < \infty$ axis. To avoid divergence in $R(r)$ we have to use the boundary condition $u(0) = 0$, as if there is an infinite wall at $r = 0$.

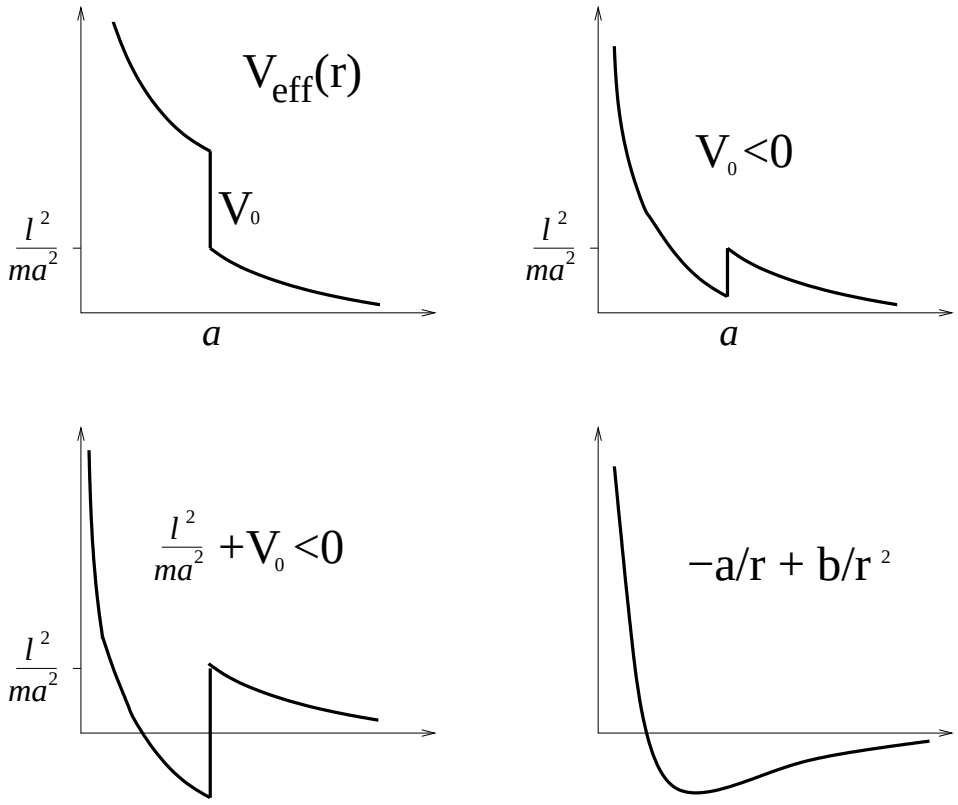
Most textbooks focus on the Coulomb interaction $V(r, \theta, \varphi) = -a/r$ for which the effective radial potential is $V_{\text{eff}}(r) = -a/r + b/r^2$. This is an extremely exceptional potential because of the following:

- There is no centrifugal barrier.
- Therefore there are no resonances with the continuum.
- It has an infinite rather than a finite number of bound states.
- The frequencies of the radial and the angular motions are degenerate.
- Hence there is no precession of the Kepler ellipse.

We are going to consider as an example scattering on a spherical target which we call either "sphere" or "well". The parameters that characterize the sphere are its radius a, the height of the potential floor V_0, and optionally the "thickness" the shielding U_0. Namely,

$$V(r, \theta, \varphi) \quad = \quad V_0\Theta(a - r) + U_0\delta(r - a) \tag{1188}$$

Disregarding the shielding the effective radial potential is $V_{\text{eff}}(r) = V_0\Theta(a - r) + b/r^2$. We consider first hard sphere ($V_0 = \infty$) and later on the scattering on a spherical well ($V_0 < 0$). The effective potential for 3 representative values of V_0 is illustrated in panels (a)-(b)-(c) of the following figure. In panels (d) we illustrate, for sake of comparison, the effective potential in case of a Coulomb interaction.



Classically it is clear that if the "impact parameter" of a particle is larger than the radius a of the scattering region then there is no scattering at all. A better phrasing which can be adopted into the quantum mechanical framework is in terms of angular momentum. Namely, there is non-negligible scattering only within the channels that satisfy

$$\frac{\ell^2}{2\mathsf{m}a^2} < E \tag{1189}$$

The statement above assumes that the "forbidden" region is unaccessible to the particle, hence it excludes the possibility of tunneling and resonances that we shall discuss later on. Whenever we neglect the latter possibilities, the scattering state is simply a free wave which is described by the spherical Bessel function $j_\ell(k_E r)$. For $k_E r \ll \ell$ this spherical Bessel function is exponentially small due to the centrifugal barrier, and therefore it is hardly affected by the presence of the sphere.

[42.9] Scattering by a soft sphere

Assuming that we have a soft sphere ($|V_0|$ is small), we would like to evaluate the phase shift using the Born approximation. Evidently the result makes sense only if the phase shift comes out small ($\delta_\ell \ll 1$). There are two limiting cases. If $ka \ll \ell$ we can use the short range approximation of the spherical Bessel function to obtain

$$\delta_\ell^{\text{Born}} \approx -\frac{2}{(2\ell+3)\left[(2l+1)!!\right]^2}\frac{\mathsf{m}V}{\hbar^2}a^2(ka)^{2\ell+1} \tag{1190}$$

On the other hand, if $ka \ll \ell$ we can use the "far field" asymptotic approximation of the spherical Bessel function which implies $[krj_\ell(kr)]^2 \approx [\sin(kr)]^2 \approx 1/2$. Then we obtain

$$\delta_\ell^{\text{Born}} \;\approx\; -\frac{1}{\hbar v_E}Va \;=\; -\frac{\mathsf{m}V}{\hbar^2}a^2(ka)^{-1} \tag{1191}$$

[42.10] Finding the phase shift by matching

In this section we would like to outline a procedure for finding exact results for the phase shifts. This would allow us to consider in the next sections scattering by "hard" spheres as well as by "deep" wells. We fist consider the the scattering in the $\ell = 0$ channel, and later generalize to any ℓ.

Considering $\ell = 0$ we first have to find the regular solution $u(r)$ of the Schrodinger equation in the region $r < a$. Then we can calculate the logarithmic derivative at the boundary $r = a$ of the scattering region:

$$\tilde{k}_0 = \left(\frac{1}{u(r)}\frac{du(r)}{dr}\right)_{r=a} \tag{1192}$$

For example if we have a high potential floor such that $E < V_0$, then the interior solution is $\psi(r) = A\sinh(\alpha r)$ leading to $\tilde{k}_0 = \alpha\coth(\alpha a)$ which for very large α becomes simply $\tilde{k}_0 = \alpha$. Once we know $\tilde{k}_0$ we can do the matching with the outside scattering solution

$$\psi(r) = A\mathrm{e}^{-ik_E r} - B\mathrm{e}^{ik_E r} = A(\mathrm{e}^{-ik_E r} - \mathrm{e}^{i2\delta_0}\mathrm{e}^{ik_E r}) = C\sin(k_E r + \delta_0) \tag{1193}$$

where δ_0 is the phase shift. The matching gives the equation

$$k_E\cot(k_E a + \delta_0) = \tilde{k}_0 \tag{1194}$$

which leads to the result

$$\delta_0 = -k_E a + \arctan(\frac{k_E}{\tilde{k}_0}) \tag{1195}$$

In the limit of $V_0 \to \infty$ we have

$$\tilde{k}_0 \approx \alpha = \sqrt{2\mathsf{m}(V_0 - E)} \to \infty \tag{1196}$$

leading to the expected solution $\delta = -ka$, which is implied by Dirichlet boundary conditions at $x = a$.

Now we generalize the scheme to any ℓ. First we have to solve the radial function for $0 < r < a$ and define the logarithmic derivative

$$k_\ell = \left(\frac{1}{R(r)}\frac{dR(r)}{dr}\right)_{r=a} \tag{1197}$$

Note that we use here $R(r)$ and not $u(r)$ and therefore in the $\ell = 0$ case we get $k_0 = \tilde{k}_0 - (1/a)$. The solution in the outside region is

$$\begin{aligned} R(r) &= Ah_\ell^-(k_E r) - Bh_\ell^+(k_E r) \\ &= A(h_\ell^-(k_E r) - \mathrm{e}^{i2\delta_\ell}h_\ell^+(k_E r)) \\ &= C(\cos(\delta_\ell)j_\ell(k_E r) + \sin(\delta_\ell)n_\ell(k_E r)) \end{aligned} \tag{1198}$$

We do not care about the normalization because the matching equation involves only logarithmic derivatives:

$$k_E\frac{\cos(\delta)j' + \sin(\delta)n'}{\cos(\delta)j + \sin(\delta)n} = k_\ell \tag{1199}$$

solving this equation for $\tan(\delta_\ell)$ we get

$$\tan(\delta_\ell) = -\frac{k_\ell j_\ell(ka) - k_E j'_\ell(ka)}{k_\ell n_\ell(ka) - k_E n'_\ell(ka)} \tag{1200}$$

which can also be written as:

$$\mathrm{e}^{i2\delta_\ell} = \left(\frac{h_\ell^-}{h_\ell^+}\right) \frac{k_\ell - (h_\ell'^-/h_\ell^-)k_E}{k_\ell - (h_\ell'^+/h_\ell^+)k_E} \tag{1201}$$

These are the general expressions for the phase shift.

======== [42.11] Scattering by a hard sphere

The phase shifts for a hard sphere ($V \to \infty$) can be found from the phase shift formula of the previous section using $k_\ell \to \infty$, leading to

$$\mathrm{e}^{i2\delta_\ell^\infty} = \frac{h^-(k_E a)}{h^+(k_E a)} \tag{1202}$$

or equivalently

$$\tan(\delta_\ell^\infty) = -\frac{j_\ell(k_E a)}{n_\ell(k_E a)} \tag{1203}$$

From the first version it is convenient to derive the result

$$\delta_\ell^\infty = -\arg(h^+(k_E a)) \approx -(k_E a - \frac{\pi}{2}\ell) \qquad \text{for } \ell \ll ka \tag{1204}$$

where we have used the asymptotic expression $h(r) \sim (-\imath)^\ell \ \mathrm{e}^{ik_E r}/r$.

From the second version it is convenient to derive the result

$$\delta_\ell^\infty \approx -\frac{1}{(2\ell+1)!!(2\ell-1)!!}(k_E a)^{2\ell+1} \qquad \text{for } \ell \gg ka \tag{1205}$$

where we have used the short range expansions $j_\ell \propto r^\ell$ and $n_\ell \propto 1/r^{\ell+1}$.

In the case of a small sphere ($k_E a \ll 1$) we have $1 \gg \delta_0 \gg \delta_1 \gg \delta_2 \ldots$ and the $\ell = 0$ cross section is dominant

$$\delta_0 = -(k_E a) \tag{1206}$$

Hence

$$\sigma_{\text{total}} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\delta_\ell) \approx \frac{4\pi}{k^2} \sin^2(\delta_0) \approx 4\pi a^2 \tag{1207}$$

We got a σ that is 4 times bigger than the classical one. The scattering is isotropic because only the $\ell = 0$ component contributes to the scattered wave.

Now we turn to the case of a large sphere ($k_E a \gg 1$). We neglect all δ_ℓ for which $\ell > k_E a$. For the non-vanishing phase shifts we get

$$\begin{aligned} \delta_\ell &= \quad -(k_E a) \qquad \text{for } \ell = 0, 2, 4, \ldots \\ \delta_\ell &= -(k_E a) + \tfrac{\pi}{2} \qquad \text{for } \ell = 1, 3, 5, \ldots \end{aligned} \tag{1208}$$

hence

$$\begin{aligned} \sigma_{total} &= \frac{4\pi}{k^2}\left(\sum_{\ell=0,2\ldots ka}(2l+1)\sin^2(k_E a) + \sum_{\ell=1,3\ldots ka}(2l+1)\cos^2(k_E a)\right) \\ &\approx \frac{4\pi}{k^2}\sum_{\ell=0,1\ldots ka}^{\ell=ka}(2l+1)\frac{1}{2} \approx \frac{2\pi}{k^2}\int_0^{ka} 2x dx = \frac{2\pi}{k^2}(k_E a)^2 = 2\pi a^2 \end{aligned} \tag{1209}$$

This time the result is 2 times the classical result. The factor of 2 is due to forward scattering which partially cancels the incident wave so as to create a shadow region behind the sphere.

[42.12] Scattering by an attractive well

So far we have discussed "soft" sphere and "hard sphere". In order to discuss the problem in its full generality we have to find the dependence of $\tilde{k}_\ell$ on the potential floor V_0 and on the optional shielding thickness U_0. In order to get insight let us consider the $\ell = 0$ case.

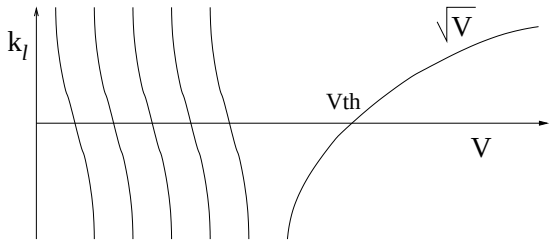
The $\ell = 0$ wavefunction inside a sphere if $V_0 > E$ is $u(r < a) = \sinh(\alpha_{in} r)$ where $\alpha_{in} = \sqrt{2\mathsf{m}(V_0 - E)}$. This leads to

$$\tilde{k}_0 = \alpha_{in}\coth(\alpha_{in} a) \approx \alpha_{in} \tag{1210}$$

where the approximation holds for large V_0. Hence $\tilde{k}_0$ goes to infinity for $V \to \infty$. This means that in this limit the wavefunction should satisfy Dirichlet (zero) boundary conditions on the boundary of the sphere. If $V_0 < E$ the $\ell = 0$ wavefunction is $u(r < a) = \sin(k_{in} r)$ with $k_{in} = \sqrt{2\mathsf{m}(E - V_0)}$. This leads to

$$\tilde{k}_0 = k_{in}\cot(k_{in} a) \tag{1211}$$

The dependence of $\tilde{k}_0$ on V_0 is demonstrated in the following figure. The threshold V_{th} distinguishes between the case of having real α_{in} as opposed to real k_{in}.



Similar plot would be obtained for any ℓ. We note that the effect of shielding is simply to shift the whole plot upwards. Namely

$$k_\ell \quad \mapsto \quad k_\ell + (2\mathsf{m}/\hbar^2)U_0 \tag{1212}$$

In the case of an attractive well ($V_0 < 0$) the log-derivative k_ℓ goes to infinity within strips that we call "off resonance" regions. Within these "off resonance" regions an attractive well is similar to a hard sphere. In the next section we

focus on resonant scattering. In particular we are going to define the "width" of the resonance regions. We shall see that the shielding can help us to make the width of the the resonance regions smaller. This would allow us to further discuss the case of well separated resonances.

[42.13] Scattering resonances of a shielded well

In what follows we fix the energy E of the scattered particle, and discuss the behavior of the phase shift and the cross section as a function of V_0, which from now on we denote simply as V. In physical applications V can be interpreted as some "gate voltage". Note that in most textbooks it is customary to fix V and to change E. Within the approximation that we are going to do this is equivalent. The phase shift is found from

$$e^{i2\delta_\ell} = \left(\frac{h_\ell^-}{h_\ell^+}\right) \frac{k_\ell(V) - (h_\ell'^-/h_\ell^-)k}{k_\ell(V) - (h_\ell'^+/h_\ell^+)k} \tag{1213}$$

Following Messiah p.391 and using the notation

$$k\left(\frac{h_\ell'^+}{h_\ell^+}\right)_{r=a} \equiv \epsilon + i\gamma \tag{1214}$$

we can write it in a simpler form as

$$e^{i2\delta_\ell} = \left(e^{i2\delta_\ell^\infty}\right) \frac{k_\ell(V) - \epsilon + i\gamma}{k_\ell(V) - \epsilon - i\gamma} \tag{1215}$$

or equivalently as

$$\tan\left(\delta_\ell - \delta_\ell^\infty\right) = \frac{\gamma}{k_\ell(V) - \epsilon} \tag{1216}$$

We can plot the right hand side as a function of V. For $V \gg V_{th}$ we have $\delta_\ell \approx \delta_\ell^\infty$ because the right hand side of the equation becomes very small. On the other hand for $V < V_{th}$ we can distinguish between on-resonance and off-resonance regions. The off-resonance regions are those where the right hand side is very small and hence $\delta_\ell \approx \delta_\ell^\infty$ as for a hard sphere. The on-resonance regions are those where the right hand side is large, and we get a big deviation from the hard sphere result.

