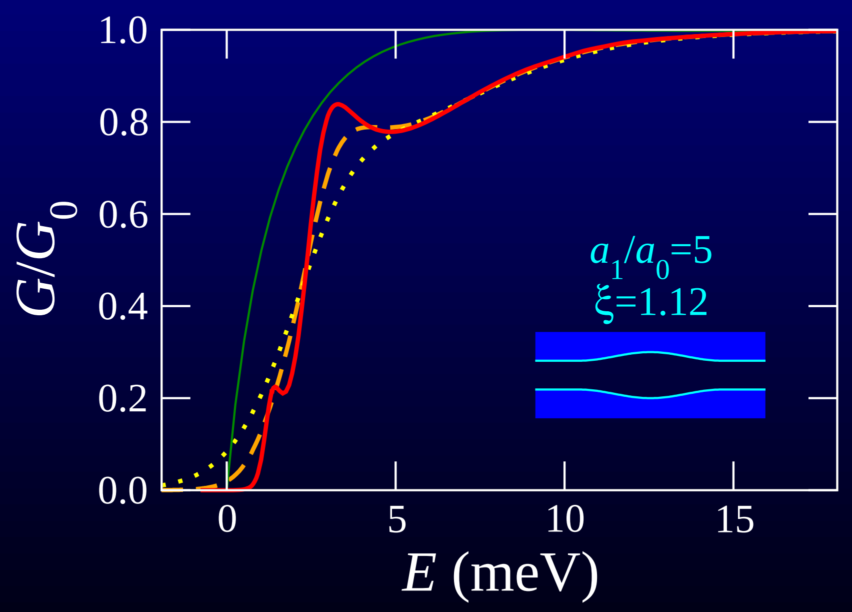
Tomaž Rejec

Transport Properties of Strongly Correlated Nanoscopic Systems

Thesis



Outline

- Introduction
- Spin-dependent anomalies at the conduction edge of quantum wires
- Zero-temperature conductance through an interacting electron region
- Summary

Mesoscopic physics

macroscopic systems

succesfully described with scale independent quantities

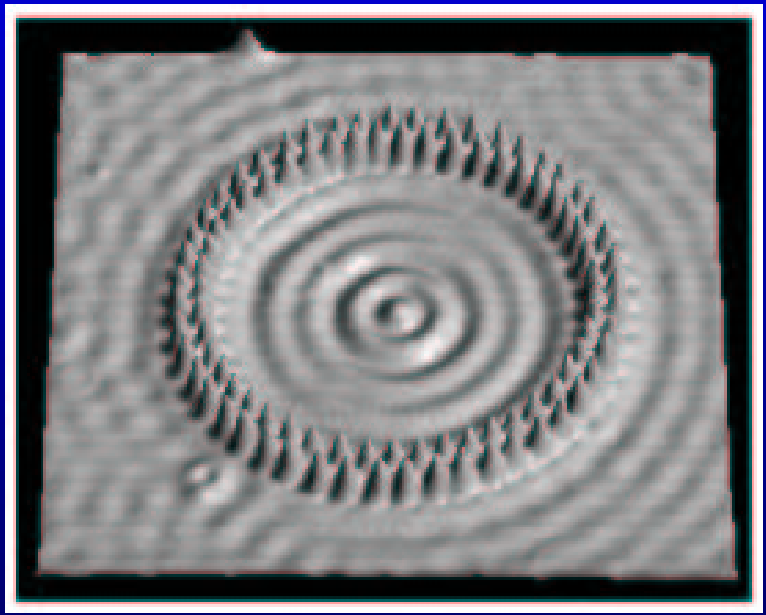
•

coherence length

•

mesoscopic (nanoscopic) systems

quantum interference, multi-particle entanglement



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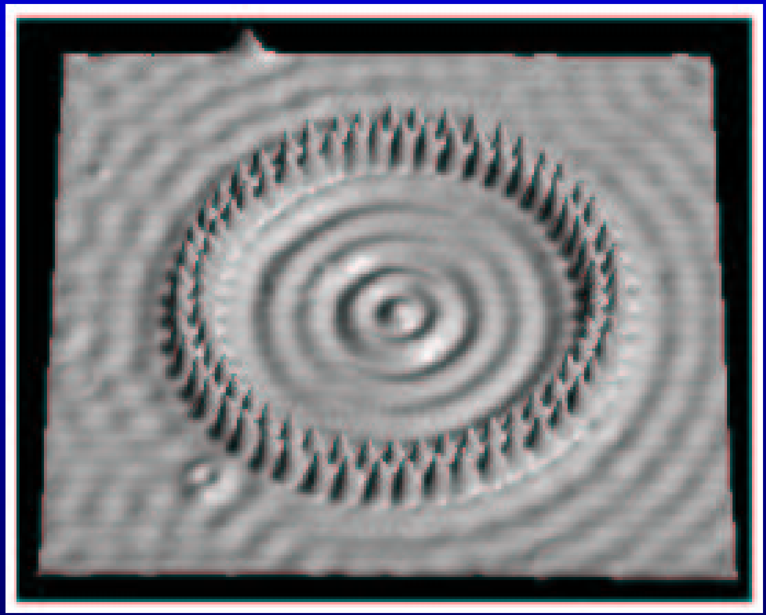
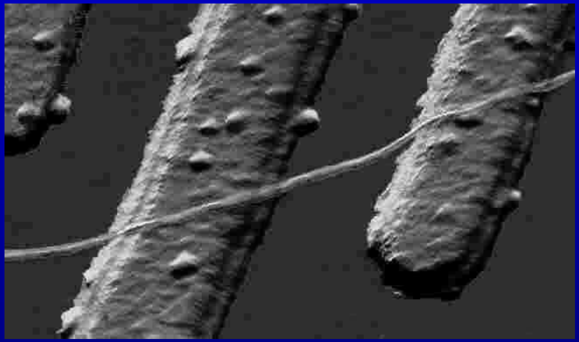
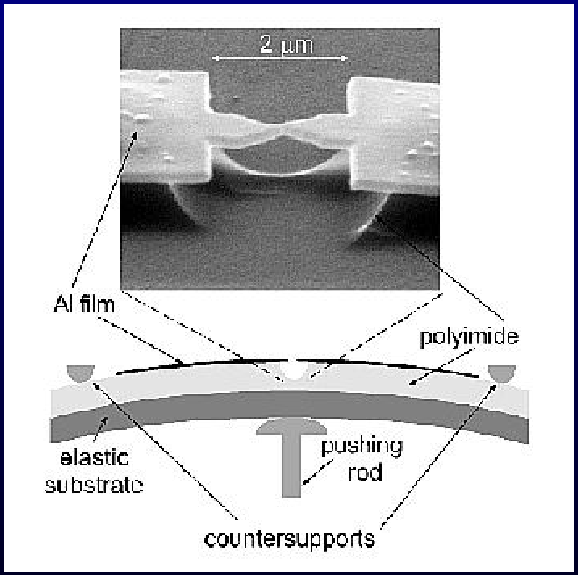


- basic physics
  - ⋆ better understanding of microscopic objects
  - ⋆ new phenomena in nanoscopic systems
- technological applications
  - ⋆ computer industry
  - ⋆ quantum computers (q-bit)
  - ⋆ chemical & biological sensors, ...

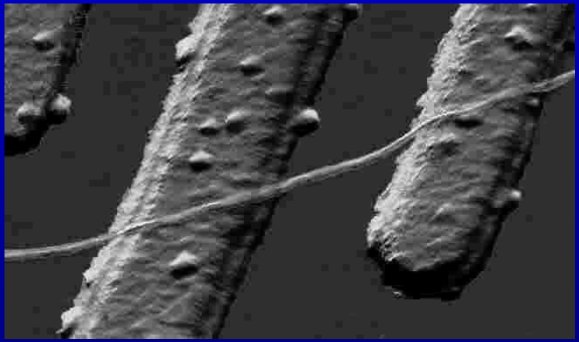
Conductance





Conductance

$$G = \frac{\delta I}{\delta V}$$



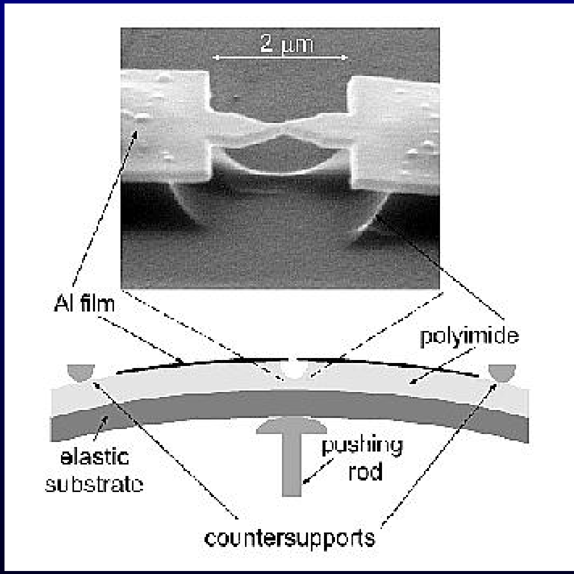
$$\delta I = e \cdot \rho\left(\epsilon_F\right) \cdot v\left(\epsilon_F\right) \cdot e\,\delta V$$

In 1D:

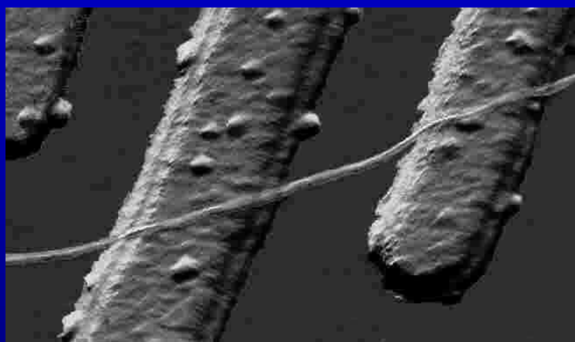
$$v\left(\epsilon\right) \propto \sqrt{\epsilon},$$

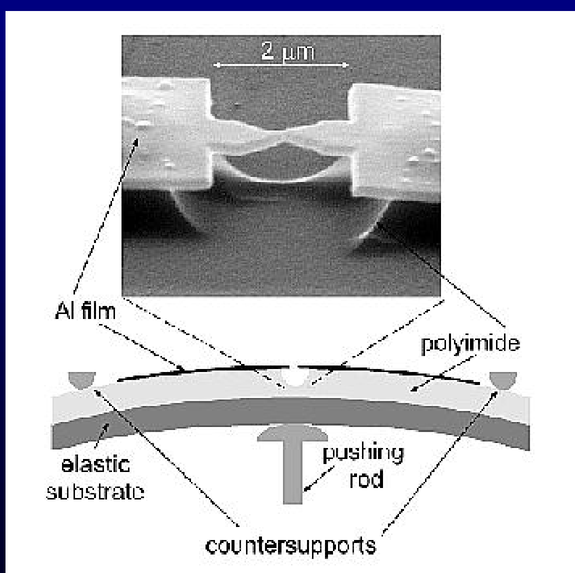
$$\rho\left(\epsilon\right) \propto 1/\sqrt{\epsilon}$$

$$G = \frac{2e^2}{h}$$



Conductance





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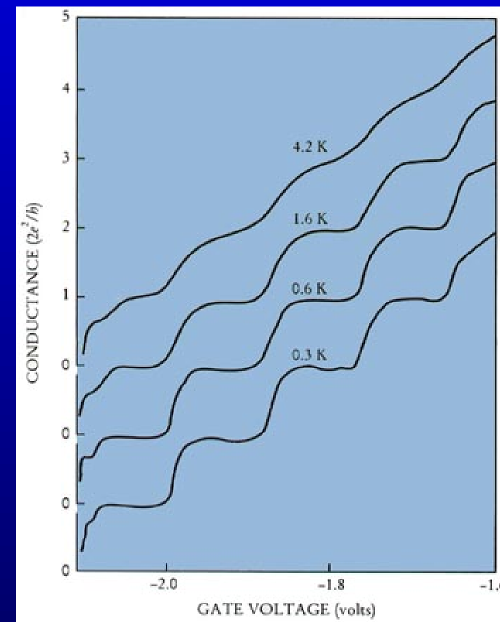
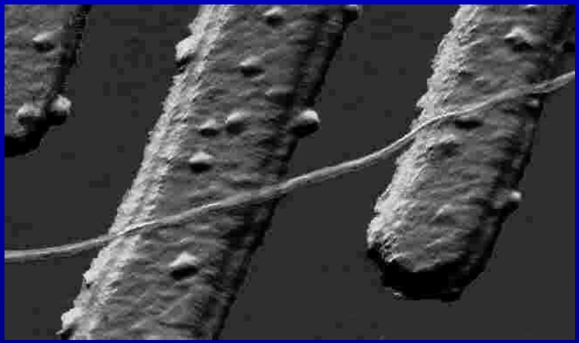


Conductance



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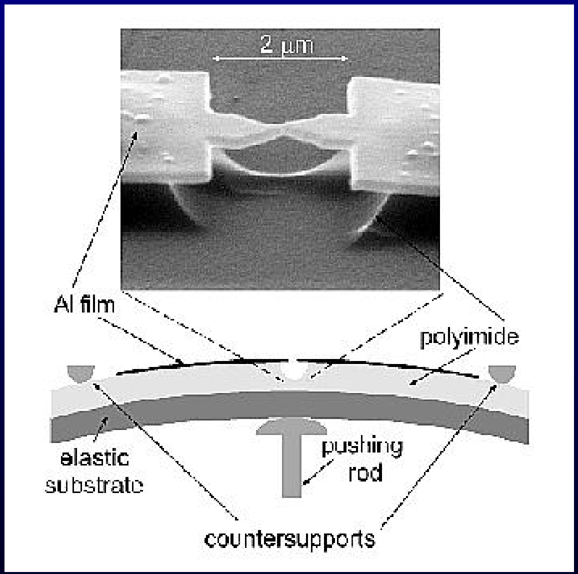
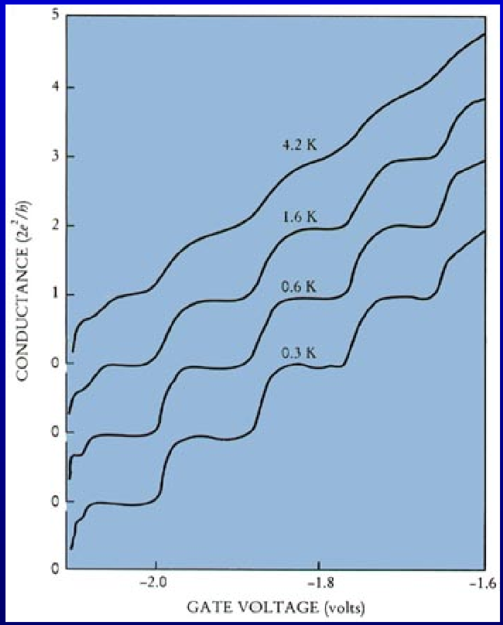




Landauer-Büttiker formula

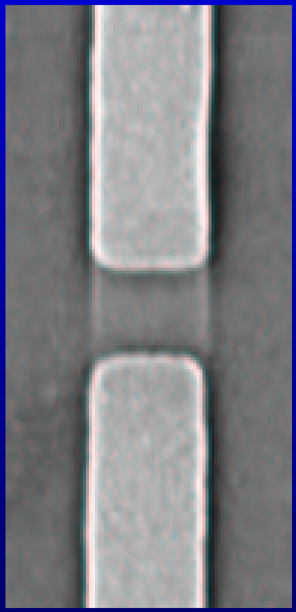
$$G = \frac{2e^2}{h} \int \mathrm{d}\epsilon \left(-\frac{\partial f(\epsilon)}{\partial \epsilon}\right) |t(\epsilon)|^2$$

Conductance quantum: $\frac{e^2}{h} = (25.8\,\mathrm{k}\Omega)^{-1}$

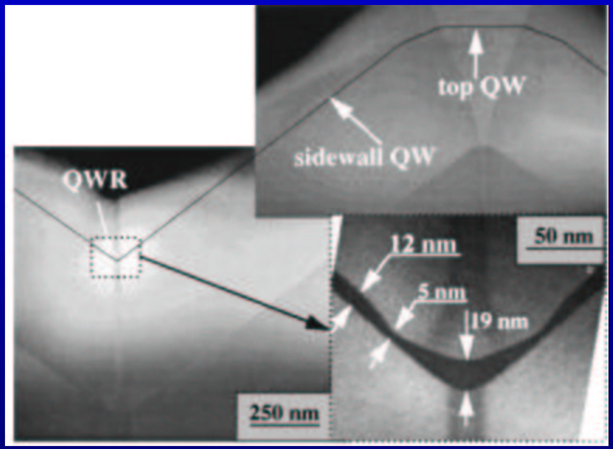
Outline

- Introduction
- Spin-dependent anomalies at the conduction edge of quantum wires
  - ⋆ System
  - ⋆ Conductance
  - ⋆ Extended Anderson Model
- Zero-temperature conductance through an interacting electron region
- Summary

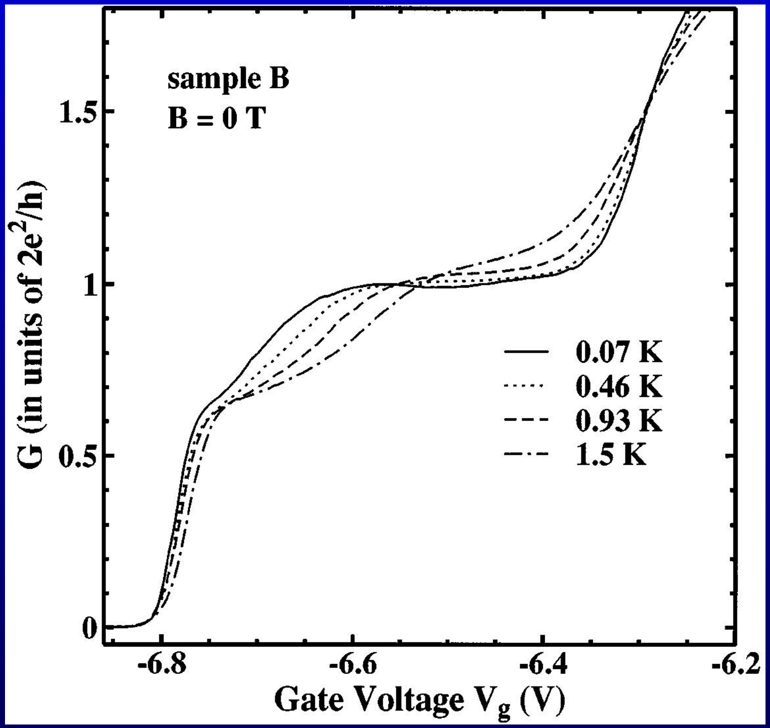
0.7 anomaly



Quantum point contact



'v'-groove quantum wire



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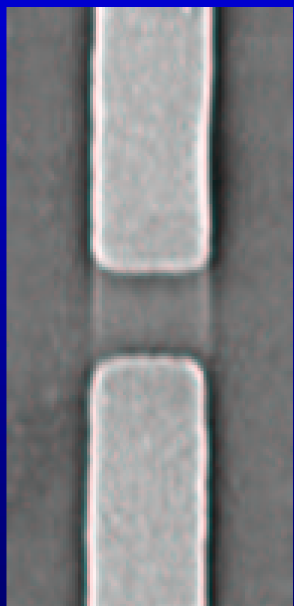