For the sake of practical analysis let us define the on-resonance regions using the inequality

$$|k_\ell(V) - \epsilon| < \gamma \tag{1217}$$

Let us define the center of a resonance $V = V_r$ by the equation $k_\ell(V) = \epsilon$. Also let us define the "velocity"

$$v_r = \left|\frac{dk_\ell}{dV}\right|^{-1} \tag{1218}$$

Then upon linearization we can rewrite the definition of the on-resonance region as $|V - V_r| < v_r\gamma$, or we can write

$$|V - V_r| < (\Gamma_r/2) \tag{1219}$$

where the width of the resonance is defined here as $\Gamma = (2\gamma)v_r$. It is clear that the distance between the locations V_r of the resonances is simply the distance between the metastable states of the well. Let us call this level spacing Δ_0. The condition for having a narrow resonance is $\Gamma_r < \Delta_0$. By inspection of the plot it should be clear that shielding (large U_0) shifts E_r such that v_r and hence Γ_r become smaller.

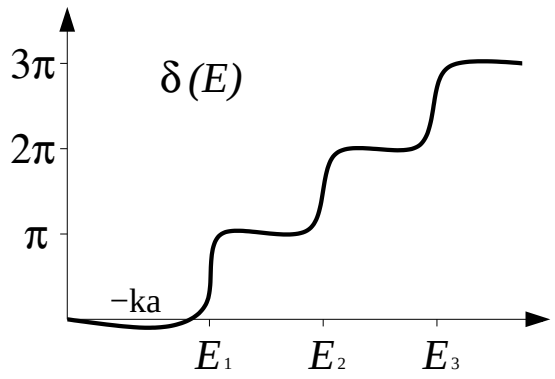
Assuming that the resonances are narrow, and using the above notations, we find that in the vicinity of a resonance the phase shift is given by the expression

$$\delta_\ell = \delta_\ell^\infty + \arctan\left(\frac{\Gamma_r/2}{V - V_r}\right) \tag{1220}$$

We note again that in most textbooks V is fixed and E is varied. Switching to the conventional notation we re-write the above as

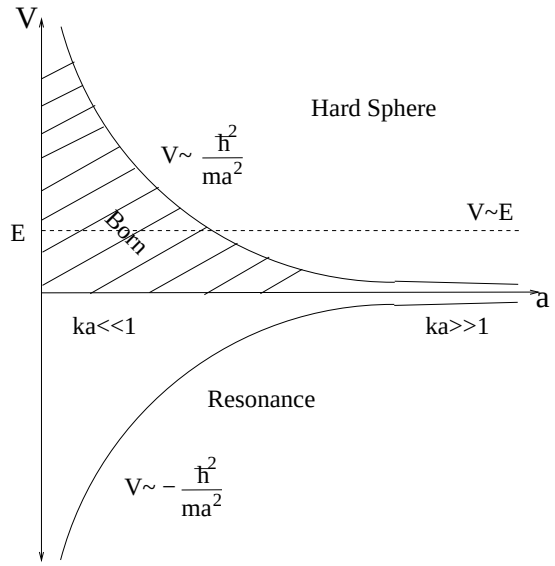
$$\delta_\ell = \delta_\ell^\infty - \arctan\left(\frac{\Gamma_r/2}{E - E_r}\right) \tag{1221}$$

An example for the behavior of $\delta_\ell(E)$ as a function of E in case of an attractive well is illustrated in the figure below. In order to ensure narrow resonance one should assume that the well is shielded by a large barrier. At low energies the s-scattering phase shift is $\delta_0(E) = -k_E a$. As the energy is raised there is an extra π shift each time that E goes through a resonance. The phase shift is defined modulo π, but in the figure it is convenient not to take the modulo so as to have a continuous plot.



[42.14] Summary of results for scattering on a sphere

We have discussed scattering on a "hard sphere", on a "deep well", and finally on a "soft sphere". Now we would like to put everything together and to draw an (a, V) diagram of all the different regimes.



Let us discuss the various regimes in this diagram. It is natural to begin with a small sphere. A small sphere means that the radius is small compared with the De-Broglie wavelength ($ka < 1$). This means that disregarding resonances the cross section is dominated by s-scattering ($\ell = 0$). On the one hand we have the Born approximation and on the other hand the hard sphere result:

$$\begin{aligned} \delta_0^{\rm Born} &\approx -\frac{2}{3}\left[\frac{\mathsf{m}V}{\hbar^2}a^2\right](ka) \\ \delta_0^{\rm Hard} &\approx -(ka) \end{aligned} \tag{1222}$$

Thus we see that the crossover from "soft" to "hard" happens at $V \sim \hbar^2/(\mathsf{m}a^2)$. What about $V < 0$? It is clear that the Born approximation cannot be valid once we encounter a resonance (at a resonance the phase shift becomes large). So we are safe as long as the well is not deep enough to contain a quasi bound state. This leads to the sufficient condition $-\hbar^2/(\mathsf{m}a^2) < V < 0$. For more negative V values we have resonances on top of a "hard sphere" behavior. Thus we conclude that for $ka < 1$ soft sphere means

$$|V| < \frac{\hbar^2}{\mathsf{m}a^2} \tag{1223}$$

We now consider the case of a large sphere ($ka \gg 1$). In the absence of resonances we have for small impact parameter ($\ell \ll ka$) either the Born or the hard sphere approximations:

$$\begin{aligned} \delta_\ell^{\rm Born} &\approx -\frac{V}{\hbar v_E}a \\ \delta_\ell^{\rm Hard} &= \mathcal{O}(1) \end{aligned} \tag{1224}$$

Also here we have to distinguish between two regimes. Namely, for $ka \gg 1$ soft sphere means

$$|V| < \frac{\hbar v_E}{a} \tag{1225}$$

If this condition breaks down we expect to have a crossover to the Hard sphere result. However, one should be aware that if $V < E$, then one cannot trust the hard sphere approximation for the low ℓ scattering.

Special Topics

[43] Quantization of the EM Field

[43.1] The Classical Equations of Motion

The equations of motion for a system which is composed of non-relativistic classical particles and EM fields are:

$$\begin{aligned} \mathsf{m}\frac{d^2\mathbf{x}_i}{dt^2} &= e\mathcal{E} - e\mathcal{B}\times\dot{\mathbf{x}}_i \\ \nabla\cdot\mathcal{E} &= 4\pi\rho \\ \nabla\times\mathcal{E} &= -\frac{\partial\mathcal{B}}{\partial t} \\ \nabla\cdot\mathcal{B} &= 0 \\ \nabla\times\mathcal{B} &= \frac{\partial\mathcal{E}}{\partial t} + 4\pi\vec{J} \end{aligned} \tag{1226}$$

where

$$\begin{aligned} \rho(x) &= e\sum_i \delta(x-\mathbf{x}_i) \\ J(x) &= e\sum_i \dot{\mathbf{x}}_i\delta(x-\mathbf{x}_i) \end{aligned} \tag{1227}$$

We also note that there is a continuity equation which is implied by the above definition and also can be regarded as a consistency requirement for the Maxwell equation:

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot J \tag{1228}$$

It is of course simpler to derive the EM field from a potential (V, A) as follows:

$$\begin{aligned} \mathcal{B} &= \nabla\times A \\ \mathcal{E} &= -\frac{\partial A}{\partial t} - \nabla V \end{aligned} \tag{1229}$$

Then we can write an equivalent system of equations of motion

$$\begin{aligned} \mathsf{m}\frac{d^2\mathbf{x}_i}{dt^2} &= e_i\mathcal{E} - e_i\mathcal{B}\times\dot{\mathbf{x}}_i \\ \frac{\partial^2 A}{\partial t^2} &= \nabla^2\vec{A} - \frac{\partial}{\partial t}\nabla V + 4\pi J \\ \nabla^2 V &= -4\pi\rho \end{aligned} \tag{1230}$$

[43.2] The Coulomb Gauge

In order to further simplify the equations we would like to use a convenient gauge which is called the "Coulomb gauge". To fix a gauge is essentially like choosing a reference for the energy. Once we fix the gauge in a given reference frame ("laboratory") the formalism is no longer manifestly Lorentz invariant. Still the treatment is exact.

Any vector field can be written as a sum of two components, one that has zero divergence and another that has zero curl. For the case of the electric field $\mathcal{E}$, the sum can be written as:

$$\mathcal{E} = \mathcal{E}_{\shortparallel} + \mathcal{E}_{\perp} \tag{1231}$$

where $\nabla \cdot \mathcal{E}_{\perp} = 0$ and $\nabla \times \mathcal{E}_{\shortparallel} = 0$. The field $\mathcal{E}_{\perp}$ is called the transverse or solenoidal or "radiation" component, while the field $\mathcal{E}_{\shortparallel}$ is the longitudinal or irrotational or "Coulomb" component. The same treatment can be done for the magnetic field $\mathcal{B}$ with the observation that from Maxwell's equations $\nabla \cdot \mathcal{B} = 0$ yields $\mathcal{B}_{\|} = 0$. That means that there is no magnetic charge and hence the magnetic field $\mathcal{B}$ is entirely transverse. So now we have

$$\text{EM field} = (\mathcal{E}_{\shortparallel}, \mathcal{E}_{\perp}, \mathcal{B}) = \text{Coulomb field} + \text{radiation field} \tag{1232}$$

Without loss of generality we can derive the radiation field from a transverse vector potential. Thus we have:

$$\begin{aligned} \mathcal{E}_{\shortparallel} &= -\nabla V \\ \mathcal{E}_{\perp} &= -\frac{\partial A}{\partial t} \\ \mathcal{B} &= \nabla \times A \end{aligned} \tag{1233}$$

This is called the Coulomb gauge, which we will use from now on. We can solve the Maxwell equation for V in this gauge, leading to the the potential

$$V(x) = \sum_j \frac{e_j}{|x - \mathbf{x}_j|} \tag{1234}$$

Now we can insert the solution into the equations of motion of the particles. The new system of equations is

$$\begin{aligned} \mathsf{m}\frac{d^2\mathbf{x}_i}{dt^2} &= \left[\sum_j \frac{e_i e_j \ \vec{n}_{ij}}{|\mathbf{x}_i - \mathbf{x}_j|^2}\right] + e_i\mathcal{E}_{\perp} - e_i\mathcal{B} \times \dot{\mathbf{x}}_i \\ \frac{\partial^2 A}{\partial t^2} &= \nabla^2 \vec{A} + 4\pi J_{\perp} \end{aligned} \tag{1235}$$

It looks as if $J_{\shortparallel}$ is missing in the last equation. In fact it can be easily shown that it cancells with the ∇V term due to the continuity equation that relates $\partial_t \rho$ to $\nabla \cdot J$, and hence $\partial_t \nabla V$ to $J_{\shortparallel}$ respectively.

═══ [43.3] Hamiltonian for the Particles

We already know from the course in classical mechanics that the Hamiltonian, from which the equations of motion of particles in EM field are derived, is

$$\mathcal{H} = \sum_i \left[\frac{1}{2\mathsf{m}_i}(\mathbf{p}_i - e_i A(\mathbf{x}_i))^2 + e_i V(\mathbf{x}_i)\right] \tag{1236}$$

This Hamiltonian assumes the presence of classical fields where A and V are the potentials from which the EM field is derived. Note that there is *no direct interaction* between the particles, in agreement with the theory of relativity. Using the Coulomb gauge we would like the Hamiltonian to give also the Coulomb term in the equations of motion. Thus,

$$\mathcal{H} = \sum_i \frac{1}{2\mathsf{m}_i}(\mathbf{p}_i - e_i A(\mathbf{x}_i))^2 + \frac{1}{2}\sum_{i,j} \frac{e_i e_j}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{1237}$$

It seems as if the *direct Coulomb interaction* between the paticles is in contradiction with relativity. In fact it is due to the non-invariant way that we separated the electric field into components. It is important to re-emphasize that our treatment is exact. As a whole the Hamiltonian that we will get (as far as the EM field is concerned) is going to be Lorentz invariant.

The factor 1/2 in the Coulomb interaction is there in order to compensate for the double counting of the interactions. What about the diagonal terms $i = j$? We can keep them if we want because they add just a finite constant term to the Hamiltonian. The "self interaction" infinite term can be regularized by assuming that each particle has a very small radius. To drop this constant from the Hamiltonian means that "infinite distance" between the particles is taken as the reference state for the energy. However, it is more convenient to keep this infinite constant in the Hamiltonian, because then we can write:

$$\mathcal{H} = \sum_i \frac{1}{2\mathsf{m}_i}(\mathbf{p}_i - e_i A(\mathbf{x}_i))^2 + \frac{1}{8\pi}\int E_{\shortparallel}^2 d^3x \tag{1238}$$

In order to get the latter expression we have used the following identity:

$$\int \frac{\rho(x)\rho(x')}{|x-x'|} d^3x d^3x' \quad = \quad \frac{1}{8\pi}\int E_{\shortparallel}^2 d^3x \tag{1239}$$

The derivation of this identity is based on Gauss law, integration by parts, and using the fact that the Laplacian of $1/|x-x'|$ is a delta function. Again we emphasize that the integral diverges unless we regularize the physical size of the particles, or else we have to subtract an infinite constant that represents the "self interaction".

[43.4] Hamiltonian for the Radiation Field

So now we need another term in the Hamiltonian from which the second equation of motion is derived

$$\frac{\partial^2 A}{\partial t^2} - \nabla^2 \vec{A} = 4\pi \vec{J}_{\perp} \tag{1240}$$

In order to decouple the above equations into "normal modes" we write $\vec{A}$ in a Fourier series:

$$\vec{A}(x) = \frac{1}{\sqrt{\text{volume}}}\sum_k \vec{A}_k \ \mathrm{e}^{ikx} = \frac{1}{\sqrt{\text{volume}}}\sum_{k,\alpha} A_{k,\alpha} \ \vec{\varepsilon}_{k,\alpha}\mathrm{e}^{ikx} \tag{1241}$$

where $\vec{\varepsilon}_{k,\alpha}$ for a given k is a set of two orthogonal unit vectors. If A were a general vector field rather than a transverse field, then we would have to include a third unit vector. Note that $\nabla \cdot A = 0$ is like $k \cdot \vec{A}_k = 0$. Now we can rewrite the equation of motion as

$$\ddot{A}_{k,\alpha} + \omega_k^2 A_{k,\alpha} = 4\pi J_{k,\alpha} \tag{1242}$$

where $\omega_k = |k|$. The disadvantage of this Fourier expansion is that it does not reflect that $A(x)$ is a real field. In fact the $A_{k,\alpha}$ should satisfy $A_{-k,\alpha} = (A_{k,\alpha})^*$. In order to have proper "normal mode" coordinates we have to replace each pair of complex $A_{k,\alpha}$ and $A_{-k,\alpha}$ by a pair of real coordinates $A'_{k,\alpha}$ and $A''_{-k,\alpha}$. Namely

$$A_{k,\alpha} = \frac{1}{\sqrt{2}}[A'_{k,\alpha} + iA''_{-k,\alpha}] \tag{1243}$$

We also use a similar decomposition for $J_{k,\alpha}$. We choose the $1/\sqrt{2}$ normalization so as to have the following identity:

$$\int J(x)\cdot A(x)\ dx \quad = \quad \sum_{k,\alpha} J^*_{k,\alpha}A_{k,\alpha} = \sum_{[k],\alpha}(J'_{k,\alpha}A'_{k,\alpha} + J''_{k,\alpha}A''_{k,\alpha}) \ = \ \sum_r J_r Q_r \tag{1244}$$

In the sum over degrees of freedom r we must remember to avoid double counting. The vectors k and $-k$ represent the same direction which we denote as $[k]$. The variable $A'_{-k,\alpha}$ is the same variable as $A'_{k,\alpha}$, and the variable $A''_{-k,\alpha}$ is the same variable as $-A''_{k,\alpha}$. We denote this set of coordinates Q_r, and the conjugate momenta as P_r. We see that each of the normal coordinates Q_r has a "mass" that equals $1/(4\pi)$ [CGS!!!]. Therefore the conjugate "momenta" are $P_r = [1/(4\pi)]\dot{Q}_r$, which up to a factor are just the Fourier components of the electric field. Now we can write the Hamiltonian as

$$\mathcal{H}_{rad} = \sum_r \left[\frac{1}{2 \cdot \text{mass}} P_r^2 + \frac{1}{2} \text{mass} \cdot \omega_r^2 \; Q_r^2 + J_r Q_r \right] \tag{1245}$$

where r is the sum over all the degrees of freedom: two independent modes for each direction and polarization. By straightforwrd algebra the sum can be written as

$$\mathcal{H}_{rad} = \frac{1}{8\pi} \int (\mathcal{E}_\perp^2 + \mathcal{B}^2) d^3x - \int \vec{J} \cdot A d^3x \tag{1246}$$

It is not difficult to see that the total Hamiltonian for the particle and the EM field can be written as

$$\mathcal{H} = \mathcal{H}_{\text{particles}} + \mathcal{H}_{\text{interaction}} + \mathcal{H}_{\text{radiation}} = \sum_i \frac{1}{2\mathsf{m}_i} (\mathbf{p}_i - e_i A(\mathbf{x}_i))^2 + \frac{1}{8\pi} \int (\mathcal{E}^2 + \mathcal{B}^2) d^3x \tag{1247}$$

This way of writing is somewhat misleading. First one should notice that we have combined the Coulomb potential term (which involves $\mathcal{E}_{||}^2$) with the "kinetic" term of the radiation field (which involves $\mathcal{E}_\perp^2$). Also notice that we should avoid double counting of the interation between the EM field and the particles. A term that corresponds to $\vec{J} \cdot A$ is already present in the first term of the Hamiltonian.