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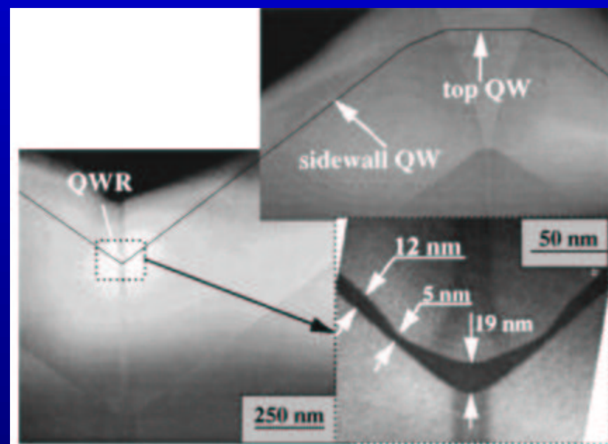

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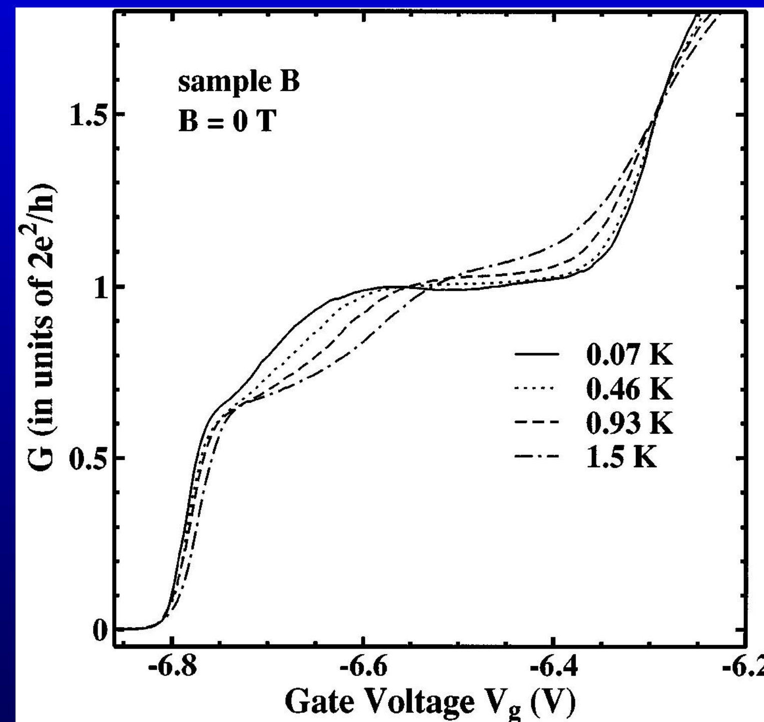
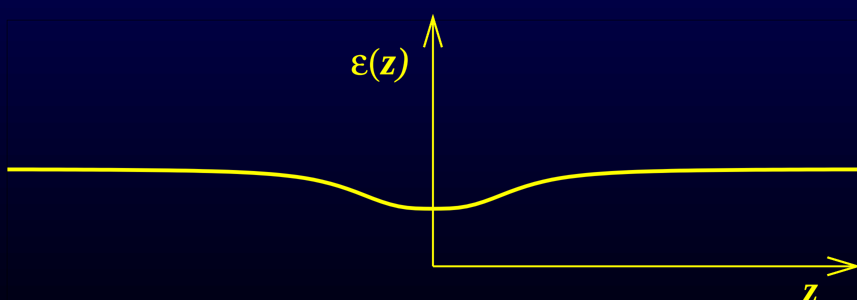
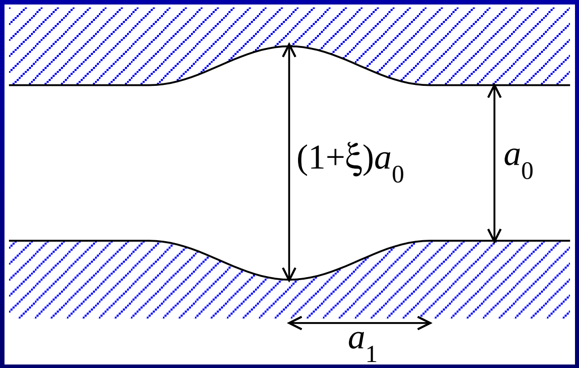




- thickness fluctuation
- nearby impurity charge
- image charge on an electrode
- self-consistent effect

Model Hamiltonian

$$-\frac{\hbar^2}{2m^*}\nabla^2\Psi\left(r,\varphi,z\right)+V\left(r,z\right)\Psi\left(r,\varphi,z\right)=E\Psi\left(r,\varphi,z\right)$$



$$\Psi(r,\varphi,z)=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\psi_{mn}\left(z\right)\Phi_{mn}\left(r,\varphi;z\right)$$

$$\psi''_{mn}\left(z\right)+\left[k^2-k^2_{mn}\left(z\right)+a_{mnn}\left(z\right)\right]\psi_{mn}\left(z\right)+$$
$$+\sum_{n\neq n'}b_{mnn'}(z)\psi'_{mn'}\left(z\right)+\sum_{n\neq n'}a_{mnn'}\left(z\right)\psi_{mn'}\left(z\right)=0$$

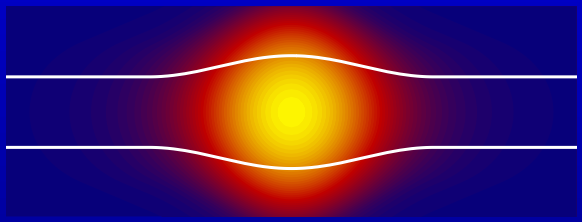
$$H=-\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+\epsilon(z)$$

Coulomb interaction:

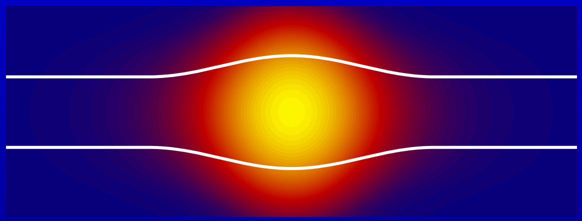
$$U(z,z')=\frac{e^2}{4\pi\epsilon\epsilon_0 d\left(z,z'\right)}$$

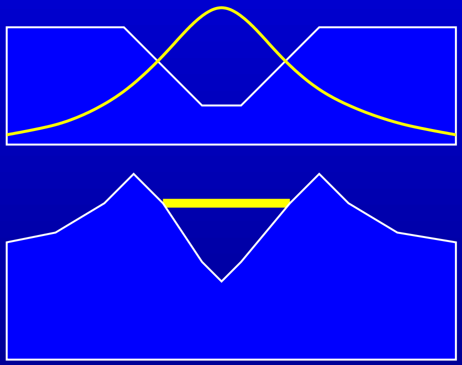
$$\frac{1}{d\left(z,z'\right)}=\int\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'\frac{\left|\Phi_{00}\left(\mathbf{r};z\right)\right|^2\left|\Phi_{00}\left(\mathbf{r}';z'\right)\right|^2}{\sqrt{\left(z-z'\right)^2+\left|\mathbf{r}-\mathbf{r}'\right|^2}}$$

Conductance



Conductance





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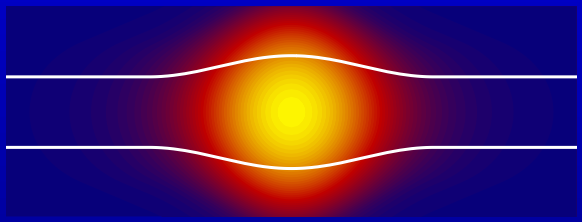

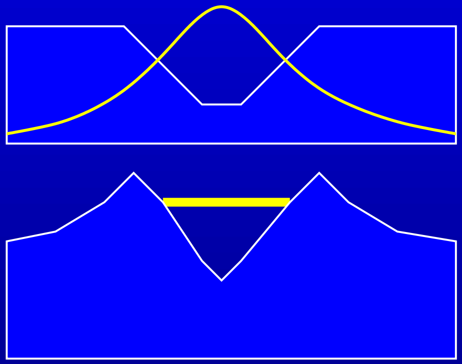

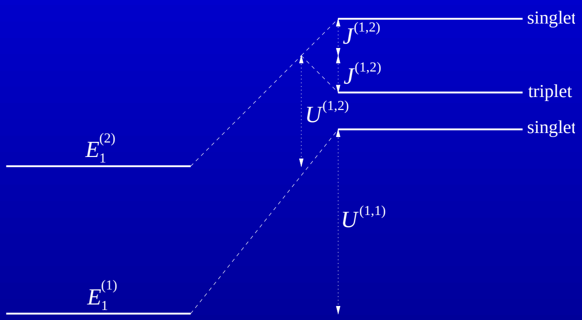

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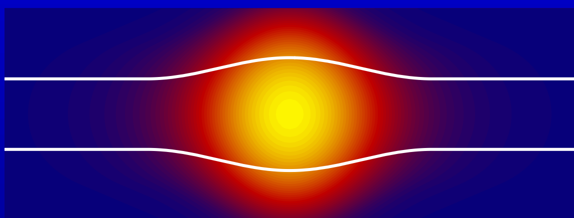

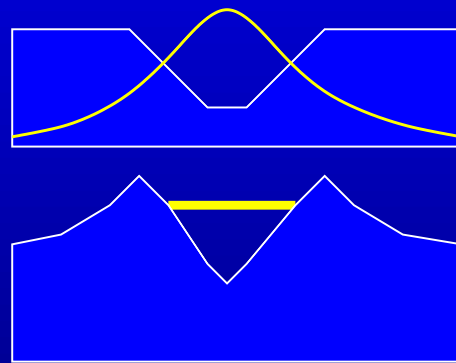

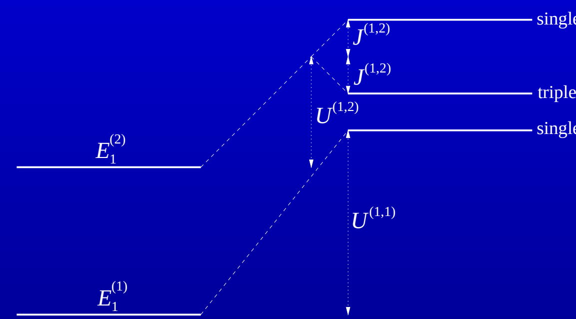

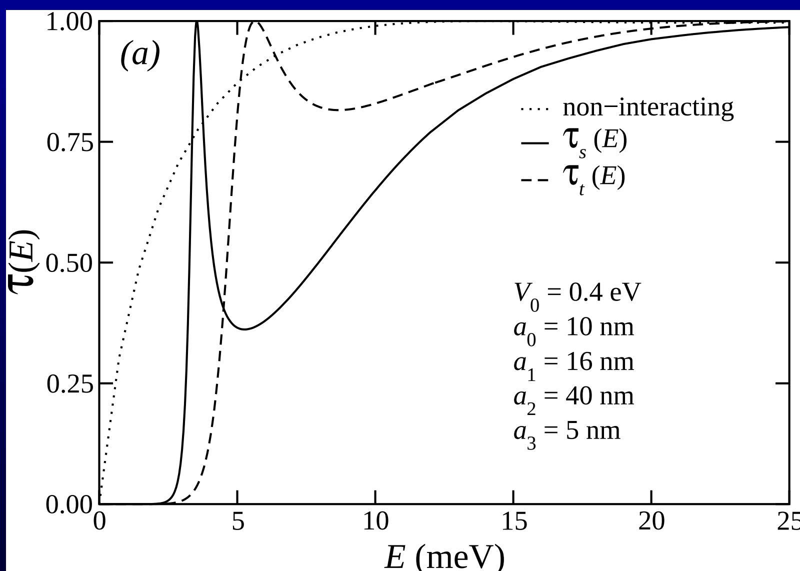

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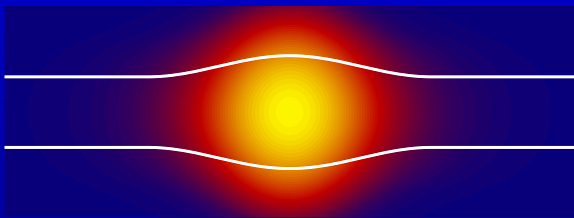
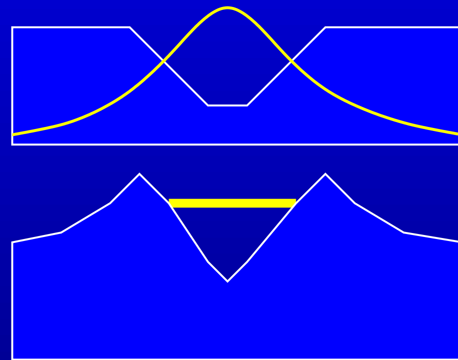
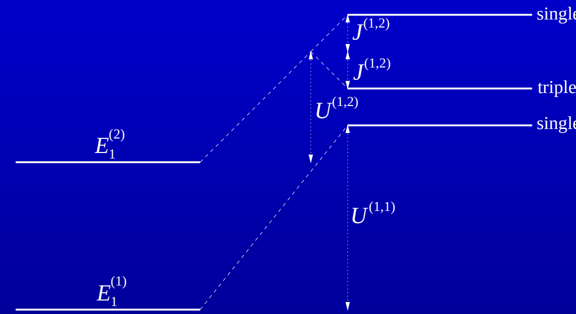
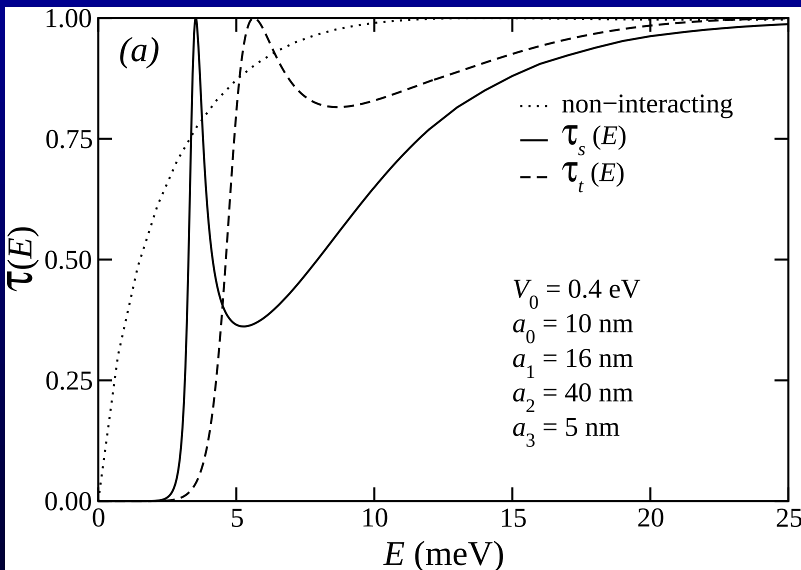
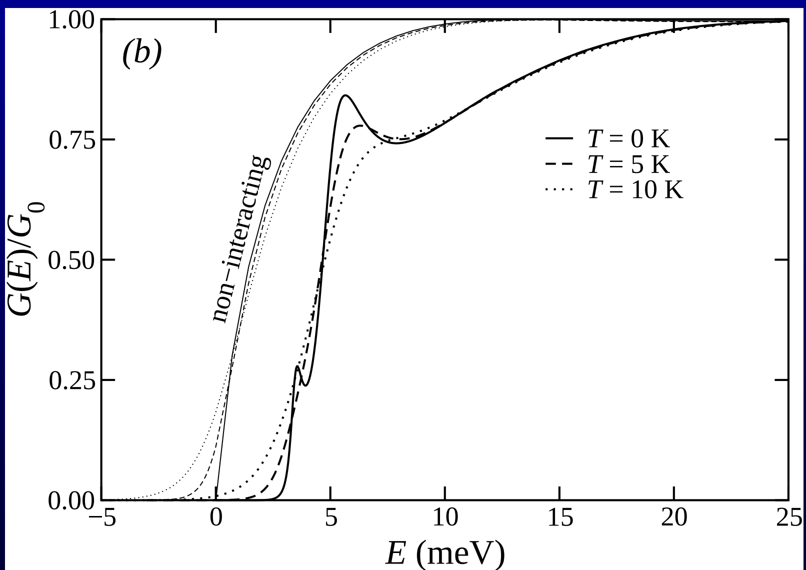