═══ [43.5] Quantization of the EM Field

Now that we know the "normal coordinates" of the EM field the quantization is trivial. For each "oscillator" of "mass" $1/(4\pi)$ we can define a and $a^\dagger$ operators such that $Q_r = (2\pi/\omega)^{1/2}(a_r + a_r^\dagger)$. Since we have two distinct variables for each direction, we use the notations $(b, b^\dagger)$ and $(c, c^\dagger)$ respectively:

$$Q_{1[k]\alpha} \;\; = A'_{k\alpha} = A'_{-k\alpha} \;\; = \sqrt{\frac{2\pi}{\omega_k}} \left(b_{[k]\alpha} + b^\dagger_{[k]\alpha} \right) \tag{1248}$$

$$Q_{2[k]\alpha} \;\; = A''_{k\alpha} = -A''_{-k\alpha} \;\; = \sqrt{\frac{2\pi}{\omega_k}} \left(c_{[k]\alpha} + c^\dagger_{[k]\alpha} \right) \tag{1249}$$

In order to make the final expressions look more elegant we use the following canonical transformation:

$$\begin{aligned} a_+ &= \frac{1}{\sqrt{2}}(b + ic) \\ a_- &= \frac{1}{\sqrt{2}}(b - ic) \end{aligned} \tag{1250}$$

It can be easily verified by calculating the commutators that the transformation from (b, c) to (a_+, a_-) is canonical. Also note that $b^\dagger b + b^\dagger b = a_+^\dagger a_+ + a_-^\dagger a_-$. Since the oscillators (normal modes) are uncoupled the total Hamiltonian is a simple sum over all the modes:

$$\mathcal{H} = \sum_{[k],\alpha} (\omega_k b^\dagger_{k,\alpha} b_{k,\alpha} + \omega_k c^\dagger_{k,\alpha} c_{k,\alpha}) = \sum_{k,\alpha} \omega_k a^\dagger_{k,\alpha} a_{k,\alpha} \tag{1251}$$

For completeness we also write the expression for the field operators:

$$A_{k,\alpha} = \frac{1}{\sqrt{2}}(A' + iA'') = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{2\pi}{\omega_k}}(b + b^\dagger) + i\sqrt{\frac{2\pi}{\omega_k}}(c + c^\dagger)\right] = \sqrt{\frac{2\pi}{\omega_k}}(a_{k,\alpha} + a^\dagger_{-k,\alpha}) \tag{1252}$$

The eigenstates of the EM field are

$$|n_1, n_2, n_3, \ldots, n_{k,\alpha}, \ldots\rangle \tag{1253}$$

We refer to the ground state as the vacuum state:

$$|\text{vacuum}\rangle = |0, 0, 0, 0, \ldots\rangle \tag{1254}$$

Next we define the one photon state as follows:

$$|\text{one photon state}\rangle = \hat{a}^\dagger_{k\alpha}\,|\text{vacuum}\rangle \tag{1255}$$

and we can also define two photon states (disregarding normalization):

$$|\text{two photon state}\rangle = \hat{a}^\dagger_{k_2\alpha_2}\hat{a}^\dagger_{k_1\alpha_1}\,|\text{vacuum}\rangle \tag{1256}$$

In particular we can have two photons in the same mode:

$$|\text{two photon state}\rangle = (\hat{a}^\dagger_{k_1\alpha_1})^2\,|\text{vacuum}\rangle \tag{1257}$$

and in general we can have N photon states or any superposition of such states.

An important application of the above formalism is for the calculation of spontaneous emission. Let us assume that the atom has an excited level E_B and a ground state E_A. The atom is prepared in the excited state, and the electromagnetic field is assume to be initially in a vacuum state. According to Fermi Golden Rule the system decays into final states with one photon $\omega_k = (E_B - E_A)$. Regarding the atom as a point-like object the interaction term is

$$\mathcal{H}_{\text{interaction}} \approx -\frac{e}{c}A(0)\cdot\hat{v} \tag{1258}$$

where $\hat{v} = \hat{p}/\mathsf{m}$ is the velocity operator. It is useful to realize that $\hat{v}_{AB} = i(E_B - E_A)\hat{x}_{AB}$. The vector $\vec{D} = \hat{x}_{AB}$ is known as the dipole matrix element. It follows that matrix element for the decay is

$$|\langle n_{k\alpha} = 1, A|\mathcal{H}_{\text{interaction}}|\text{vacuum}, B\rangle|^2 = \frac{1}{\text{volume}}\left(\frac{e}{c}\right)^2 2\pi\omega_k|\vec{\varepsilon}_{k,\alpha}\cdot D|^2 \tag{1259}$$

In order to calculate the decay rate we have to multiply this expression by the density of the final states, to integrate over all the possible directions of k, and to sum over the two possible polarizations α.

[44] Quantization of a Many Body System

[44.1] Second Quantization

If we regard the electromagnetic field as a collection of oscillators then we call $a^\dagger$ and a raising and lowering operators. This is "first quantization" language. But we can also call $a^\dagger$ and a creation and destruction operators. Then it is "second quantization" language. So for the electromagnetic field the distinction between "first quantization" and "second quantization" is merely a linguistic issue. Rather than talking about "exciting" an oscillator we talk about "occupying" a mode.

For particles the distinction between "first quantization" and "second quantization" is not merely a linguistic issue. The quantization of *one* particle is called "first quantization". If we treat several distinct particles (say a proton and an electron) using the same formalism then it is still "first quantization".

If we have many (identical) electrons then a problem arises. The Hamiltonian commutes with "transpositions" of particles, and therefore its eigenstates can be categorized by their symmetry under permutations. In particular there are two special subspaces: those of states that are symmetric for *any* transposition, and those that are antisymmetric for *any* transposition. It turns out that in nature there is a "super-selection" rule that allows only one of these two symmetries, depending on the type of particle. Accordingly we distinguish between Fermions and Bosons. All other sub-spaces are excluded as "non-physical".

We would like to argue that the "first quantization" approach, is simply the wrong language to describe a system of identical particles. We shall show that if we use the "correct" language, then the distinction between Fermions and Bosons comes out in a natural way. Moreover, there is no need for the super-selection rule!

The key observation is related to the definition of Hilbert space. If the particles are distinct it makes sense to ask "where is each particle". But if the particles are identical this question is meaningless. The correct question is "how many particles are in each site". The space of all possible occupations is called "Fock space". Using mathematical language we can say that in "first quantization", Hilbert space is the external product of "one-particle spaces". In contrast to that, Fock space is the external product of "one site spaces".

When we say "site" we mean any "point" in space. Obviously we are going to demand at a later stage "invariance" of the formalism with respect to the choice of one-particle basis. The formalism should look the same if we talk about occupation of "position states" or if we talk about occupation of "momentum states". Depending on the context we talk about occupation of "sites" or of "orbitals" or of "modes" or in general we talk about occupation of "one particle states".

Given a set of sites $|r\rangle$ the Fock space is spanned by the basis $\{|n_1, n_2, ...n_r, ...\rangle\}$. We can define a subspace of all N particles states

$$\text{span}_N\{|n_1, n_2, ..., n_r, ...\rangle\} \tag{1260}$$

that includes all the superpositions of basis states with $\sum_r n_r = N$ particles. On the other hand, if we use the first quantization approach, we can define Hilbert subspaces that contains only totally symmetric or totally anti-symmetric states:

$$\begin{aligned}&\text{span}_S\{|r_1, r_2, ..., r_N\rangle\}\\ &\text{span}_A\{|r_1, r_2, ..., r_N\rangle\}\end{aligned} \tag{1261}$$

The mathematical claim is that there is a one-to-one correspondence between Fock span_N states and Hilbert span_S or span_A states for Bosons and Fermions respectively. The identification is expressed as follows:

$$|n_1, n_2, ..., n_r, ...\rangle \iff \frac{1}{N!}\sqrt{C_N^n}\sum_P \xi^P \; P|r_1, r_2, ..., r_N\rangle \tag{1262}$$

where $r_1, ..., r_N$ label the occupied sites, P is an arbitrary permutation operator, ξ is $+1$ for Bosons and -1 for Fermions, and $C_N^n = N!/(n_1!n_2!...)$. We note that in the case of Fermions the representation of an N particle Fock

state in first quantization can be written as a Slater determinant:

$$\langle x_1,...,x_N|n_1,n_2,...,n_r,...\rangle = \frac{1}{\sqrt{N!}}\begin{vmatrix} \langle x_1|r_1\rangle & \cdots & \langle x_1|r_N\rangle \\ \vdots & & \vdots \\ \langle x_N|r_1\rangle & \cdots & \langle x_N|r_N\rangle \end{vmatrix} \tag{1263}$$

In the following section we discuss only the Fock space formalism. Nowadays the first quantization Hilbert space approach is used mainly for the analysis of $N = 2$ systems. For larger number of particles the Fock formalism is much more convenient, and all the issue of "symmetrization" is avoided.

═══ [44.2] Raising and Lowering Operators

First we would like to discuss the mathematics of a single "site". The basis states $|n\rangle$ can be regarded as the eigenstates of a number operator:

$$\hat{n}|n\rangle = n|n\rangle \tag{1264}$$
$$\hat{n} \longrightarrow \begin{pmatrix} 0 & & & 0 \\ & 1 & & \\ & & 2 & \\ 0 & & & \ddots \end{pmatrix}$$

In general a lowering operator has the property

$$\hat{a}\,|n\rangle = f(n)\,|n-1\rangle \tag{1265}$$

and its matrix representation is:

$$\hat{a} \longrightarrow \begin{pmatrix} 0 & * & & \\ & \ddots & \ddots & \\ & & \ddots & * \\ 0 & & & 0 \end{pmatrix} \tag{1266}$$

The adjoint is a raising operator:

$$\hat{a}^{\deg}\,|n\rangle = f(n+1)\,|n+1\rangle \tag{1267}$$

and its matrix representation is:

$$\hat{a}^\dagger \longrightarrow \begin{pmatrix} 0 & & & 0 \\ * & \ddots & & \\ & \ddots & \ddots & \\ & & * & 0 \end{pmatrix} \tag{1268}$$

By appropriate gauge we can assume without loss of generality that $f(n)$ is real and non-negative. so we can write

$$f(n) = \sqrt{g(n)} \tag{1269}$$

From the definition of $\hat{a}$ it follows that

$$\hat{a}^\dagger\hat{a}|n\rangle = g(n)|n\rangle \tag{1270}$$

and therefore

$$\hat{a}^\dagger \hat{a} = g\left(\hat{n}\right) \tag{1271}$$

There are 3 cases of interest

- The raising/lowering is unbounded ($-\infty < n < \infty$)
- The raising/lowering is bounded from one side (say $0 \leq n < \infty$)
- The raising/lowering is bounded from both sides (say $0 \leq n < \mathcal{N}$)

The simplest choice for $g(n)$ in the first case is

$$g(n) = 1 \tag{1272}$$

In such a case $\hat{a}$ becomes the translation operator, and the spectrum of n stretches from $-\infty$ to ∞. The simplest choice for $g(n)$ in the second case is

$$g(n) = n \tag{1273}$$

this leads to the same algebra as in the case of an harmonic oscillator. The simplest choice for $g(n)$ in the third case is

$$g(n) = (\mathcal{N} - n)n \tag{1274}$$

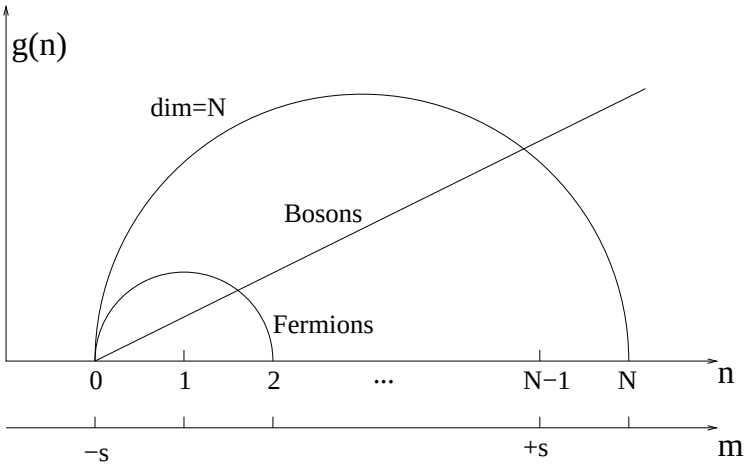
Here it turns out that the algebra is the same as that for angular momentum. To see that it is indeed like that define

$$m \;=\; n - \frac{\mathcal{N}-1}{2} \;=\; -s, \ldots, +s \tag{1275}$$

where $s = (\mathcal{N}-1)/2$. Then it is possible to write

$$g(m) = s(s+1) - m(m+1) \tag{1276}$$

In the next sections we are going to discuss the "Bosonic" case $\mathcal{N} = \infty$ with $g(n) = n$, and the "Fermionic" case $\mathcal{N} = 2$ with $g(n) = n(1-n)$. Later we are going to argue that these are the only two possibilities that are relevant to the description of many body occupation.



It is worthwhile to note that the algebra of "angular momentum" can be formally obtained from the Bosonic algebra using a trick due to Schwinger. Let us define two Bosonic operators c_1 and c_2, and

$$a^\dagger \;=\; c_2^\dagger c_1 \tag{1277}$$

The $a^\dagger$ operator moves a particle from site 1 to site 2. Consider how a and $a^\dagger$ operate within the subspace of $(N-1)$ particle states. It is clear that a and $a^\dagger$ act like lowering/raising operators with respect to $m = (c_2^\dagger c_2 - c_1^\dagger c_1)/2$. Obviously the lowering/raising operation in bounded from both ends. In fact it is easy to verify that a and $a^\dagger$ have the same algebra as that of "angular momentum".