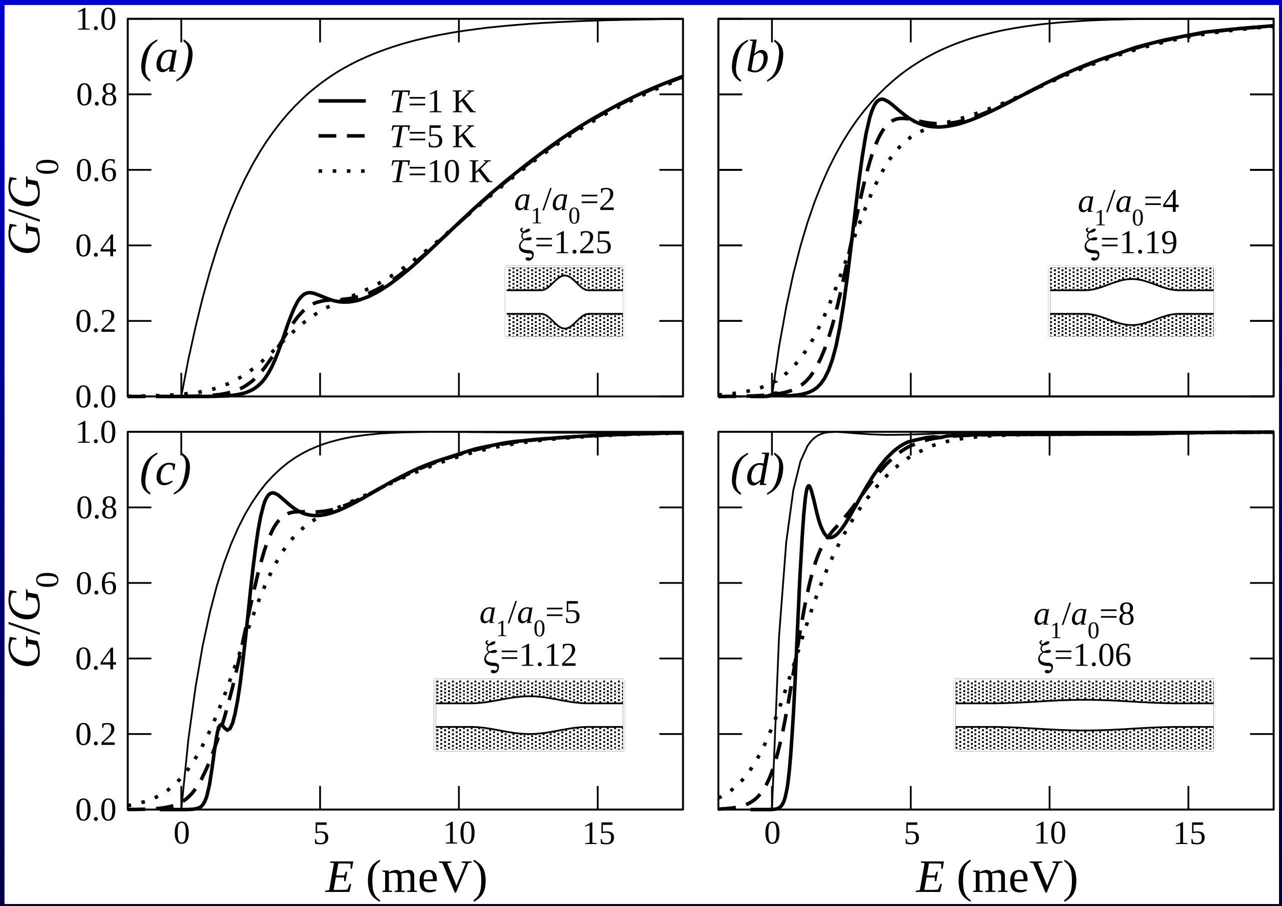


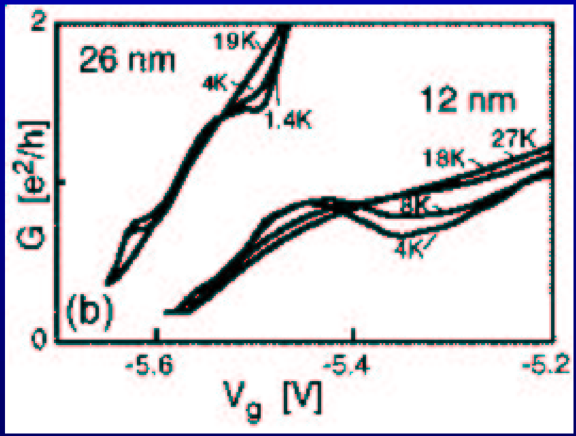




$$G = \frac{2e^2}{h} \int \mathrm{d}\epsilon \left(-\frac{\partial f\,(\epsilon)}{\partial \epsilon} \right) \left(\frac{1}{4} \left| t^{(0)}\,(\epsilon) \right|^2 + \frac{3}{4} \left| t^{(1)}\,(\epsilon) \right|^2 \right)$$

Results

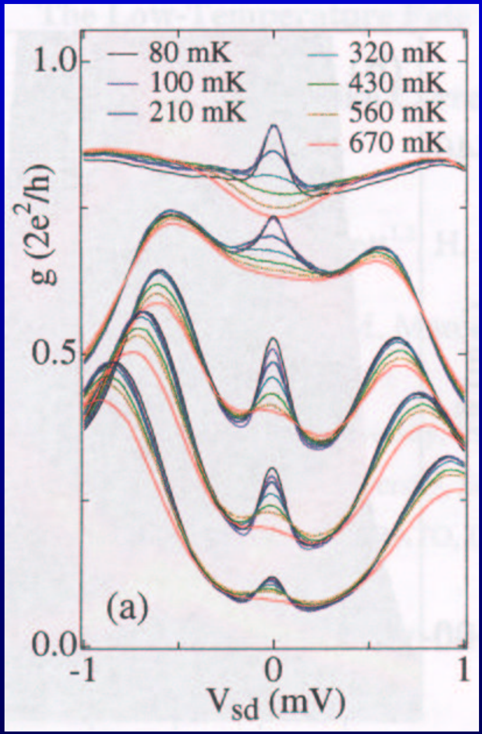

(a)
(b)
(c)
(d)
T=1 K
T=5 K
T=10 K
a1/a0=2
ξ=1.25
a1/a0=4
ξ=1.19
a1/a0=5
ξ=1.12
a1/a0=8
ξ=1.06
G/G0
E (meV)
0.0
0.2
0.4
0.6
0.8
1.0
0
5
10
15


26 nm
19K
4K
1.4K
12 nm
27K
18K
8K
4K
(b)
G [e2/h]
Vg [V]
2
0
-5.6
-5.4
-5.2

Extended Anderson model

- $d_\sigma^\dagger$ creates an electron in the single-electron bound state
- $c_{k\sigma}^\dagger$ creates an electron in a scattering state $|k\rangle$
- we retain only those Coulomb matrix elements which involve both localized and conduction electrons, omitting all terms which would give rise to states in which the localized state is unoccupied

$$H = \sum_k \epsilon_k n_k + \epsilon_d n_d + \sum_{k\sigma} (V_k n_{d\bar{\sigma}} c_{k\sigma}^\dagger d_\sigma + \text{h.c.}) +$$
$$+ U n_{d\uparrow} n_{d\downarrow} + \sum_{kk'\sigma} M_{kk'} n_d c_{k\sigma}^\dagger c_{k'\sigma} + \sum_{kk'} J_{kk'} \mathbf{S}_d \cdot \mathbf{s}_{kk'}$$

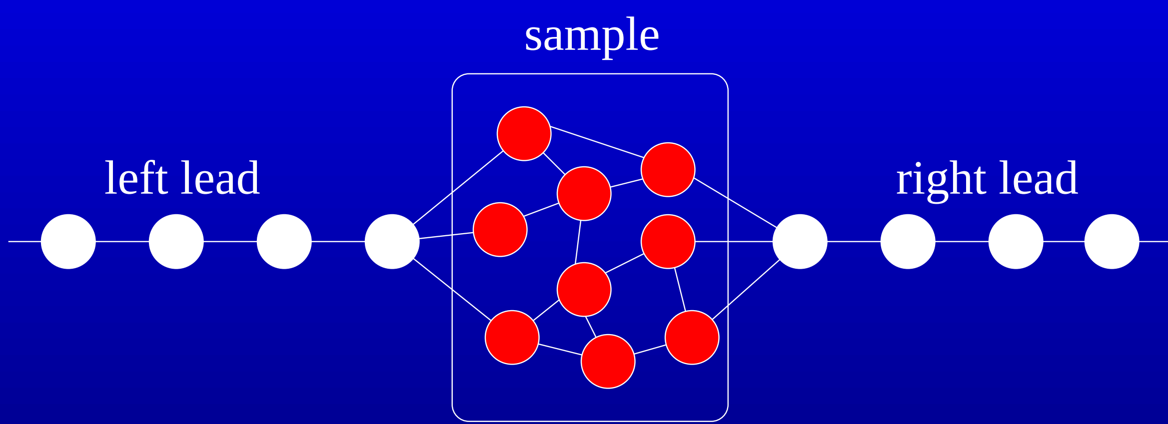


Kondo physics at low temperatures

Outline

- Introduction
- Spin-dependent anomalies at the conduction edge of quantum wires
- Zero-temperature conductance through an interacting electron region
  - ⋆ Model
  - ⋆ Conductance formulae for noninteracting systems
  - ⋆ Proof of validity for Fermi liquid systems
  - ⋆ Tests
- Summary

Model Hamiltonian



$$H = H_L + V_L + H_C + V_R + H_R$$

$$H_{\mathrm{C}} = H_C^{(0)} + U$$

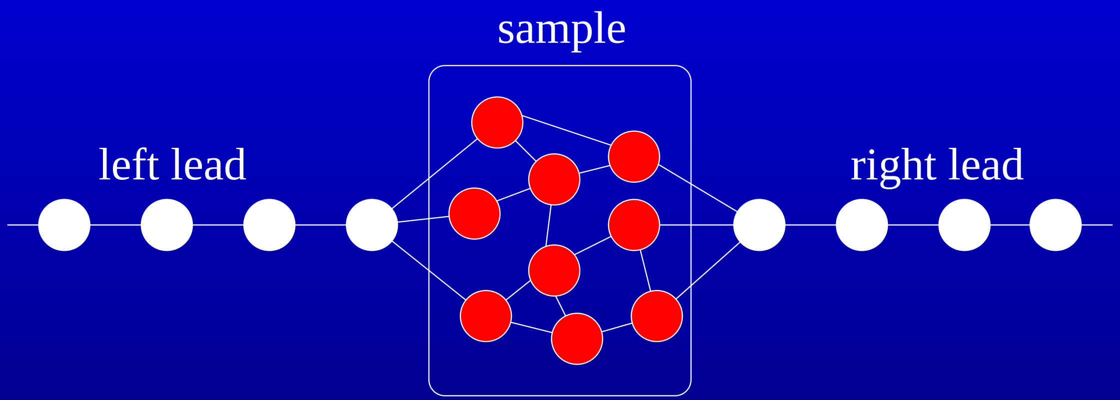
$$H_C^{(0)} = \sum_{\substack{i,j\in C\\ \sigma}} H_{Cji}^{(0)} d_{j\sigma}^{\dagger} d_{i\sigma}$$

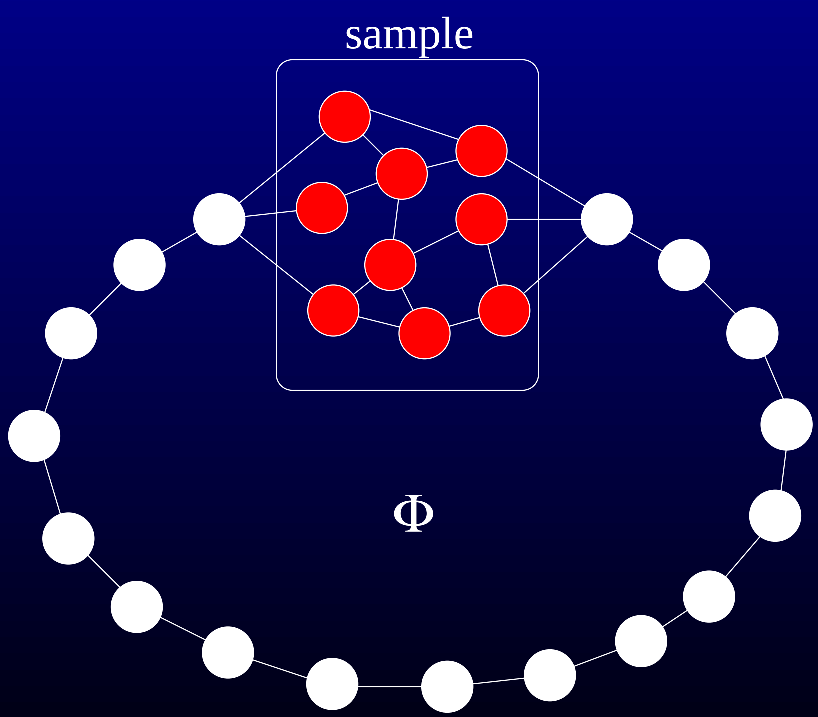
$$U = \frac{1}{2} \sum_{\substack{i,j\in C\\ \sigma,\sigma'}} U_{ji}^{\sigma\sigma'} n_{j\sigma} n_{i\sigma'}$$

$$H_{\mathrm{L}(R)} = -t \sum_{\substack{i,i+1\in L(R)\\ \sigma}} c_{i\sigma}^{\dagger} c_{i+1\sigma} + \mathrm{h.c.}$$

$$V_{L(R)} = \sum_{\substack{j\in L(R)\\ i\in C\\ \sigma}} V_{L(R)ji} c_{j\sigma}^{\dagger} d_{i\sigma} + \mathrm{h.c.}$$

Auxiliary system



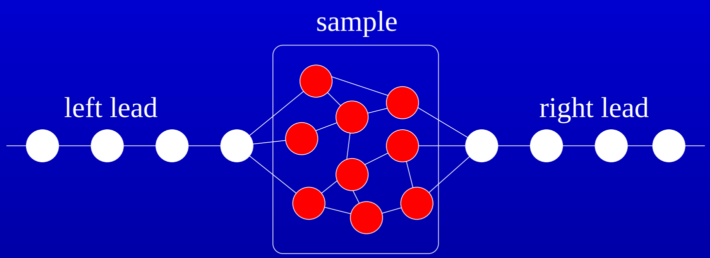


$$\Phi = \oint \mathbf{A} \cdot \mathrm{d}\mathbf{x}$$

$$t_{ji} \longrightarrow t_{ji} e^{i\frac{e}{\hbar}\int_{\mathbf{x}_i}^{\mathbf{x}_j} \mathbf{A}\cdot \mathrm{d}\mathbf{x}}$$

$$\Phi = \frac{\hbar}{e}\phi$$

Conductance formulae for noninteracting systems



left lead: $a_L e^{iki} + b_L e^{-iki}$

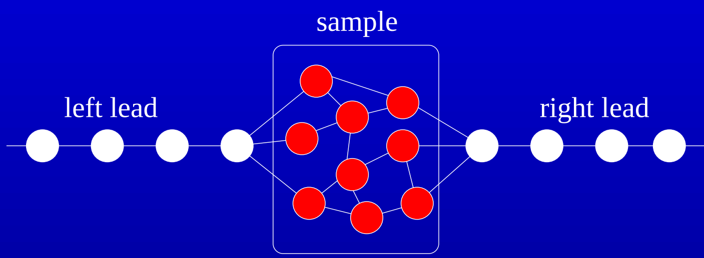
right lead: $b_R e^{iki} + a_R e^{-iki}$

$$\begin{pmatrix} b_L \\ b_R \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_L \\ a_R \end{pmatrix}$$

Landauer-Büttiker formula:

$$G = \frac{2e^2}{h} \left| t\left(\epsilon_F\right) \right|^2$$

Conductance formulae for noninteracting systems



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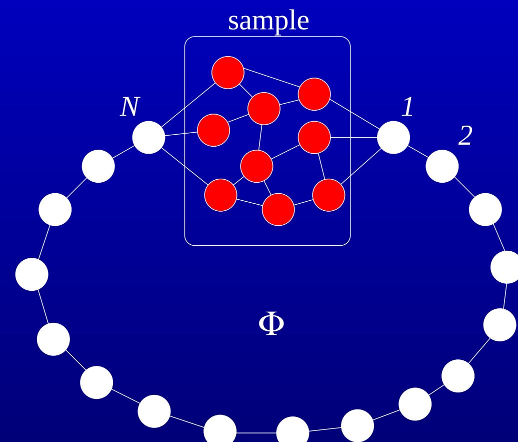
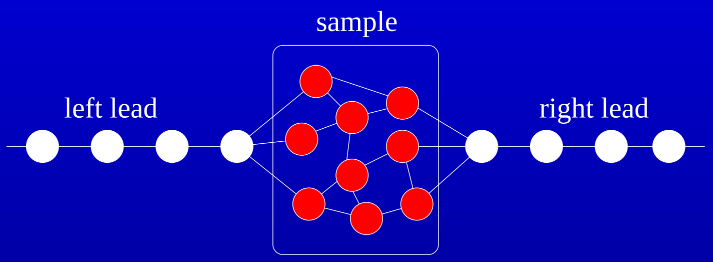


- $a_L, b_L \quad \overset{N,\phi}{\longleftrightarrow} \quad a_R, b_R$
- $t = t'$ (time-reversal symmetry, $B = 0$)
- $t = |t|\, e^{i\varphi}$

$$|t| \cos\phi = \cos\left(kN - \varphi\right)$$

Conductance formulae for noninteracting systems



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- $t = t'$ (time-reversal symmetry, $B = 0$)
- $t = |t|\, e^{i\varphi}$

$$|t| \cos\phi = \cos\left(kN - \varphi\right)$$

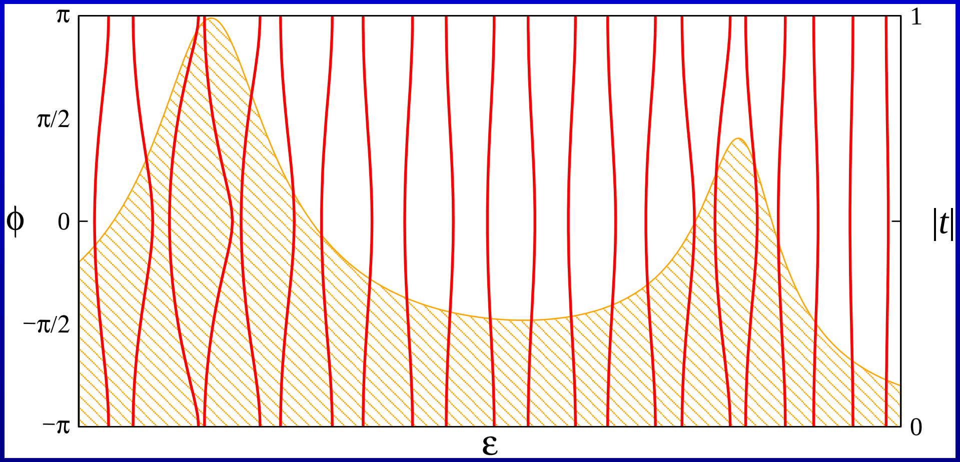
- $N \gg \frac{1}{\rho(\epsilon)} \frac{\partial |t|}{\partial \epsilon}$

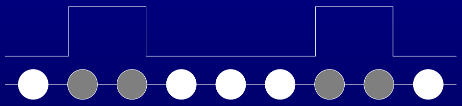
$$\frac{\partial \arccos\left(\mp |t| \cos\phi\right)}{\partial \cos\phi} = \pi N \rho\left(\epsilon\right) \frac{\partial \epsilon}{\partial \cos\phi}$$

- $E = 2 \sum_{\epsilon_n \leq \epsilon_F} \varepsilon_n$

$$\frac{1}{\pi} \frac{\partial \arccos^2\left(\mp |t| \cos\phi\right)}{\partial \cos\phi} = \pi N \rho\left(\epsilon_F\right) \frac{\partial E}{\partial \cos\phi}$$

Conductance formulae for noninteracting systems

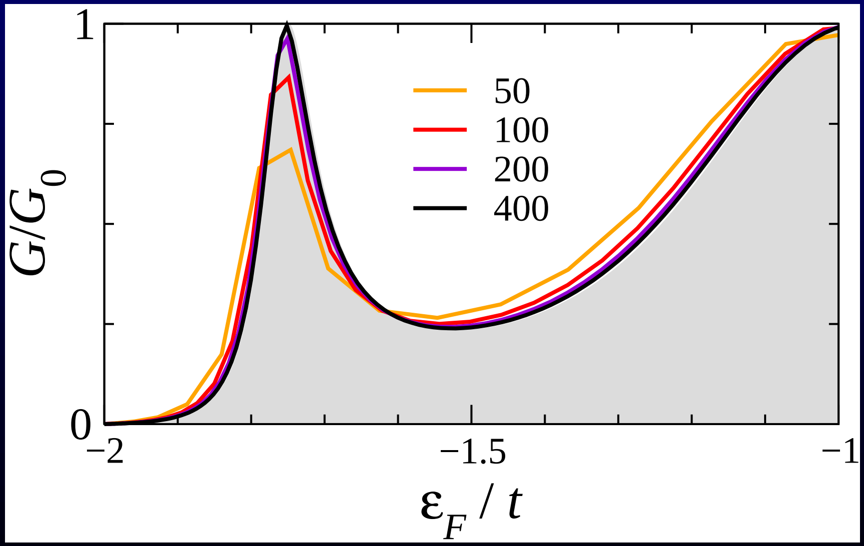




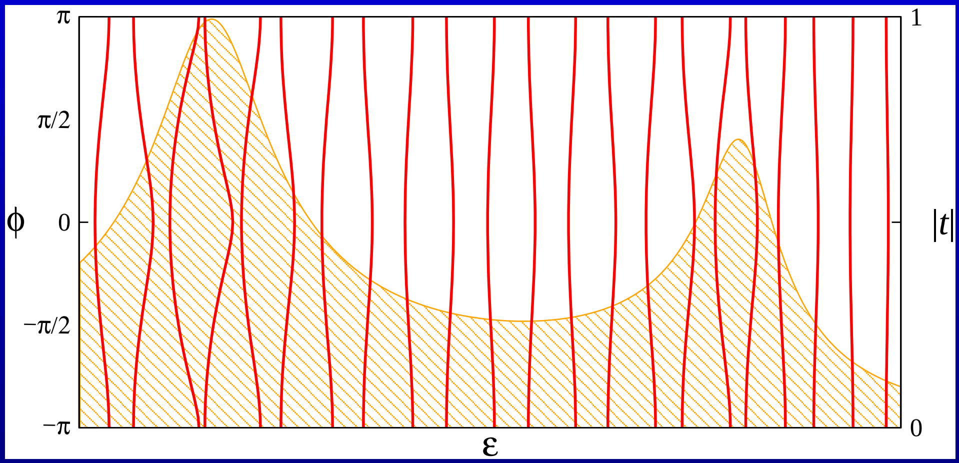
$$I(\phi) = \frac{e}{\hbar}\frac{\partial E(\phi)}{\partial \phi}$$