======= [44.3] Algebraic characterization of creation operators

We can characterize a raising/lowering operator as follows:

$$\hat{n}\left(\hat{a}\left|n\right\rangle\right) = \left(n-1\right)\left(\hat{a}\left|n\right\rangle\right) \qquad \text{for any } n \tag{1278}$$

which is equivalent to

$$\hat{n}\hat{a}\left|n\right\rangle = \hat{a}\left(n-1\right)\left|n\right\rangle \qquad \text{for any } n \tag{1279}$$

which is equivalent to

$$\hat{n}\hat{a}\left|n\right\rangle = \hat{a}\left(\hat{n}-1\right)\left|n\right\rangle \qquad \text{for any } n \tag{1280}$$

which is equivalent to

$$\hat{n}\hat{a} = \hat{a}\left(\hat{n}-1\right) \tag{1281}$$

which can be written as

$$[\hat{n},\hat{a}] = \text{step } \hat{a} \tag{1282}$$

with step $= -1$. The opposite path also holds. If the latter commutation holds then $\hat{a}$ is a ladder operator with respect to $\hat{n}$

$$\hat{a}\left|n\right\rangle = (\text{prefactor})\left|n + \text{step}\right\rangle \tag{1283}$$

In fact it is possible to make a more interesting statement. Given that

$$[a, a^\dagger]_\mp \;=\; 1 \tag{1284}$$

We deduce that a and $a^\dagger$ are lowering and raising operators with respect to $n = a^\dagger a$. Furthermore they are of either Bosonic or Fermionic type, depending on whether it is commutation or anti-commutation relation. The proof is based on the relations

$$||a|n\rangle|| \;=\; \langle n|a^\dagger a|n\rangle \;=\; n \tag{1285}$$
$$||a^\dagger|n\rangle|| \;=\; \langle n|aa^\dagger|n\rangle \;=\; 1 \pm n \tag{1286}$$

which are most easily derived using the identity

$$[AB, C] = A[B,C]_\mp - [C,A]_\mp B \tag{1287}$$

[44.4] Creation Operators for "Bosons"

For a "Bosonic" site we define

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{1288}$$

hence

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{1289}$$

and

$$\left[\hat{a},\hat{a}^\dagger\right] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1 \tag{1290}$$

If we have many sites then we define

$$\hat{a}_r^\dagger = 1\otimes 1\otimes\cdots\otimes\hat{a}^\dagger\otimes\cdots\otimes 1 \tag{1291}$$

which means

$$\hat{a}_r^\dagger\,|n_1,n_2,\ldots,n_r,\ldots\rangle = \sqrt{n_r+1}\,|n_1,n_2,\ldots,n_r+1,\ldots\rangle \tag{1292}$$

and hence

$$[\hat{a}_r,\hat{a}_s] = 0 \tag{1293}$$

and

$$\left[\hat{a}_r,\hat{a}_s^\dagger\right] = \delta_{r,s} \tag{1294}$$

We have defined our set of creation operators using a particular one-particle basis. What will happen if we switch to a different basis? Say from the position basis to the momentum basis? In the new basis we would like to have the same type of "occupation rules", namely,

$$\left[\hat{a}_\alpha,\hat{a}_\beta^\dagger\right] = \delta_{\alpha\beta} \tag{1295}$$

Let's see that indeed this is the case. The unitary transformation matrix from the original $|r\rangle$ basis to the new $|\alpha\rangle$ basis is

$$T_{r,\alpha} = \langle r|\alpha\rangle \tag{1296}$$

Then we have the relation

$$|\alpha\rangle = \sum_r |r\rangle\,\langle r|\alpha\rangle = \sum_r T_{r,\alpha}\,|r\rangle \tag{1297}$$

and therefore

$$\hat{a}_\alpha^\dagger = \sum_r T_{r,\alpha}\hat{a}_r^\dagger \tag{1298}$$

Taking the adjoint we also have

$$\hat{a}_\alpha = \sum_r T^*_{r,\alpha} \hat{a}_r \tag{1299}$$

Now we find that

$$\left[\hat{a}_\alpha, \hat{a}^\dagger_\beta\right] = \sum_{r,s} \left[T^*_{r\alpha}\hat{a}_r, T_{s\beta}\hat{a}^\dagger_s\right] = T^*_{r\alpha}T_{s\beta}\delta_{rs} = \left(T^\dagger\right)_{\alpha r} T_{r\beta} = \left(T^\dagger T\right)_{\alpha\beta} = \delta_{\alpha\beta} \tag{1300}$$

This result shows that $\hat{a}_\alpha$ and $\hat{a}^\dagger_\beta$ are indeed destruction and creation operators of the same "type" as $\hat{a}_r$ and $\hat{a}^\dagger_r$. Can we have the same type of invariance for other types of occupation? We shall see that the only other possibility that allows "invariant" description is $\mathcal{N} = 2$.

[44.5] Creation Operators for "Fermions"

In analogy with the case of a "Boson site" we define a "Fermion site" using

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{1301}$$

and

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad \text{with mod(2) plus operation} \tag{1302}$$

The representation of the operators is, using Pauli matrices:

$$\begin{aligned}
&\hat{n} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\left(\hat{1} + \sigma_3\right) \\
&\hat{a} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\left(\sigma_1 - i\sigma_2\right) \\
&\hat{a}^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\left(\sigma_1 + i\sigma_2\right) \\
&\hat{a}^\dagger\hat{a} = \hat{n} \\
&\hat{a}\hat{a}^\dagger = \hat{1} - \hat{n} \\
&\left[\hat{a}, \hat{a}^\dagger\right]_+ = \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 1
\end{aligned} \tag{1303}$$

while

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1 - 2\hat{n} \tag{1304}$$

Now we would like to proceed with the many-site system as in the case of "Bosonic sites". But the problem is that the algebra

$$\left[\hat{a}_r, \hat{a}^\dagger_s\right] = \delta_{r,s}(1 - 2\hat{a}^\dagger_r\hat{a}_r) \tag{1305}$$

is manifestly not invariant under a change of one-particle basis. The only hope is to have

$$\left[\hat{a}_r, \hat{a}^\dagger_s\right]_+ = \delta_{r,s} \tag{1306}$$

which means that a_r and a_s for $r \neq s$ should anti-commute rather than commute. Can we define the operators a_r in such a way? It turns out that there is such a possibility:

$$\hat{a}_r^\dagger \left| n_1, n_2, \ldots, n_r, \ldots \right\rangle = (-1)^{\sum_{s(>r)} n_s} \left| n_1, n_2, \ldots, n_r + 1, \ldots \right\rangle \tag{1307}$$

For example, it is easily verified that we have:

$$a_2^\dagger a_1^\dagger |0,0,0,\ldots\rangle = -a_1^\dagger a_2^\dagger |0,0,0,\ldots\rangle = |1,1,0,\ldots\rangle \tag{1308}$$

With the above convention if we create particles in the "natural order" then the sign comes out plus, while for any "violation" of the natural order we get a minus factor.

[44.6] One Body Additive Operators

Let us assume that we have an additive quantity V which is not the same for different one-particle states. One example is the (total) kinetic energy, another example is the (total) potential energy. It is natural to define the many body operator that corresponds to such a property in the basis where the one-body operator is diagonal. In the case of potential energy it is the position basis:

$$V = \sum_\alpha V_{\alpha,\alpha} \hat{n}_\alpha = \sum_\alpha \hat{a}_\alpha^\dagger V_{\alpha,\alpha} \hat{a}_\alpha \tag{1309}$$

This counts the amount of particles in each α and multiplies the result with the value of V at this site. If we go to a different one-particle basis then we should use the transformation

$$\begin{aligned} \hat{a}_\alpha &= \sum_k T_{k,\alpha}^* \hat{a}_k \\ \hat{a}_\alpha^\dagger &= \sum_{k'} T_{k',\alpha} \hat{a}_{k'}^\dagger \end{aligned} \tag{1310}$$

leading to

$$V = \sum_{k,k`} \hat{a}_{k'}^\dagger V_{k',k} \hat{a}_k \tag{1311}$$

Given the above result we can calculate the matrix elements from a transition between two different occupations:

$$|\langle n_1 - 1, n_2 + 1 | V | n_1, n_2 \rangle|^2 = (n_2 + 1)\, n_1 \, |V_{2,1}|^2 \tag{1312}$$

What we get is quite amazing: in the case of Bosons we get an amplification of the transition if the second level is already occupied. In the case of Fermions we get "blocking" if the second level is already occupied. Obviously this goes beyond classical reasoning. The latter would give merely n_1 as a prefactor.

[44.7] Two Body "Additive" Operators

It is straightforward to make a generalization to the case of two body "additive" operators. Such operators may represent the two-body interaction between the particles. For example we can take the Coulomb interaction, which is diagonal in the position basis. Thus we have

$$U = \frac{1}{2} \sum_{\alpha \neq \beta} U_{\alpha\beta,\alpha\beta} \hat{n}_\alpha \hat{n}_\beta + \frac{1}{2} \sum_\alpha \; U_{\alpha\alpha,\alpha\alpha} \; \hat{n}_\alpha \left(\hat{n}_\alpha - 1 \right) \tag{1313}$$

Using the relation

$$\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\beta \hat{a}_\alpha = \begin{cases} \hat{n}_\alpha \hat{n}_\beta & \text{for } \alpha \neq \beta \\ \hat{n}_\alpha(\hat{n}_\alpha - 1) & \text{for } \alpha = \beta \end{cases} \tag{1314}$$

We get the simple expression

$$U = \frac{1}{2} \sum_{\alpha,\beta} \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \; U_{\alpha\beta,\alpha\beta} \; \hat{a}_\beta \hat{a}_\alpha \tag{1315}$$

and for a general one-particle basis

$$U = \frac{1}{2} \sum_{k'l',kl} \hat{a}^\dagger_{k'} \hat{a}^\dagger_{l'} \; U_{k'l',kl} \; \hat{a}_l \hat{a}_k \tag{1316}$$

We call such operator "additive" (with quotations) because in fact they are not really additive. An example for a genuine two body additive operator is $[A, B]$, where A and B are one body operators. This observation is very important in the theory of linear response (Kubo).

[44.8] Matrix Elements With N Particle States

Let's take an N particle state of a Fermionic system

$$|R_N\rangle = \hat{a}^\dagger_N \ldots \hat{a}^\dagger_2 \hat{a}^\dagger_1 |0\rangle \tag{1317}$$

For the one body operator we get

$$\langle R_N|V|R_N\rangle = \sum_k \langle k|V|k\rangle \tag{1318}$$

because only the terms with $k = k'$ do not vanish. For the two body operator we get

$$\langle R_N|U|R_N\rangle = \frac{1}{2} \sum_{k,l \in R} \underset{direct}{\langle kl|U|kl\rangle} - \underset{exchange}{\langle kl|U|lk\rangle} \tag{1319}$$

because the only non-vanishing terms are those with either $k' = k$ and $l' = l$ or with $k' = l$ and $l' = k$. The other possibilities give zero.

[45] Wigner function and Wigner-Weyl formalism

[45.1] The classical description of a state

Classical states are described by a probability function. Given a random variable $\hat{x}$, we define $\rho(x) = \text{Prob}(\hat{x} = x)$ as the probability of the event $\hat{x} = x$, where the possible values of x are called the spectrum of the random variable $\hat{x}$. For a random variable continuous spectrum we define the probability density function via $\rho(x)dx = \text{Prob}(x < \hat{x} < x + dx)$. The expectation value of a random variable $\hat{A} = A(\hat{x})$ is defined as

$$\langle \hat{A} \rangle = \sum \rho(x)\ A(x) \tag{1320}$$

and for a continuous variable as. For simplicity we use form now on notation as if the random variables have discrete spectrum, with the understanding that in case of continuous spectrum we should replace the $\sum$ by an integral with the appropriate *measure* (e.g. dx or $dp/(2\pi)$).

Let us consider two random variables $\hat{x}, \hat{p}$. One can ask what is the joined probability function for these two variables. This is a valid question only in classical mechanics. In quantum mechanics one usually cannot ask this question since not all variables can be measured in the same measurement. In order to find the joined probability function of these two variables in quantum mechanics one needs to build a more sophisticated method. The solution is to regard the expectation value as the fundamental outcome and to define the probability function as an expectation value In the case of one variable such as $\hat{x}$ or $\hat{p}$, we define probability functions as

$$\begin{aligned} \rho(X) &\equiv \langle\ \delta(\hat{x} - X)\ \rangle \\ \rho(P) &\equiv \langle\ 2\pi\delta(\hat{p} - P)\ \rangle \end{aligned} \tag{1321}$$

Now we can also define the joined probability function as

$$\rho(X, P) = \langle 2\pi\ 2\pi\delta(\hat{p} - P)\ \delta(\hat{x} - X)\ \rangle \tag{1322}$$

This probability function is normalized so that

$$\int \rho(X, P)\frac{dXdP}{2\pi} = \left\langle \int \delta(\hat{p} - P)dP \int \delta(\hat{x} - X)dX \right\rangle = 1 \tag{1323}$$

In the next section we shall define essentially the same object in the framework of quantum mechanics.

[45.2] Wigner function

Wigner function is a real normalized function which is defined as

$$\rho_{\text{w}}(X, P) = \left\langle\ \left[\ 2\pi\delta(\hat{p} - P)\ \delta(\hat{x} - X)\ \right]_{\text{sym}}\ \right\rangle \tag{1324}$$

In what follow we define what do we mean by symmetrization ("sym"), and we relate $\rho_{\text{w}}(X, P)$ to the conventional probability matrix $\rho(x', x'')$. We recall that the latter is defined as

$$\rho(x', x'') = \left\langle P^{x'x''} \right\rangle = \left\langle\ |x''\rangle\langle x'|\ \right\rangle \tag{1325}$$

The "Wigner function identity" that we are going to prove is

$$\rho_{\text{w}}(X, P) = \int \rho\left(X + \frac{1}{2}r, X - \frac{1}{2}r\right) \text{e}^{-iPr}dr \tag{1326}$$

Thus to go from the probability matrix to the Wigner function is merely a Fourier transform, and can be loosely regarded as a change from "position representation" to "phase space representation".

Moreover we can use the same transformation to switch the representation of an observable $\hat{A}$ from $A(x', x'')$ to $A(X, P)$. Then we shall prove that

$$\text{trace}(A\rho) = \int A(X,P)\rho_{\text{w}}(X,P)\frac{dXdP}{2\pi} \tag{1327}$$

This means that expectation values of observables can be calculated using a semi-classical calculation. This extension of the Wigner function idea is called Wigner-Weyl formalism.

[45.3] Mathematical derivations

Fourier transform reminder:

$$\begin{aligned} F(k) &= \int f(x)\mathrm{e}^{-ikx}dx \\ f(x) &= \int \frac{dk}{2\pi}F(k)\mathrm{e}^{ikx} \end{aligned} \tag{1328}$$

Inner product is invariant under change of representation

$$\int f(x)g^*(x)dx = \int \frac{dk}{2\pi}F(k)G^*(k) \tag{1329}$$

For the matrix representation of an operator A we use the notation

$$A(x', x'') = \langle x'|A|x''\rangle \tag{1330}$$

It is convenient to replace the row and column indexes by diagonal and off-diagonal coordinates:

$$\begin{aligned} X &= \frac{1}{2}(x' + x'') = \text{the diagonal coordinate} \\ r &= x' - x'' = \text{the off diagonal coordinate} \\ x' &= X + \frac{1}{2}r \\ x'' &= X - \frac{1}{2}r \end{aligned} \tag{1331}$$

and to use the alternate notation

$$A(X,r) = \left\langle X + \frac{1}{2}r\middle|A\middle|X - \frac{1}{2}r\right\rangle \tag{1332}$$

Using this notation, the transformation to phase space representations can be written as

$$A(X,P) = \int A(X,r)\mathrm{e}^{-iPr}dr \tag{1333}$$

Note that if A is hermitian then $A(X,-r) = A^*(X,+r)$, and consequently $A(X,P)$ is a real function. Moreover, the

trace of two hermitian operators can be written as a phase space integral

$$\begin{aligned}\mathrm{trace}(\widehat{A}\widehat{B}) &= \int A(x',x'')B(x'',x')dx'dx'' = \int A(X,+r)B(X,-r)dr \\ &= \int A(X,+r)B^*(X,r)dr = \int A(X,P)B(X,P)\frac{dXdP}{2\pi}\end{aligned} \tag{1334}$$

This we call the Wigner-Weyl identity.

A useful operator identity

$$\mathrm{e}^{\hat{A}+\hat{B}} = \mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}\mathrm{e}^{\frac{1}{2}[\hat{A},\hat{B}]} \tag{1335}$$

In the case of $\hat{x},\hat{p}$ we have $[\hat{x},\hat{p}] = i$ and therefore

$$\mathrm{e}^{\hat{x}+\hat{p}} = \mathrm{e}^{\hat{x}}\mathrm{e}^{\hat{p}}\mathrm{e}^{\frac{1}{2}i} = \mathrm{e}^{\frac{1}{2}\hat{p}}\mathrm{e}^{\hat{x}}\mathrm{e}^{\frac{1}{2}\hat{p}} \tag{1336}$$

Another useful identity is

$$|X\rangle\langle X| = \delta(\hat{x}-X) \tag{1337}$$

In order to prove this identity it is easier to use discrete notations $|n_0\rangle\langle n_0| = \delta_{\hat{n},n_0}$. The left hand side is a projector $P \mapsto P_{nm}$ whose only non-zero matrix element is $n = m = n_0$. The right hand side is a function of $f(\hat{n})$ such that $f(n) = 1$ for $n = n_0$ and zero otherwise. Therefore the right hand side is also diagonal in n with the same representation. Finally we note the following identity

$$|x'\rangle\langle x''| = \Big|X-(r/2)\Big\rangle\Big\langle X+(r/2)\Big| = \mathrm{e}^{i(r/2)\hat{p}}|X\rangle\langle X|\mathrm{e}^{i(r/2)\hat{p}} = \mathrm{e}^{i(r/2)\hat{p}}\delta(\hat{x}-X)\mathrm{e}^{i(r/2)\hat{p}} \tag{1338}$$

and we can also write

$$\delta(\hat{x}-X) = \int \frac{dp}{2\pi}\mathrm{e}^{ip(\hat{x}-X)} \tag{1339}$$

so it is natural to define

$$\Big[\ 2\pi\delta(\hat{p}-P)\ \delta(\hat{x}-X)\ \Big]_{\mathrm{sym}} \equiv \int \frac{drdp}{2\pi}\ \mathrm{e}^{ir(\hat{p}-P)+ip(\hat{x}-X)} \tag{1340}$$

From a classical point of view this is a trivial mathematical identity, while quantum mechanically a properly symmetrized version of the delta functions product is implied. The derivation of the Wigner function identity follows in a straightforward fashion:

$$\begin{aligned}\rho_{\mathrm{W}}(X,P) &= \Big\langle\ \Big[\ 2\pi\delta(\hat{p}-P)\ \delta(\hat{x}-X)\ \Big]_{\mathrm{sym}}\ \Big\rangle \\ &= \Big\langle\ \int \frac{drdp}{2\pi}\ \mathrm{e}^{ir(\hat{p}-P)+ip(\hat{x}-X)}\ \Big\rangle \\ &= \Big\langle\ \int \frac{drdp}{2\pi}\ \mathrm{e}^{i\frac{1}{2}r(\hat{p}-P)}\ \mathrm{e}^{ip(\hat{x}-X)}\ \mathrm{e}^{i\frac{1}{2}r(\hat{p}-P)}\ \Big\rangle \\ &= \Big\langle\ \int dr\ \mathrm{e}^{i\frac{1}{2}r(\hat{p}-P)}\ \delta(\hat{x}-X)\ \mathrm{e}^{i\frac{1}{2}r(\hat{p}-P)}\ \Big\rangle \\ &= \Big\langle\ \int dr\mathrm{e}^{-irP}\ |X-(r/2)\rangle\langle X+(r/2)|\ \Big\rangle \\ &= \int dr\ \mathrm{e}^{-irP}\ \rho(X,r)\end{aligned} \tag{1341}$$

[45.4] Applications of the Wigner Weyl formalism

In analogy with the Wigner representation at ρ we can define a Wigner-Weyl (WW) representation of any hermitian operator. The matrix elements of the operator $\hat{x}$ can be written as $\langle x'|\hat{x}|x''\rangle$

$$\langle\, x'|\hat{x}|x''\rangle = x'\delta(x'-x'') = X\delta(r) \stackrel{WW}{\to} X \tag{1342}$$

Similarly $\hat{p} \stackrel{WW}{\to} P$ and in general $f(\hat{x}) \stackrel{WW}{\to} f(X)$, and $g(\hat{p}) \stackrel{WW}{\to} g(P)$. Next in line are

$$\begin{aligned} \hat{x}\hat{p} &\stackrel{WW}{\longrightarrow} XP + \frac{1}{2}i \\ \hat{p}\hat{x} &\stackrel{WW}{\longrightarrow} XP - \frac{1}{2}i \\ \frac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x}) &\stackrel{WW}{\longrightarrow} XP \end{aligned} \tag{1343}$$

In general for appropriate ordering we get that $f(\hat{x},\hat{p})$ is represented by $f(X,P)$. But in practical applications $f(\hat{x},\hat{p})$ will not have the desired ordering, and therefore this recipe should be considered as a leading term in a semiclassical $\hbar$ expansion.

Below we list the two major applications of the Wigner Weyl identity. The first one is the calculation of the partition function.

$$\mathcal{Z}(\beta) = \sum_r \mathrm{e}^{-\beta E_r} = \sum_r \langle r|\mathrm{e}^{-\beta H}|r\rangle = \mathrm{trace}(\mathrm{e}^{-\beta H}) = \int \frac{dXdP}{2\pi}(\mathrm{e}^{-\beta H(X,P)}) + \mathcal{O}(\hbar) \tag{1344}$$

The second one is the calculation of the number of eigenstates up to a given energy E

$$\begin{aligned} \mathcal{N}(E) &= \sum_{E_r \le E} 1 = \sum_r \Theta(E-E_r) = \mathrm{trace}[\Theta(E-\hat{H})] \\ &\approx \int \frac{dXdP}{2\pi}\Theta(E-H(X,P)) = \int_{H(X,P)\le E} \frac{dXdP}{2\pi} \end{aligned} \tag{1345}$$

[45.5] Wigner function for a Gaussian wavepacket

A Gaussian wavepacket in the position representation is written as

$$\Psi(x) = \frac{1}{\sqrt{\sqrt{2\pi}\sigma}}\mathrm{e}^{-\frac{(x-x_0)^2}{4\sigma^2}}\mathrm{e}^{ip_0x} \tag{1346}$$

The probability density matrix is

$$\rho(X,r) = \Psi^*(X+\frac{1}{2}r)\Psi(X-\frac{1}{2}r) = \frac{1}{\sqrt{2\pi}\sigma}\mathrm{e}^{-\frac{((X-x_0)+\frac{1}{2}r)^2}{4\sigma^2}-\frac{((X-x_0)-\frac{1}{2}r)^2}{4\sigma^2}-ip_0r} = \frac{1}{\sqrt{2\pi}\sigma}\mathrm{e}^{-\frac{(X-x_0)^2}{2\sigma^2}-\frac{r^2}{8\sigma^2}-ip_0r} \tag{1347}$$

Transforming to the Wigner representation

$$\rho_{\mathrm{w}}(X,P) = \int \frac{1}{\sqrt{2\pi}\sigma}\mathrm{e}^{-\frac{(X-x_0)^2}{2\sigma^2}-\frac{r^2}{8\sigma^2}-i(P-p_0)r}dr = \frac{1}{\sigma_x\sigma_p}\mathrm{e}^{-\frac{(X-x_0)^2}{2\sigma_x^2}-\frac{(P-p_0)^2}{2\sigma_p^2}} \tag{1348}$$

where $\sigma_x = \sigma$ and $\sigma_p = \frac{1}{2\sigma}$. It follows that $\sigma_x\sigma_p = 1/2$. Let us no go backwards. Assume that have a Gaussian in phase space, which is characterized by some σ_x and σ_p. Does it represent a legitimate quantum mechanical state? The normalization condition $\mathrm{trace}(\rho) = 1$ is automatically satisfied. We also easily find that

$$\mathrm{trace}(\rho^2) = \int \frac{1}{\sigma_x^2\sigma_p^2} \mathrm{e}^{-\frac{(X-x_0)^2}{\sigma_x^2} - \frac{(P-p_0)^2}{\sigma_p^2}} \frac{dXdP}{2\pi} = \frac{1}{2\sigma_x\sigma_p} \tag{1349}$$

We know that $\mathrm{trace}(\rho^2) = 1$ implies pure state. If $\mathrm{trace}(\rho^2) < 1$ it follows that we have a mixed state, whereas $\mathrm{trace}(\rho^2) > 1$ is not physical. It is important to remember that not any $\rho(X, P)$ corresponds to a legitimate quantum mechanical state. There are classical states that do not have quantum mechanical analog (e.g. point like preparation). Also the reverse is true: not any quantum state has a classical analogue. The latter is implied by the possibility to have negative regions in phase space. These is discussed in the next example.

======= [45.6] The Winger function of a bounded particle

Wigner function may have some modulation on a fine scale due to an interference effect. The simplest and most illuminating example is the Wigner function of the nth eigenstate of a particle in a one dimensional box ($0 < x < L$). The eigen-wavefunction that correspond to wavenumber $k = (\pi/L) \times \text{integer}$ can be written as the sum of a right moving and a left moving wave $\psi(x) = (1/\sqrt{2})(\psi_1(x) + \psi_2(x))$ within $0 < x < L$, and $\psi(x) = 0$ otherwise. The corresponding Wigner function is zero outside of the box. Inside the box it can be written as

$$\rho_{\mathrm{w}}(X, P) \;=\; \frac{1}{2}\rho_1(X, P) + \frac{1}{2}\rho_2(X, P) + \rho_{12}(X, P) \tag{1350}$$

where ρ_{12} is the interference component. The semiclassical components are concentrated at $P = \pm k$, while the interference component is concentrated at $P = 0$. The calculation of $\rho_1(X, P)$ in the interval $0 < x < L/2$ is determined solely by the presence of the hard wall at $x = 0$. The relevant component of the wavefunction is

$$\psi_1(x) = \frac{1}{\sqrt{L}}\Theta(x)\mathrm{e}^{ikx} \tag{1351}$$

and hence

$$\begin{aligned}\rho_1(X, P) \;&=\; \int_{-\infty}^{\infty} \psi_1(X + (r/2))\psi_1^*(X - (r/2))\mathrm{e}^{-iPr}dr \;=\; \frac{1}{L}\int_{-\infty}^{\infty} \Theta(X + (r/2))\Theta(X - (r/2))\mathrm{e}^{-i(P-k)r}dr \\ &=\; \frac{1}{L}\int_{-2X}^{2X} \mathrm{e}^{-i(P-k)r}dr \;=\; \frac{4X}{L}\mathrm{sinc}(2X(P-k))\end{aligned} \tag{1352}$$

This shows that as we approach the sharp feature the non-classical nature of Wigner function is enhanced, and the classical (delta) approximation becomes worse. The other components of Wigner function are similarly calculated, and for the interference component we get

$$\rho_{12}(X, P) = -2\cos(2kX) \times \frac{4X}{L}\mathrm{sinc}(2XP) \tag{1353}$$

It is easily verified that integration of $\rho_{\mathrm{w}}(X, P)$ over P gives $\rho(x) = 1 + 1 - 2\cos(2kX) = 2(\sin(kX))^2$.

In many other cases the energy surface in phase space is "soft" (no hard walls) and then one can derive a uniform semiclassical approximation [Berry, Balazs]:

$$\rho_{\mathrm{w}}(X, P) = \frac{2\pi}{\Delta_{sc}(X, P)}\mathrm{Ai}\left(\frac{\mathcal{H}(X, P) - E}{\Delta_{sc}(X, P)}\right) \tag{1354}$$

where for $\mathcal{H} = p^2/(2\mathsf{m}) + V(x)$

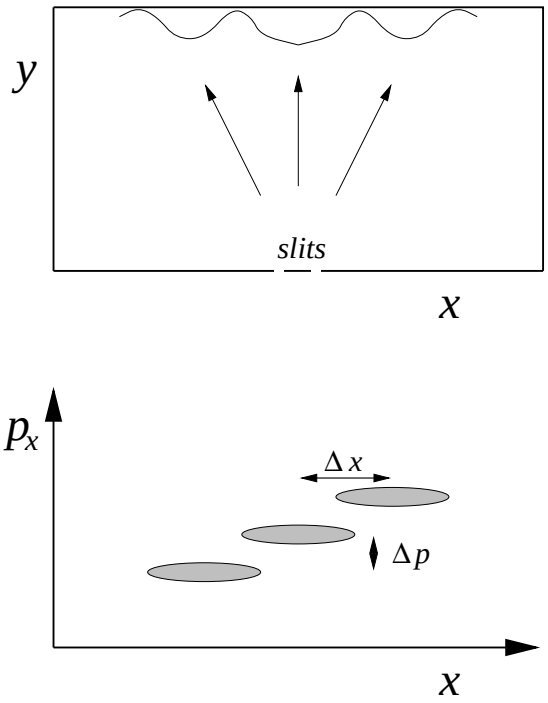
$$\Delta_{sc} = \frac{1}{2}\left[\hbar^2\left(\frac{1}{\mathsf{m}}|\nabla V(X)|^2 + \frac{1}{\mathsf{m}^2}(P\cdot\nabla)^2 V(X)\right)\right]^{1/3} \tag{1355}$$

What can we get out of this expression? We see that $\rho_{\rm w}(X,P)$ decays exponentially as we go outside of the energy surface. Inside the energy surface we have oscillations due to interference.

The interference regions of the Wigner function might be very significant. A nice example is given by Zurek. Let us assume that we have a superposition of $N \gg 1$ non-overlapping Gaussian. we can write the Wigner function as $\rho = (1/N)\sum \rho_j + \rho_{\rm intrfr}$. We have trace$(\rho) = 1$ and also trace$(\rho^2) = 1$. This implies that trace$(\rho_{\rm intrfr}) = 0$, while trace$(\rho^2_{\rm intrfr}) \sim 1$. The latter conclusion stems from the observation that the classical contribution is $N \times (1/N)^2 \ll 1$. Thus the interference regions of the Wigner function dominate the calculation.

[45.7] The Winger picture of a two slit experiment

The textbook example of a two slit experiment will be analyzed below. The standard geometry is described in the upper panel of the following figure. The propagation of the wavepacket is in the y direction. The wavepacket is scattered by the slits in the x direction. The distance between the slits is d. The interference pattern is resolved on the screen. In the lower panel the phase-space picture of the dynamics is displayed. Wigner function of the emerging wavepacket is projected onto the (x, p_x) plane.



The wavepacket that emerges from the two slits is assumed to be a superposition

$$\varphi(x) \approx \frac{1}{\sqrt{2}}(\varphi_1(x) + \varphi_2(x)) \tag{1356}$$

The approximation is related to the normalization which assumes that the slits are well separated. Hence we can regard $\varphi_1(x) = \varphi_0(x + (d/2))$ and $\varphi_2(x) = \varphi_0(x - (d/2))$ as Gaussian wavepackets with a vanishingly small overlap. The probability matrix of the superposition is

$$\rho(x', x'') = \varphi(x')\varphi^*(x'') = (\varphi_1(x') + \varphi_2(x'))(\varphi_1^*(x'') + \varphi_2^*(x'')) = \frac{1}{2}\rho_1 + \frac{1}{2}\rho_2 + \rho_{\rm interference} \tag{1357}$$

All the integrals that are encountered in the calculation are of the Wigner function are of the type

$$\int \varphi_0\left((X-X_0)+\frac{1}{2}(r-r_0)\right)\ \varphi_0\left((X-X_0)-\frac{1}{2}(r-r_0)\right)\ \mathrm{e}^{-iPr}dr \quad\equiv\quad \rho_0(X-X_0,P)\ \mathrm{e}^{-iPr_0} \tag{1358}$$

where $X_0=\pm d/2$ and $r_0=0$ for the classical part of the Wigner function, while $X_0=0$ and $r_0=\pm d/2$ for the interference part. Hence we get the result

$$\rho_{\rm w}(X,P) \quad=\quad \frac{1}{2}\rho_0\left(X+\frac{d}{2},P\right)\ +\ \frac{1}{2}\rho_0\left(X-\frac{d}{2},P\right)\ +\ \cos(Pd)\ \rho_0(X,P) \tag{1359}$$

Note that the momentum distribution can be obtained by integrating over X

$$\rho(P)=(1+\cos(Pd))\rho_0(P)=2\cos^2(\frac{Pd}{2})\rho_0(P) \tag{1360}$$

In order to analyze the dynamics it is suggestive to write $\rho(X,P)$ schematically as a sum of partial-wavepackets, each characterized by a different transverse momentum:

$$\rho_{\rm w}(X,P)=\sum_{n=-\infty}^{\infty}\rho_n(X,P) \tag{1361}$$

By definition the partial-wavepacket ρ_n equals ρ for $|P-n\times(2\pi\hbar/d)|<\pi\hbar/d$ and equals zero otherwise. Each partial wavepacket represents the possibility that the particle, being scattered by the slits, had acquired a transverse momentum which is an integer multiplet of

$$\Delta p=(2\pi\hbar/d) \tag{1362}$$

The corresponding angular separation is $\Delta\theta=\Delta p/P=\lambda_B/d$, as expected. The associated spatial separation is

$$\Delta x=(\Delta p/m)\cdot t \tag{1363}$$

where $t=y/(P/m)$ is the time up to the screen. It is important to distinguish between the "preparation" zone $y<d$, and the far-field (Franhaufer) zone $d^2/\lambda_B\ll y$. In the latter $\hbar\ll\Delta x\Delta p$ and consequently the individual partial-wavepackets can be resolved.