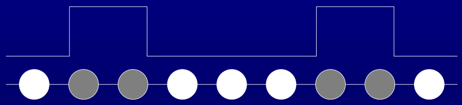
$$|t| = \sin\left(\frac{\pi^2\hbar}{2e} N\rho(\epsilon_F)\langle|I(\phi)|\rangle\right)$$

$$\langle|I(\phi)|\rangle = \frac{e}{\pi\hbar}\left[E(\pi) - E(0)\right]$$



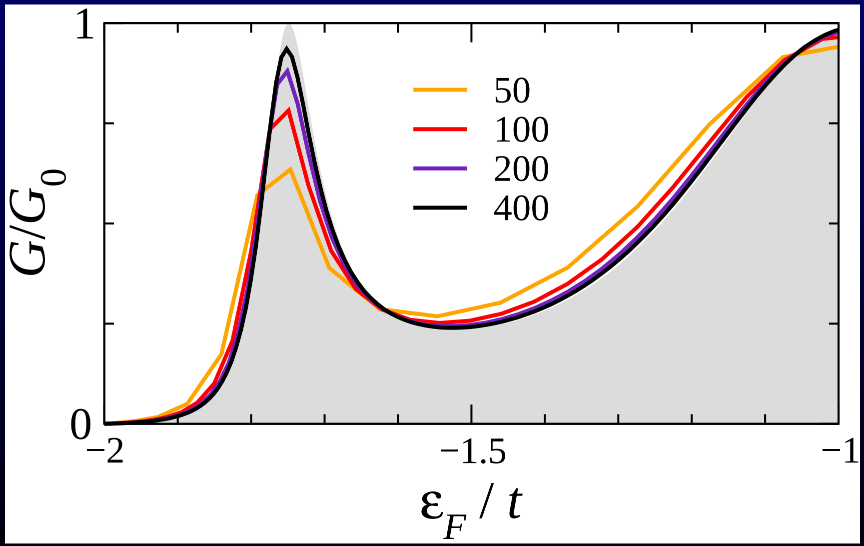
Conductance formulae for noninteracting systems



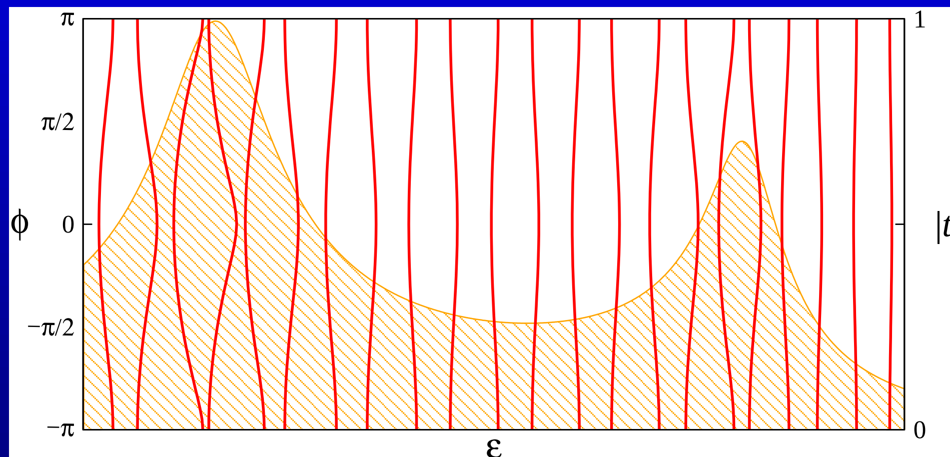


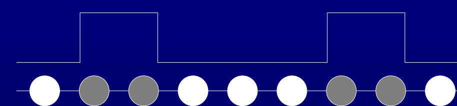
$$I\left(\phi\right)=\frac{e}{\hbar}\frac{\partial E\left(\phi\right)}{\partial\phi}$$

$$\left|t\right|=\frac{\pi\hbar}{e}N\rho\left(\epsilon_F\right)\left|I\left(\frac{\pi}{2}\right)\right|$$



Conductance formulae for noninteracting systems

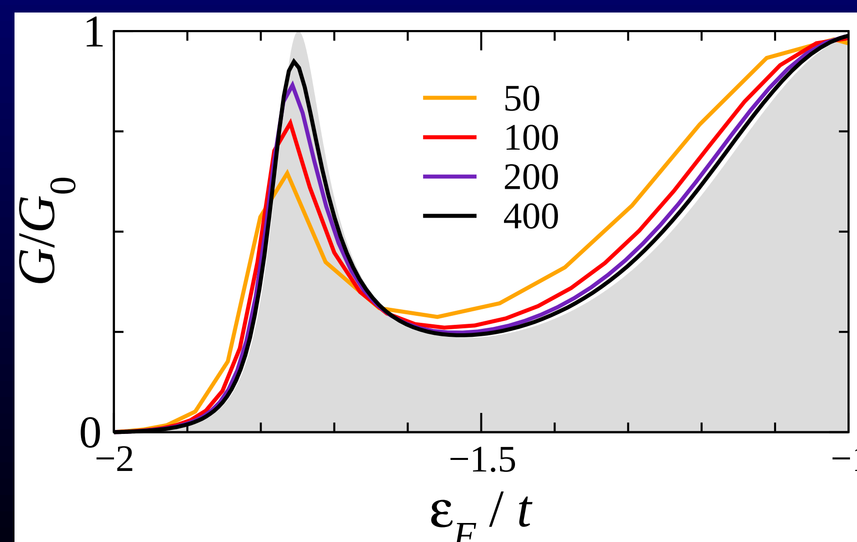




$$D = -\frac{N}{2}\left.\frac{\partial^2 E}{\partial \phi^2}\right|_{\min}$$

$$\pi^2 \rho\left(\epsilon_F\right) D = -\frac{|t|}{\sqrt{1-|t|^2}} \arccos |t|$$

$$|t| = \begin{cases} 2\pi\rho\left(\epsilon_F\right) D, & |t| \to 0, \\ \frac{1}{2} + \frac{3\pi^2}{2}\rho\left(\epsilon_F\right) D, & |t| \to 1. \end{cases}$$



Proof of validity for Fermi liquid systems

In Fermi liquid systems, the $T = 0$ conductance is still given with the Landauer-Büttiker formula

$$G = \frac{2e^2}{h} \left| t\left(\epsilon_F\right) \right|^2$$

if the transmission amplitude is defined by the Fisher-Lee relation

$$t\left(\epsilon\right) = \frac{1}{-i\pi\rho\left(\epsilon\right)} e^{-ik\left(n'-n\right)} G_{n'n}\left(\epsilon + i\delta\right).$$

Alternatively, the transmission amplitude for the corresponding (noninteracting) quasiparticle Hamiltonian may be used

$$\tilde{\mathbf{H}} = \mathbf{Z}^{1/2}\left[\mathbf{H}^{(0)} + \mathbf{\Sigma}\left(\epsilon_F + i\delta\right)\right]\mathbf{Z}^{1/2}, \quad \mathbf{Z}^{-1} = \mathbf{1} - \left.\frac{\partial \mathbf{\Sigma}\left(\omega + i\delta\right)}{\partial \omega}\right|_{\omega=\epsilon_F}$$

as

$$G_{n'n}\left(\epsilon_F + i\delta\right) = \tilde{G}_{n'n}\left(\epsilon_F + i\delta\right).$$

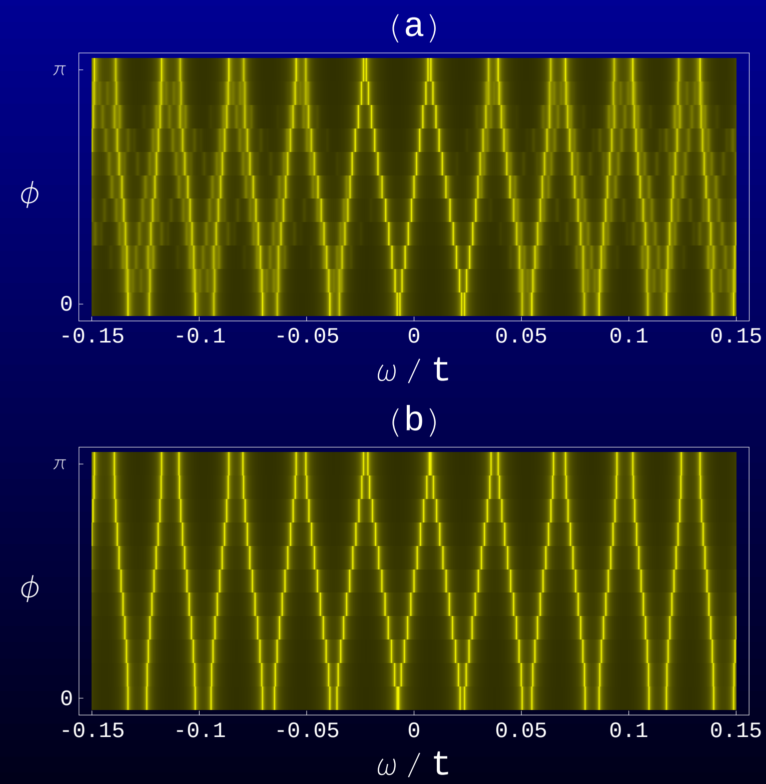
Proof of validity for Fermi liquid systems