═══ [45.8] Thermal states

A stationary state $\partial\rho/\partial t$ has to satisfy $[\mathcal{H},\rho]=0$. This means that ρ is diagonal in the energy representation. It can be further argued that in typical circumstances the thermalized mixture is of the canonical type. Namely

$$\hat{\rho}=\sum|r\rangle p_r\langle r|=\frac{1}{\mathcal{Z}}\sum|r\rangle\mathrm{e}^{-\beta E_r}\langle r|=\frac{1}{\mathcal{Z}}\mathrm{e}^{-\beta\hat{H}} \tag{1364}$$

Let us consider some typical examples. The first example is spin 1/2 in a magnetic field. In this case the energies are $E_\uparrow=\epsilon/2$ and $E_\downarrow=\epsilon/2$. Therefore ρ takes the following form:

$$\rho=\frac{1}{2\cosh(\frac{1}{2}\beta\epsilon)}\begin{pmatrix}\mathrm{e}^{\beta\frac{\epsilon}{2}} & 0\\ 0 & \mathrm{e}^{-\beta\frac{\epsilon}{2}}\end{pmatrix} \tag{1365}$$

Optionally one can represent the state of the spin by the polarization vector

$$\vec{M}=(0,0,\tanh(\frac{1}{2}\beta\epsilon)) \tag{1366}$$

The second example is free particle. The Hamiltonian is $H = \hat{p}^2/2m$. Hence ρ is diagonal in the p representation, and identical with the classical expression in the Wigner function representation. Hence its partition function can be calculated as

$$\mathcal{Z} = \int \frac{dk}{(2\pi)/L} \mathrm{e}^{-\beta\frac{k^2}{2m}} = \int \frac{dXdP}{2\pi} \mathrm{e}^{-\beta\frac{P^2}{2m}} = L\left(\frac{m}{2\pi\beta}\right)^{\frac{1}{2}} \tag{1367}$$

The $\hat{x}$ representation of the canonical state can be calculated by inverse Fourier transform of the Wigner function, or it can be regarded as a special case of the harmonic oscillator result (see next example):

$$\rho(x', x'') \;=\; \left(\frac{1}{L}\right) \mathrm{e}^{-\frac{m}{2\beta}[x'-x'']^2} \tag{1368}$$

The third example is harmonic oscillator. Here the calculation is less trivial because the Hamiltonian is not diagonal neither in the x nor in the p representation. The eigenstates of the Hamiltonian are $H|n\rangle = E_n|n\rangle$ with $E_n = \left(\frac{1}{2} + n\right)\omega$. The probability matrix $\rho_{nn'}$ is

$$\rho_{nn'} = \frac{1}{\mathcal{Z}}\delta_{nn'}\mathrm{e}^{-\beta\omega\left(\frac{1}{2}+n\right)} \tag{1369}$$

where the partition function is

$$\mathcal{Z} = \sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n} = \left(2\sinh\left(\frac{1}{2}\beta\omega\right)\right)^{-1} \tag{1370}$$

In the $\hat{x}$ representation

$$\rho(x', x'') = \sum_n \langle x'|n\rangle p_n \langle n|x''\rangle = \sum_n p_n \varphi^n(x')\varphi^n(x'') \tag{1371}$$

The last sum can be evaluated by using properties of Hermite polynomials, but this is very complicated. A much simpler strategy is to use of the Feynman path integral method. The calculation is done as for the propagator $\langle x'|\exp(-i\mathcal{H}t)|\rangle$ with the time t replaced by $-i\beta$. The result is

$$\rho(x', x'') \propto \mathrm{e}^{-\frac{m\omega}{2\sinh(\beta\omega)}\left(\cosh(\beta\omega)\left[x''^2+x'^2\right)-2x'x''\right]} \tag{1372}$$

which leads to the Wigner function

$$\rho_{\mathrm{w}}(X, P) \propto \mathrm{e}^{-\beta\left(\frac{\tanh\left(\frac{1}{2}\beta\omega\right)}{\frac{1}{2}\beta\omega}\right)\left[\frac{P^2}{2m}+\frac{1}{2}m\omega^2X^2\right]} \tag{1373}$$

It is easily verified that in the zero temperature limit we get a minimal wavepacket that represent the pure ground state of the oscillator, while in high temperatures we get the classical result which represents a mixed thermal state.

[46] Theory of Quantum Measurements

[46.1] The reduced probability matrix

In this section we consider the possibility of having a system that has interacted with its surrounding. So we have "system $\otimes$ environment" or "system $\otimes$ measurement device" or simply a system which is a part of a larger thing which we can call "universe". The question that we would like to ask is as follows: Assuming that we know what is the sate of the "universe", what is the way to calculate the state of the "system"?

The mathematical formulation of the problem is as follows. The pure states of the "system" span $N_{\rm sys}$ dimensional Hilbert space, while the states of the "environment" span $N_{\rm env}$ dimensional Hilbert space. So the state of the "universe" is described by $N \times N$ probability matrix $\rho_{i\alpha,j\beta}$, where $N = N_{\rm sys}N_{\rm env}$. This means that if we have operator A which is represented by the matrix $A_{i\alpha,j\beta}$, then it expectation value is

$$\langle A\rangle = {\rm trace}(A\rho) = \sum_{i,j,\alpha,\beta} A_{i\alpha,j\beta}\ \rho_{j\beta,i\alpha} \tag{1374}$$

The probability matrix of the "system" is defined in the usual way. Namely, the matrix element $\rho^{\rm sys}_{j,i}$ is defined as the expectation value of $P^{ji} = |i\rangle\langle j| \otimes \mathbf{1}$. Hence

$$\rho^{\rm sys}_{j,i} = \langle P^{ji}\rangle = {\rm trace}(P^{ji}\rho) = \sum_{k,\alpha,l,\beta} P^{ji}_{k\alpha,l\beta}\rho_{l\beta,k\alpha} = \sum_{k,\alpha,l,\beta} \delta_{k,i}\delta_{l,j}\delta_{\alpha,\beta}\ \rho_{l\beta,k\alpha} = \sum_{\alpha} \rho_{j\alpha,i\alpha} \tag{1375}$$

The common terminology is to say that $\rho^{\rm sys}$ is the *reduced* probability matrix, which is obtained by *tracing out* the environmental degrees of freedom. Just to show mathematical consistency we note that for a general system operator of the type $A = A^{\rm sys} \otimes \mathbf{1}^{\rm env}$ we get as expected

$$\langle A\rangle = {\rm trace}(A\rho) = \sum_{i,\alpha,j\beta} A_{i\alpha,j\beta}\rho_{j\beta,i\alpha} = \sum_{i,j} A^{\rm sys}_{i,j}\rho^{\rm sys}_{j,i} = {\rm trace}(A^{\rm sys}\rho^{\rm sys}) \tag{1376}$$

Of particular interest is the case where the universe is in a pure state $\Psi_{i\alpha}$. The prescription above implies that the state of the system is

$$\rho^{\rm sys}_{j,i} \ = \ \sum_{\alpha} \Psi_{j\alpha}\Psi^*_{i\alpha} \tag{1377}$$

Let us consider for example

$$\Psi \ = \ \sqrt{p_1}\ \psi^{(1)} \otimes \chi^{(1)} + \sqrt{p_2}\ \psi^{(2)} \otimes \chi^{(2)} \tag{1378}$$

where $\psi^{(1)}$ and $\psi^{(2)}$ are orthonormal states of the system. Later on we shall see that such linear combination may come out as a result of an interaction. Depending on the state of the system the environment, or the measurement apparatus, ends up in a different state χ. Accordingly we do not assume that $\chi^{(1)}$ and $\chi^{(2)}$ are orthogonal, though we normalize each of them and pull out the normalization factors as p_1 and p_2. One say that the χ states are the "relative states" of the environment with respect to the system ψ states. It is straightforward to show that

$$\rho^{\rm sys}_{j,i} \ = \ p_1\ \rho^{(1)}_{j,i} + p_2\ \rho^{(2)}_{j,i} + 2\sqrt{p_1p_2}|\langle\chi^{(1)}|\chi^{(2)}\rangle|\ \rho^{\rm interference}_{j,i} \tag{1379}$$

At the same time the environment is in the state

$$\rho^{\rm env} \ = \ p_1\ |\chi^{(1)}\rangle\langle\chi^{(1)}| + p_2\ |\chi^{(2)}\rangle\langle\chi^{(2)}| \tag{1380}$$

[46.2] Purity and the Von Neumann entropy

The purity of a state can be characterized by the Von Neumann entropy:

$$S[\rho] = -\text{trace}(\rho \log \rho) = -\sum_r p_r \log p_r \tag{1381}$$

In the case of a pure state we have $S[\rho] = 0$, while in the case of a uniform mixture of N states we have $S[\rho] = \log(N)$. From the above it should be clear that while the "universe" might have zero entropy, it is likely that a subsystem would have a non-zero entropy. For example if the universe is a zero entropy singlet, then the state of each spin is unpolarized with log(2) entropy.

We would like to emphasize that the Von Neumann entropy $S[\rho]$ should not be confused with the Boltzmann entropy $S[\rho|A]$. The definition of the latter requires to introduce a partitioning A of phase space into cells. In the quantum case this "partitioning" is realized by introducing a complete set of projectors (a basis). The p_r in the case of the Boltzmann entropy are probabilities in a given basis and not eigenvalues. In the case of an isolated system out of equilibrium the Von Neumann entropy is a constant of the motion, while the appropriately defined Boltzmann entropy increases with time. In the case of a canonical thermal equilibrium the Von Neumann entropy $S[\rho]$ turns out to be equal to the thermodynamic entropy $\mathcal{S}$. The latter is defined via the equation $dQ = Td\mathcal{S}$, where $T = 1/\beta$ is an integration factor which is called the absolute temperature.

If the Von Neumann entropy were defined for a classical distributions $\rho = \{p_r\}$, it would have all the classical "information theory" properties of the Shanon entropy. In particular if we have two subsystems A and B one would expect

$$S[\rho^{\rm A}],\ S[\rho^{\rm B}] \quad \leq \quad S[\rho^{\rm AB}] \quad \leq \quad S[\rho^{\rm A}] + S[\rho^{\rm B}] \tag{1382}$$

This property is also satisfied in the quantum mechanical case provided the subsystems are not entangled in a sense that we define below.

[46.3] Entanglement

Let us consider a system consisting of two sub-systems, "A" and "B", with no correlation between them. Then, the state of the system can be factorized:

$$\rho^{A+B} = \rho^A \rho^B \tag{1383}$$

But in reality the state of the two sub-systems can be correlated. In classical statistical mechanics ρ^A and ρ^B are probability functions, while ρ^{A+B} is the joint probability function. In the classical state we can always write

$$\rho^{A+B}(x,y) = \sum_{x',y'} \rho^{A+B}(x',y')\delta_{x,x'}\delta_{y,y'} \tag{1384}$$

where x and y labels classical definite states of subsystems A and B respectively. This means schematically that we can write

$$\rho^{A+B} = \sum_r p_r \rho^{(A_r)} \rho^{(B_r)} \tag{1385}$$

where $r = (x', y')$ is an index that distinguish pure classical states of $A \otimes B$, and $p_r = \rho^{A+B}(x', y')$ are probabilities such that $\sum p_r = 1$, and $\rho^{(A_r)} \mapsto \delta_{x,x'}$ is a pure classical state of subsystem A, and $\rho^{(B_r)} \mapsto \delta_{y,y'}$ is a pure classical state of subsystem B. Thus any classical state of $A \otimes B$ can be expressed as a *mixture* of product states.

By definition a quantum state is *not entangled* if it is a product state or a mixture of product states. Using explicit matrix representation it means that it is possible to write

$$\rho^{A+B}_{i\alpha,j\beta} = \sum_r p_r \; \rho^{(A_r)}_{i,j} \rho^{(B_r)}_{\alpha,\beta} \tag{1386}$$

It follows that an entangled state, unlike a non-entangled state cannot have a classical interpretation. The simplest implication of non-entanglement is the validity of the entropy inequality that was mentioned in the previous section. We can use this mathematical observation in order to argue that the zero entropy singlet state is an entangled state: It cannot be written as a product of pure states, neither it cannot be a mixture of product states.

The case where ρ^{A+B} is a zero entropy pure state deserves further attention. As in the special case of a singlet, we can argue that if the state cannot be written as a product, then it must be an entangled state. Moreover we shall see below that the entropies of the subsystems satisfy $S[\rho^{\rm A}] = S[\rho^{\rm B}]$. This looks counter intuitive at first sight because subsystem A might be a tiny device which is coupled to a huge environment B. We emphasize that the assumption here is that the "universe" $A \otimes B$ is prepared in a zero order pure state.

In case that the "universe" is in a pure state we cannot write its ρ as a *mixture* of product states, but we can write its Ψ as a *superposition* of product states. The most trivial way to do it is to choose an arbitrary basis $|i\alpha\rangle = |i\rangle \otimes |\alpha\rangle$ and to expand the wavefunction as

$$|\Psi\rangle = \sum_{i,\alpha} \Psi_{i\alpha} |i\alpha\rangle \tag{1387}$$

This is of course a very non-efficient way. By summing over α we can write

$$|\Psi\rangle = \sum_i \sqrt{p_i} |i\rangle \otimes |B_i\rangle \tag{1388}$$

where $|B_i\rangle \propto \sum_\alpha \Psi_{i\alpha}|\alpha\rangle$ is called the "relative state" of subsystem B to the ith state of subsystem A, while p_i is the associated normalization factor. Note that the states $|B_i\rangle$ are in general not orthogonal. The natural question that arise is whether we can find a decomposition such that the $|B_i\rangle$ are orthonormal. The answer is positive: Such decomposition exists and it is unique. It is called Schmidt decomposition, and it is based on singular value decomposition (SVD). Let us regard $\Psi_{i\alpha} = W_{i,\alpha}$ as an $N_A \times N_B$ matrix. From linear algebra it is known that any matrix can be written in a unique way as a product:

$$W_{(N_A \times N_B)} = U^A_{(N_A \times N_A)} D_{(N_A \times N_B)} U^B_{(N_B \times N_B)} \tag{1389}$$

where U^A and U^B are the so called left and right unitary matrices, while D is a diagonal matrix with so called (positive) singular values. Thus we can re-write the above matrix multiplication as

$$\Psi_{i\alpha} = \sum_r U^A_{i,r} \; \sqrt{p_r} \; U^B_{r,\alpha} \tag{1390}$$

Substitution of this expression leads to the result

$$|\Psi\rangle = \sum_r \sqrt{p_r} |A_r\rangle \otimes |B_r\rangle \tag{1391}$$

where $|A_r\rangle$ and $|B_r\rangle$ are implied by the unitary transformations. We note that the normalization of Ψ implies $\sum p_r = 1$. Furthermore the probability matrix is $\rho^{A+B}_{i\alpha,j\beta} = W_{i,\alpha} W^*_{j,\beta}$, and therefore the calculation of the reduced probability matrix can be written as:

$$\begin{array}{lll} \rho^A = & WW^\dagger & = (U^A) D^2 (U^A)^\dagger \\ \rho^B = & (W^T)(W^T)^\dagger & = [(U^B)^\dagger D^2 (U^B)]^* \end{array} \tag{1392}$$

This means that the matrices ρ^A and ρ^B are similar in the mathematical sense, and they have the same eigenvalues $\{p_r\}$. It follows automatically that the associated entropy of the subsystems is the same.

[46.4] Measurements, the notion of collapse

In elementary textbooks the quantum measurement process is described as inducing "collapse" of the wavefunction. Assume that the system is prepared in state $\rho_{\text{initial}} = |\psi\rangle\langle\psi|$ and that one measures $\hat{P} = |\varphi\rangle\langle\varphi|$. If the result of the measurement is $\hat{P} = 1$ then it is said that the system has collapsed into the state $\rho_{\text{final}} = |\varphi\rangle\langle\varphi|$. The probability for this "collapse" is given by the projection formula $\text{Prob}(\varphi|\psi) = |\langle\varphi|\psi\rangle|^2$.

If one regard $\rho(x, x')$ or $\psi(x)$ as representing *physical reality*, rather than a probability matrix or a probability amplitude, then one immediately gets into puzzles. Recalling the EPR experiment this world imply that once the state of one spin is measured at Earth, then immediately the state of the other spin (at the Moon) would change from unpolarized to polarized. This would suggest that some spooky type of "interaction" over distance has occurred.

In fact we shall see that the quantum theory of measurement does not involve any assumption of spooky "collapse" mechanism. Once we recall that the notion of quantum state has a statistical interpretation the mystery fades away. In fact we can show that *there is "collapse" also in classical physics*!

Consider the thought experiment which is known as the "Monty Hall Paradox". There is a car behind one of three doors. The car is like a classical "particle", and each door is like a "site". The initial classical state is such that the car has equal probability to be behind any of the three doors. You are asked to make a guess. Let us say that you peak door #1. Now the organizer opens door #2 and you see that there is no car behind it. This is like a measurement. Now the organizer allows you to change your mind. The naive reasoning is that now the car has equal probability to be behind either of the two remaining doors. So you may claim that it does not matter. But it turns out that this simple answer is very very wrong! The car is no longer in a state of equal probabilities: Now the probability to find it behind door #3 has increased. A standard calculation reveals that the probability to find it behind door #3 is twice large compared with the probability to find it behind door #2. So we have here an example for a classical collapse.

If the reader is not familiar with this well knows "paradox", the following may help to understand why we have this collapse (I thanks my colleague Eitan Bachmat for providing this explanation). Imagine that there are billion doors. You peak door #1. The organizer opens all the other doors except door #234123. So now you know that the car is either behind door #1 or behind door #234123. You want the car. What are you going to do? It is quite obvious that the car is almost definitely behind door #234123. It is also clear the that the collapse of the car into site #234123 does not imply any physical change in the position of the car.

[46.5] Quantum measurements, Schroedinger's cat

What do we mean by quantum measurement? In order to clarify this notion let us consider a system and a detector which are prepared independently as

$$\Psi = \left[\sum_a \psi_a |a\rangle\right] \otimes |q = 0\rangle \tag{1393}$$

As a result of an interaction we assume that the detector correlates with the system as follows:

$$\hat{U}_{\text{measurement}}\Psi = \sum \psi_a |a\rangle \otimes |q = a\rangle \tag{1394}$$

We call such type of unitary evolution "ideal measurement". If the system is in a definite a state, then it is not affected by the detector. Rather, we gain information on the state of the system. One can think of q as representing a memory device in which the information is stored. This memory device can be of course the brain of a human observer. Form the point of view of the observer, the result at the end of the measurement process is to have a definite a. This is interpreted as a "collapse" of the state of the system. Some people wrongly think that "collapse" is something that goes beyond unitary evolution. But in fact this term just makes over dramatization of the above unitary process.

The concept of measurement in quantum mechanics involves psychological difficulties which are best illustrated by considering the "Schroedinger's cat" experiment. This thought experiment involves a radioactive nucleus, a cat, and

a human being. The half life time of the nucleus is an hour. If the radioactive nucleus decays it triggers a poison which kills the cat. The radioactive nucleus and the cat are inside an isolated box. At some stage the human observer may open the box to see what happens with the cat... Let us translate the story into a mathematical language. A time $t = 0$ the state of the universe (nucleus⊗cat⊗observer) is

$$\Psi \;=\; |\uparrow = \text{radioactive}\rangle \;\otimes\; |q = 1 = \text{alive}\rangle \;\otimes |Q = 0 = \text{ignorant}\rangle \tag{1395}$$

where q is the state of the cat, and Q is the state of the memory bit inside the human observer. If we wait a very long time the nucleus would definitely decay, and as a result we will have a definitely dead cat:

$$U_{\text{waiting}}\Psi \;=\; |\downarrow = \text{decayed}\rangle \;\otimes\; |q = -1 = \text{dead}\rangle \;\otimes\; |Q = 0 = \text{ignorant}\rangle \tag{1396}$$

If the observer opens the box he/she would see a dead cat:

$$U_{\text{seeing}}U_{\text{waiting}}\Psi \;=\; |\uparrow = \text{decayed}\rangle \;\otimes\; |q = -1 = \text{dead}\rangle \;\otimes\; |Q = -1 = \text{shocked}\rangle \tag{1397}$$

But if we wait only one hour then

$$U_{\text{waiting}}\Psi \;=\; \frac{1}{\sqrt{2}}\Big[|\uparrow\rangle \otimes |q = +1\rangle + |\downarrow\rangle \otimes |q = -1\rangle\Big] \;\otimes\; |Q = 0 = \text{ignorant}\rangle \tag{1398}$$

which means that from the point of view of the observer the system (nucleus+cat) is in a superposition. The cat at this stage is neither definitely alive nor definitely dead. But now the observer open the box and we have:

$$U_{\text{seeing}}U_{\text{waiting}}\Psi \;=\; \frac{1}{\sqrt{2}}\Big[|\uparrow\rangle \otimes |q = +1\rangle \otimes |Q = +1 = \text{happy}\rangle \;+\; |\downarrow\rangle \otimes |q = -1\rangle \otimes |Q = -1 = \text{shocked}\rangle\Big] \tag{1399}$$

We see that now, form the point of view of the observer, the cat is in a definite(!) state. This is regarded by the observer as "collapse" of the superposition. We have of course two possibilities: one possibility is that the observer sees a definitely dead cat, while the other possibility is that the observer sees a definitely alive cat. The two possibilities "exist" in parallel, which leads to the "many worlds" interpretation. Equivalently one may say that only one of the two possible scenarios is realized from the point of view of the observer, which leads to the "relative state" concept of Everett. Whatever terminology we use, "collapse" or "many worlds" or "relative state", the bottom line is that we have here merely a unitary evolution.

═══ [46.6] Measurements, formal treatment

In this section we describe mathematically how an ideal measurement affects the state of the system. First of all let us write how the U of a measurement process looks like. The formal expression is

$$\hat{U}_{\text{measurement}} = \sum_a \hat{P}^{(a)} \otimes \hat{D}^{(a)} \tag{1400}$$

where $\hat{P}^{(a)} = |a\rangle\langle a|$ is the projection operator on the state $|a\rangle$, and $\hat{D}^{(a)}$ is a translation operator. Assuming that the measurement device is prepared in a state of ignorance $|q = 0\rangle$, the effect of $\hat{D}^{(a)}$ is to get $|q = a\rangle$. Hence

$$\hat{U}\Psi = \left[\sum_a \hat{P}^{(a)} \otimes \hat{D}^{(a)}\right]\left(\sum_{a'} \psi_{a'}|a'\rangle \otimes |q = 0\rangle\right) = \sum_a \psi_a|a\rangle \otimes \hat{D}^{(a)}|q = 0\rangle = \sum_a \psi_a|a\rangle \otimes |q = a\rangle \tag{1401}$$

A more appropriate way to describe the state of the system is using the probability matrix. Let us describe the above measurement process using this language. After "reset" the state of the measurement apparatus is $\sigma^{(0)} = |q{=}0\rangle\langle q{=}0|$.

The system is initially in an arbitrary state ρ. The measurement process correlates that state of the measurement apparatus with the state of the system as follows:

$$\hat{U}\rho\otimes\sigma^{(0)}\hat{U}^{\dagger}=\sum_{a,b}\hat{P}^{(a)}\rho\hat{P}^{(b)}\otimes[\hat{D}^{(a)}]\sigma^{(0)}[\hat{D}^{(b)}]^{\dagger}=\sum_{a,b}\hat{P}^{(a)}\rho\hat{P}^{(b)}\otimes|q{=}a\rangle\langle q{=}b| \tag{1402}$$

Tracing out the measurement apparatus we get

$$\rho^{\text{sys}} \;=\; \sum_{a}\hat{P}^{(a)}\rho\hat{P}^{(a)}=\sum_{a}p_{a}\rho^{(a)} \tag{1403}$$

Where p_a is the trace of the projected probability matrix $\hat{P}^{(a)}\rho\hat{P}^{(a)}$, while $\rho^{(a)}$ is its normalized version. We see that the effect of the measurement is to turn the superposition into a mixture of a states, unlike unitary evolution for which

$$\rho^{\text{sys}} \;=\; U_{\text{system}}\;\rho\;U^{\dagger}_{\text{system}} \tag{1404}$$

So indeed a measurement process looks like a non-unitary process: it turns a pure superposition into a mixture. A simple example is in order. Let us assume that the system is a spin 1/2 particle. The spin is prepared in a pure polarization state $\rho=|\,\psi\rangle\langle\psi\,|$ which is represented by the matrix

$$\rho_{ab}=\psi_{a}\psi_{b}^{*}=\begin{pmatrix}|\,\psi_{1}\,|^{2} & \psi_{1}\psi_{2}^{*}\\ \psi_{2}\psi_{1}^{*} & |\,\psi_{2}\,|^{2}\end{pmatrix} \tag{1405}$$

where 1 and 2 are (say) the "up" and "down" states. Using a Stern-Gerlech apparatus we can measure the polarization of the spin in the up/down direction. This means that the measurement apparatus projects the state of the spin using

$$P^{(1)}=\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}\qquad\text{and}\qquad P^{(2)}=\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix} \tag{1406}$$

leading after the measurement to the state

$$\rho=P^{(1)}\rho P^{(1)}+P^{(2)}\rho P^{(2)}=\begin{pmatrix}|\,\psi_{1}\,|^{2} & 0\\ 0 & |\,\psi_{2}\,|^{2}\end{pmatrix} \tag{1407}$$

Thus the measurement process has eliminated the off-diagonal terms in ρ and hence turned a pure state into a mixture. It is important to remember that this non-unitary non-coherent evolution arise because we look only on the state of the system. On a universal scale the evolution is in fact unitary.

[47] Theory of Quantum Computation

[47.1] Motivating Quantum Computation

Present day secure communication is based on the RSA two key encryption method. The RSA method is based on the following observation: Let N be the product of two unknown big prime numbers p and q. Say that we want to find are what are its prime factors. The simple minded way would be to try to divide N by 2, by 3, by 5, by 7, and so on. This requires a huge number ($\sim N$) of operations. It is assumed that N is so large such that in practice the simple minded approached is doomed. Nowadays we have the technology to build classical computers that can handle the factoring of numbers as large as $N \sim 2^{300}$ in a reasonable time. But there is no chance to factor larger numbers, say of the order $N \sim 2^{308}$. Such large numbers are used by Banks for the encryption of important transactions. In the following sections we shall see that factoring of a large number N would become possible once we have a quantum computer.

Computational complexity: A given a number N can be stored in an n-bit register. The size of the register should be $n \sim \log(N)$, rounded upwards such that $N \leq 2^n$. As explained above in order to factor a number which is stored in an n bit register by a classical computer we need an exponentially large number ($\sim N$) of operations. Obviously we can do some of the operations in parallel, but then we need an exponentially large hardware. Our mission is to find an efficient way to factor an n-bit number that do not require exponentially large resources. It turns out that a quantum computer can do the job with hardware/time resources that scale like power of n, rather than exponential in n. This is done by finding a number N_2 that has a common divisor with N. Then it is possible to use Euclid's algorithm in order to find this common divisor, which is either p or q.

Euclid's algorithm: There is no efficient algorithm to factor a large number $N \sim 2^n$. The classical computational complexity of this task is exponentially large in n. But if we have two numbers $N_1 = N$ and N_2 we can quite easily and efficiently find their greater common divisor $\mathrm{GCD}(N_1, N_2)$ using Euclid's algorithm. Without loss of generality we assume that $N_1 > N_2$. The two numbers are said to be co-prime if $\mathrm{GCD}(N_1, N_2) = 1$. Euclid's algorithm is based on the observation that we can divide N_1 by N_2 and take the reminder $N_3 = \mathrm{mod}(N_1, N_2)$ which is smaller than N_2. Then we have $\mathrm{GCD}(N_1, N_2) = \mathrm{GCD}(N_2, N_3)$. We iterate this procedure generating a sequence $N_1 > N_2 > N_3 > N_4 > \cdots$ until the reminder is zero. The last non-trivial number in this sequence is the greater common divisor.

The RSA encryption method: The RSA method is based on the following mathematical observation. Given two prime numbers p and q define $N = pq$. Define also a and b such that $ab = 1 \mod [(p-1)(q-1)]$. Then we have the relations

$$B = A^a \mod [N] \tag{1408}$$
$$A = B^b \mod [N] \tag{1409}$$

This mathematical observation can be exploited as follows. Define

$$\text{public key} = (N, a) \tag{1410}$$
$$\text{private key} = (N, b) \tag{1411}$$

If anyone want to encrypt a message A, one can use for this purpose the public key. The coded message B cannot be decoded unless one knows the private key. This is based on the assumption that the prime factors p and q and hence b are not known.

[47.2] The factoring algorithm

In order to factor N we have to find a number $\tilde{N}$ such that $\mathrm{GCD}(N, \tilde{N}) > 1$. The quantum computer will help us to find such $\tilde{N}$. The factoring algorithm goes as follows:

(1) We have to store N inside an n-bit register.

(2) We pick a large number M which is smaller than N. We assume that M is co-prime to N. This assumption can be easily checked using Euclid'd algorithm. If by chance the chosen M is not co-prime to N then we are lucky and we can factor N without quantum computer. So we assume that we are not lucky, and M is co-prime to N.

(3) We build a processor that can calculate the function $f(x) = M^x \mod (N)$. On the basis of Fermat theorem it can be argued that this function has a period r which is smaller than N.

(4) Using a quantum computer we find one of the Fourier components of $f(x)$ and hence its period r. This means that $M^r = 1 \mod (N)$.

(5) If r is not even we have to run the quantum computer a second time with a different M. There is a mathematical theorem that guarantees that with probability of order one we should be able to find M for which r is even.

(6) Assuming that r is even we define $Q = M^{r/2} \mod (N)$. We have $Q^2 = 1 \mod (N)$, and therefore $(Q-1)(Q+1) = 0 \mod (N)$. Consequently both $(Q-1)$ and $(Q+1)$ must have either p or q as common divisors with N.

(6) Using Euclid'd algorithm we find the GCD of N and $\tilde{N} = (Q-1)$, hence getting either p or q.

The bottom line is that given N and M an an input, we would like to find the period r of the functions

$$f(x) = M^x \mod (N) \tag{1412}$$

Why do we need a quantum computer to find the period? Recall that the period is expected to be of order N. Therefore the x register should be n_c bits, where n_c is larger or equal to n. Then we have to make order of 2^{n_c} operations for the purpose of evaluating $f(x)$ so as to find out its period. It is assumed that n is large enough such that this procedure is not practical. We can of course try to do parallel computation of $f(x)$. But for that we need hardware which is larger by factor of 2^n. It is assumed that to have such computational facility is equally not practical. We say that factoring a large number has an exponentially complexity.

The idea of quantum processing is that the calculation of $f(x)$ can be done "in parallel" without having to duplicate the hardware. The miracle happens due to the superposition principle. A single quantum register of size n_c can be prepared at $t = 0$ with all the possible input x values in superposition. The calculation of $f(x)$ is done in parallel on the prepared state. The period of $f(x)$ in found via a Fourier analysis. In order to get good resolution n_c should be larger than n so as to have $2^{n_c} \gg 2^n$. Neither the memory, nor the number of operation, are required to be exponentially large.

═══ [47.3] The quantum computation architecture

We shall regard the computer as a machine that has registers for memory and gates for performing operations. The complexity of the computation is determined by the total number of memory bits which has to be used times the number of operations. In other words the complexity of the calculation is the product memory × time. As discussed in the previous section classical parallel computation do not reduce the complexity of a calculation. Both classical and quantum computers work according to the following scheme:

$$|\text{output}\rangle = U[\text{input}]|0\rangle \tag{1413}$$

This means that initially we set all the bits or all the qubits in a zero state (a reset operation), and then we operate on the registers using gates, taking the input into account. It is assumed that there is a well define set of elementary gates. An elementary gate (such as "AND") operates on few bits (2 bits in the case of ANS) at a time. The size of the hardware is determined by how many elementary gates are required in order to realize the whole calculation.

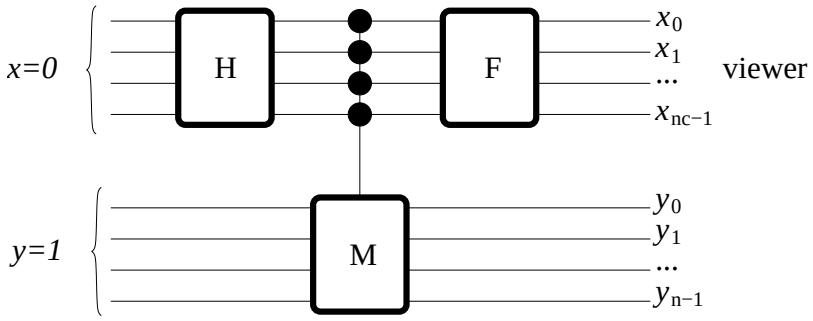
The quantum analog of the digital bits ("0" or "1") are the qubits, which can be regarded as spin 1/2 elements. These are "analog" entities because the "spin" can point in any direction (not just "up" or "down"). The set of states such that each spin is aligned either "up" or "down" is called the *computational basis*. Any other state of a register can be written a superposition:

$$|\Psi\rangle = \sum_{x_0,x_1,x_2,\ldots} \psi(x_0, x_1, x_2...)\ |x_0, x_1, x_2, ...\rangle \tag{1414}$$

The architecture of the quantum computer which is requited in order to find the period r of the function $f(x)$ is illustrated in the figure below. We have two registers:

$$x = (x_0, x_1, x_2, ..., x_{n_c-1}) \tag{1415}$$
$$y = (y_0, y_0, y_2, ..., y_{n-1}) \tag{1416}$$

The y register is used by the CPU for processing mod(N) operations and therefore it requires n bits. The x register has n_c bits and it is used to store the inputs for the function $f(x)$. In order to find the period of $f(x)$ the size n_c of the latter register should be some number (say 100) times n. Such large n_c is required if we want to determine the period with large accuracy.



We are now ready to describe the quantum computation. In later sections we shall give more details, and in particular we shall see that the realization of the various unitary operations which are listed below does not require an exponentially large hardware. The preliminary stage is to make a "reset" of the registers, so as to have

$$\Psi = |x; y\rangle = |0, 0, 0, ..., 0, 0; 1, 0, 0, ..., 0, 0\rangle \tag{1417}$$

Note that it is convenient to start with $y = 1$ rather than $y = 0$. Then come a sequence of unitary operations

$$U = U_F U_M U_H \tag{1418}$$

where

$$U_H = U_{\text{Hadamard}} \otimes \mathbf{1} \tag{1419}$$
$$U_M = \sum_x |x\rangle\langle x| \otimes U_M^{(x)} \tag{1420}$$
$$U_F = U_{\text{Fourier}} \otimes \mathbf{1} \tag{1421}$$

The first stage is a unitary operation U_H that sets the x register in a democratic state. It can realized by operating on Ψ with the Hadamard gate. Disregarding normalization we get

$$\Psi = \sum_x |x\rangle \otimes |y{=}1\rangle \tag{1422}$$

The second stage is an x controlled operation U_M. This stage is formally like a quantum measurement: The x register is "measured" by the y register. The result is

$$\Psi = \sum_x |x\rangle \otimes |y{=}f(x)\rangle \tag{1423}$$

Now the y register is entangled with the x register. The fourth stage is to perform Fourier transform on the x register:

$$\Psi = \sum_x \left[\sum_{x'} \mathrm{e}^{i\frac{2\pi}{N_c}xx'} |x'\rangle \right] \otimes |f(x)\rangle \tag{1424}$$

We replace the dummy integer index x' by $k = (2\pi/N_c)x'$ and re-write the result as

$$\Psi = \sum_k |k\rangle \otimes \left[\sum_x \mathrm{e}^{ikx} |f(x)\rangle \right] \tag{1425}$$

The final stage is to measure the x register. The probability to get k as the result is

$$\mathrm{Prob}(k) = \left|\left| \sum_x \mathrm{e}^{ikx} |f(x)\rangle \right|\right| \tag{1426}$$

The only non-zero probabilities are associated with $k = \text{integer} \times (2\pi/r)$. Thus we are likely to find one of these k values, from which we can deduce the period r. Ideally the error is associated with the finite length of the x register. By making the x register larger the visibility of the Fourier components becomes better.

═══ [47.4] Elementary quantum gates

The simplest gates are one quibit gates. They can be regarded as spin rotations. Let us list some of them:

$$\begin{aligned}
T &= \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{e}^{i\pi/4} \end{pmatrix} \qquad (1427)\\
S &= T^2 = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \\
Z &= S^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z = i\mathrm{e}^{-i\pi S_z} \\
X &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x = i\mathrm{e}^{-i\pi S_x} = \text{NOT gate} \\
Y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y = i\mathrm{e}^{-i\pi S_y} = iR^2 \\
R &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(1 - i\sigma_y) = \mathrm{e}^{-i(\pi/2)S_y} = \text{90deg Rotation} \\
H &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = i\mathrm{e}^{-i\pi S_n} = \text{Hadamard gate}
\end{aligned}$$

We have $R^4 = -1$ which is a 2π rotation in $SU(2)$. We have $X^2 = Y^2 = Z^2 = H^2 = 1$ which implies that these are π rotations in $U(2)$. We emphasize that though the operation of H on "up" or "down" states looks like $\pi/2$ rotation, it is in fact a π rotation around a 45^o inclined axis:

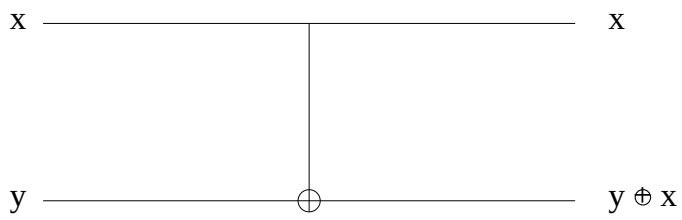
$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right) \cdot \vec{\sigma} = \vec{n} \cdot \vec{\sigma} \tag{1428}$$

More interesting are elementary gates that operate on two qubits. In classical computers it is popular to use "AND" and "OR" gates. In fact with "AND" and the one-bit operation "NOT" one can build any other gate. The "AND" cannot be literally realized as quantum gate because it does not correspond to unitary operation. But we can build

the same logical circuits with "CNOT" (controlled NOT) and the other one-qubit gates. The definition of CNOT is as follows:

$$U_{\rm CNOT} = \begin{pmatrix} 1 & 0 & & \\ 0 & 1 & & 0 \\ & & 0 & 1 \\ & 0 & 1 & 0 \end{pmatrix} \tag{1429}$$

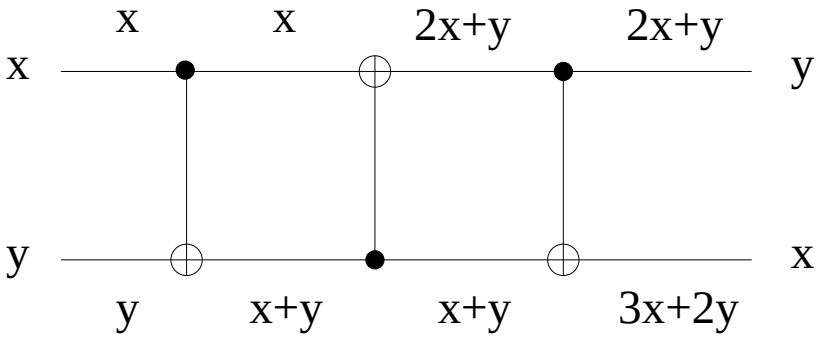
The control bit is not affected while the y bit undergoes NOT provided the x bit is turned on. The gate is schematically illustrated in the following figure:



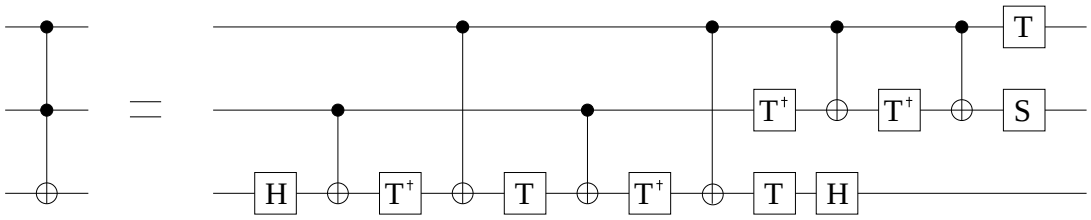
I is amusing to see how SWAP can be realized by combining 3 CNOT gates:

$$U_{\rm SWAP} = \begin{pmatrix} 1 & & & \\ & 0 & 1 & \\ & 1 & 0 & \\ & & & 1 \end{pmatrix} \tag{1430}$$

which is illustrated is the following diagram:



The generalization of CNOT to the case where we have two qubit control register is known as Toffoli. The NOT operation is performed only if both control bits are turned on:



The realization of the Toffoli gate opens the way to the quantum realization of an AND operation. Namely, by setting $y = 0$ at the input, the output would be $y = x_1 \wedge x_2$. For generalization of the Toffoli gate to the case where the x register is of arbitrary size see p.184 of Nielsen and Chuang.

[47.5] The Hadamard Transform

In the following we discuss the Hadamard and the Fourier transforms. These are unitary operations that are defined on the multi-qubit x register. A given basis state $|x_0, x_1, x_3, ...\rangle$ can be regarded as the binary representation of an integer number:

$$x = \sum_{r=0}^{n_c} x_r 2^r \tag{1431}$$

We distinguish between algebraic multiplication for which we use the notation xx'. and scalar product for which we use the notation $x \cdot x'$,

$$\begin{aligned} x \cdot x' &= \sum_r x_r x'_r \\ xx' &= \sum_{r,s} x_r x'_s 2^{r+s} \end{aligned} \tag{1432}$$

So far we have defined the single qubit Hadamard gate. If we have an multi-qubit register it is natural to define

$$U_{\text{Hadamard}} = H \otimes H \otimes H \otimes \cdots \tag{1433}$$

The operation of a single-qubit Hadamard gate can be written as

$$|x_1\rangle \xrightarrow{H} \frac{1}{\sqrt{2}} \left(|0\rangle + (-1)^{x_1} |1\rangle\right) \tag{1434}$$

If we have a multi-qubit register we simply have to perform (in parallel) an elementary Hadamard transform on each qubit:

$$\begin{aligned} |x_0, x_1, ..., x_r, ...\rangle \xrightarrow{H} \quad & \prod_r \frac{1}{\sqrt{2}} \left(|0\rangle + (-1)^{x_r} |1\rangle\right) = \frac{1}{\sqrt{2^{n_c}}} \prod_r \left[\sum_{k_r=0,1} (-1)^{k_r x_r} |k_r\rangle \right] \\ & = \frac{1}{\sqrt{N_c}} \sum_{k_0, k_1, ...} (-1)^{k_0 x_0 + k_1 x_1 + ...} |k_0, k_1, ..., k_r, ...\rangle = \frac{1}{\sqrt{N_c}} \sum_k (-1)^{k \cdot x} |k\rangle \end{aligned} \tag{1435}$$

The Hadmard transform is useful in order to prepare a "democratic" superposition state as follows:

$$|0, 0, ..., 0\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes ... \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \mapsto \frac{1}{\sqrt{N_c}} \begin{pmatrix} 1 \\ 1 \\ . \\ . \\ . \\ 1 \end{pmatrix} \tag{1436}$$

To operate with a unitary operator on this state is like making parallel computation on all the possible x basis states.

[47.6] The quantum Fourier transform

The definitions of the Hadamard transform and the quantum Fourier transform are very similar in style:

$$U_{\text{Hadamard}}|x\rangle = \frac{1}{\sqrt{N_c}}\sum_k (-1)^{k\cdot x}|k\rangle \tag{1437}$$

$$U_{\text{Fourier}}|x\rangle = \frac{1}{\sqrt{N_c}}\sum_k \mathrm{e}^{-i\frac{2\pi}{N_c}kx}|k\rangle \tag{1438}$$

Let us write the definition of the quantum Fourier transform using different style so as to see that it is indeed a Fourier transform operation in the conventional sense. First we notice that its matrix representation is

$$\langle x'|U_{\text{Fourier}}|x\rangle = \frac{1}{\sqrt{N_c}}\mathrm{e}^{-i\frac{2\pi}{N_c}x'x} \tag{1439}$$

If we operate with it on the state $|\psi\rangle = \sum_x \psi_x|x\rangle$ we get $|\varphi\rangle = \sum_x \varphi_x|x\rangle$, where the column vector φ_x is obtained from ψ_x by a multiplication with the matrix that represents U_{Fourier}. Changing the name of the dummy index form x to k we get the relation

$$\varphi_k = \frac{1}{\sqrt{N_c}}\sum_{x=0}^{N_c-1}\mathrm{e}^{-i\frac{2\pi}{N_c}kx}\psi_x \tag{1440}$$

This is indeed the conventional definition of

$$\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ .\\ .\\ .\\ \psi_{N_c-1}\end{pmatrix} \xrightarrow{FT} \begin{pmatrix}\varphi_0\\ \varphi_1\\ \varphi_2\\ .\\ .\\ .\\ \varphi_{N_c-1}\end{pmatrix} \tag{1441}$$

The number of memory bits which are required to store these vectors in a classical register is of order $N \sim 2^n$. The number of operations which is involved in the calculation of a Fourier transform seems to be of order N^2. In fact there is an efficient "Fast Fourier Transform" (FFT) algorithm that reduces the number of required operations to $N \log N = n2^n$. But this is still an exponentially large number in n. In contrast to that a quantum computer can store these vectors in n qubit register. Furthermore, the "quantum" FT algorithm can perform the calculation with only $n^2 \log n \log\log n$ operations. We shall not review here how the Quantum Fourier transform is realized. This can be found in the textbooks. As far as this presentation is concerned the Fourier transform can be regarded as a complicated variation of the Hadamard transform.

A few words are in order here regarding quantum computation versus classical analog computation. In an analog computer every analog "bit" can have a voltage within some range, so ideally each analog bit can store infinite amount of information. This is of course not the case in practice because the noise in the circuit defines some effective finite resolution. Consequently the performance is not better compared with a digital computers. In this context the analog resolution is a determining factor in the definition of the memory size. Closely related is optical computation. This can be regarded as a special type of analog computation. Optical Fourier Transform of a "mask" can be obtained on a "screen" that is placed in the focal plane of a lens. The FT is done in one shot. However, also here we have the same issue: Each pixel of the mask and each pixel of the screen is a hardware element. Therefore we still need an exponentially large hardware just to store the vectors. At best the complexity of FT with optical computer is of order 2^n.

[47.7] The U_M operation

The CNOT/Toffoli architecture can be generalized so as to realize any operation of the type $y = f(x_1, x_2, ...)$, as an x-controlled operation, where y is a single qubit. More generally we have

$$x = (x_0, x_1, x_2 ... x_{n_c - 1}) \tag{1442}$$
$$y = (y_0, y_1, y_2, ... y_{n-1}) \tag{1443}$$

and we can realize unitary controlled operations

$$U = \sum_x P^x \otimes U^{(x)} = P^0 \otimes U^{(0)} + P^1 \otimes U^{(1)} + P^2 \otimes U^{(2)} + ... \tag{1444}$$

This is formally like a measurement of the x register by the y register. Note that x is a constant of motion, and that U has a block diagonal form:

$$\langle\ x', y'|U|\ x, y\rangle = \delta_{x',x} U^{(x)}_{y',y} = \begin{pmatrix} U^0 & & & \\ & U^1 & & \\ & & U^2 & \\ & & & ... \end{pmatrix} \tag{1445}$$

Of particular interest is the realization of $y = M^x \mod (N)$. We define

$$U^{(x)}_M |y\rangle = |M^x y\rangle \tag{1446}$$

If M is co-prime to N then U is merely a permutation matrix, and therefore it is unitary. The way to realize this operation is implied by the formula

$$M^x = M^{\sum_s x_s 2^s} = \prod_s \left(M^{2^s}\right)^{x_s} = \prod_{s=0}^{n-1} M_s^{x_s} \tag{1447}$$

which requires n stages of processing. The circuit is illustrated in the figure below. In the s stage we have to perform a controlled multiplication of y by $M_s \equiv M^{2^s} \mod (N)$.