If we knew the matrix elements of the quasiparticle Hamiltonian, we could form a finite ring system

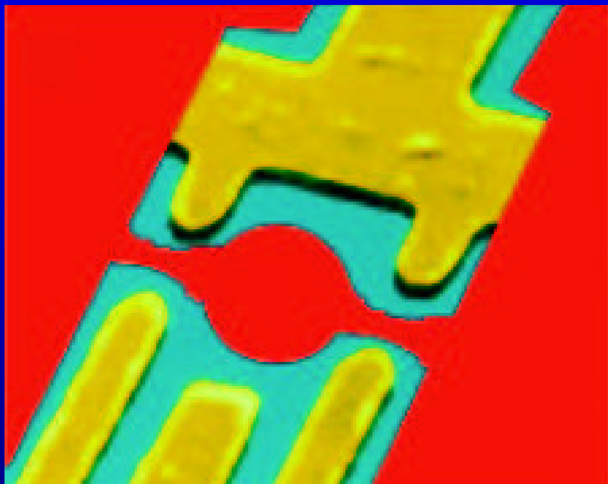
$$\tilde{\mathbf{H}}\left(N,\phi;M\right)=\mathbf{Z}^{1/2}\left[\mathbf{H}^{(0)}\left(N,\phi\right)+\mathbf{\Sigma}\left(\epsilon_F+i\delta\right)\right]\mathbf{Z}^{1/2}$$

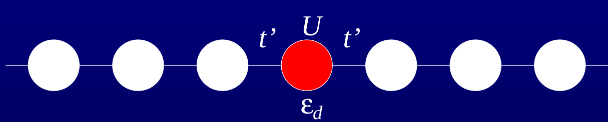
and proceed as we did for noninteracting systems. Alternatively, the single-electron energy of the quasiparticle Hamiltonian at the Fermi energy can be extracted from the ground-state energy of the interacting system

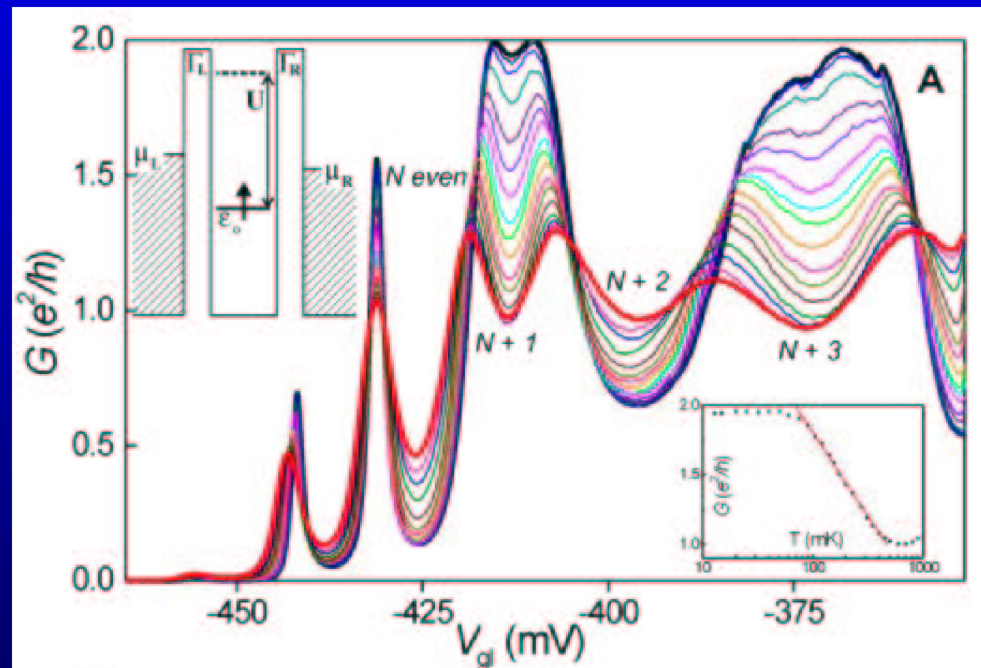
$$E\left[N,\phi;M+1\right]-E\left[N,\phi;M\right]=$$
$$=\tilde{\epsilon}\left(N,\phi;M;1\right)+\mathcal{O}\left(N^{-\frac{3}{2}}\right)$$



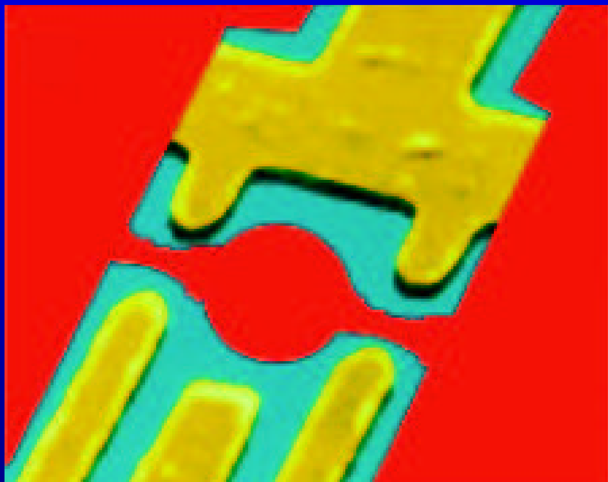
Tests

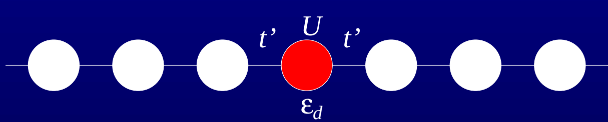



t'
U
t'
ε_d

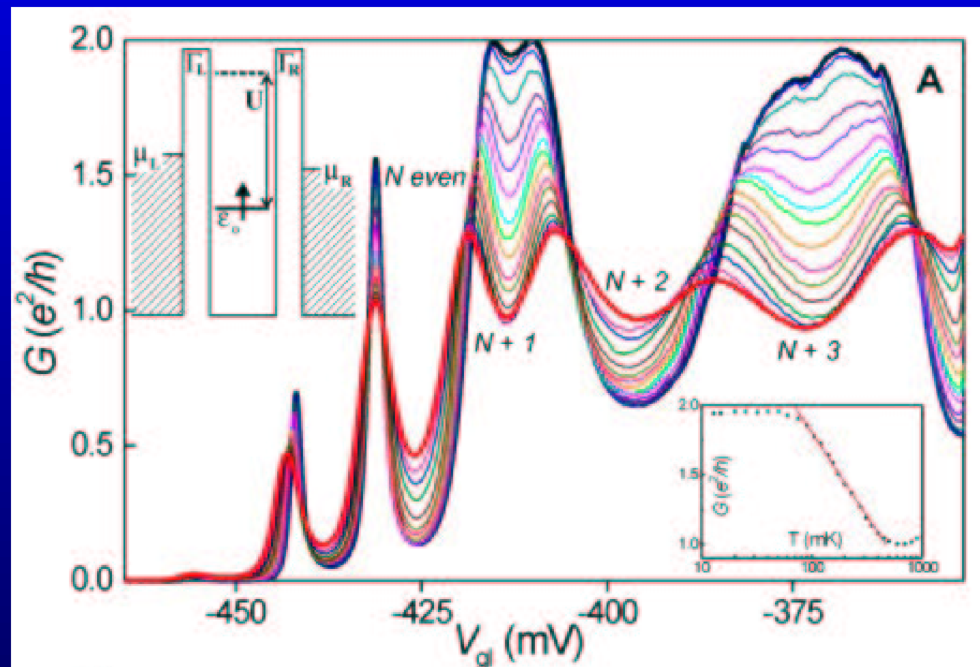

A
N even
N + 1
N + 2
N + 3
U
μ_L
μ_R
Γ_L
Γ_R
ε_0
$G(e^2/h)$
V_{gl} (mV)
T (mK)

Tests

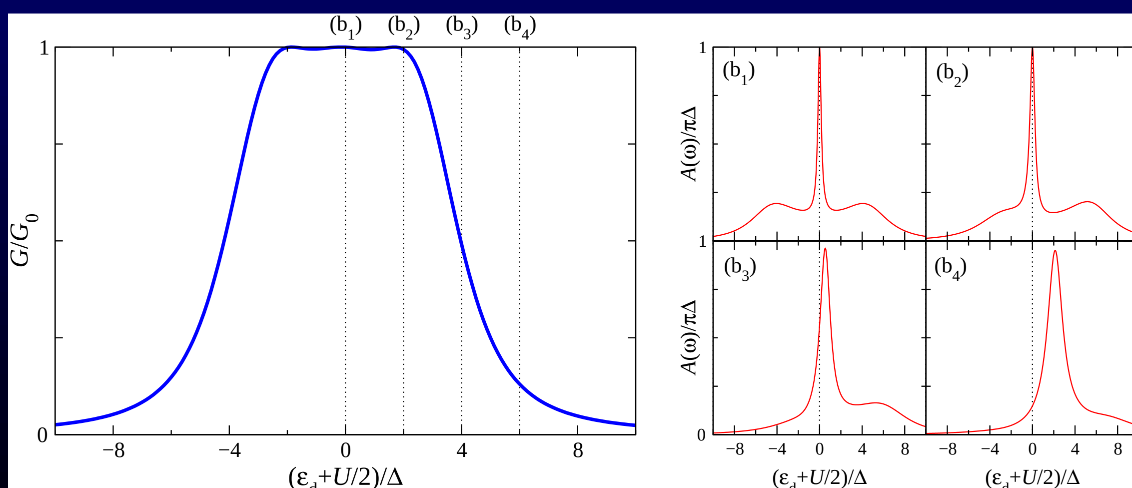




t'
U
t'
εd

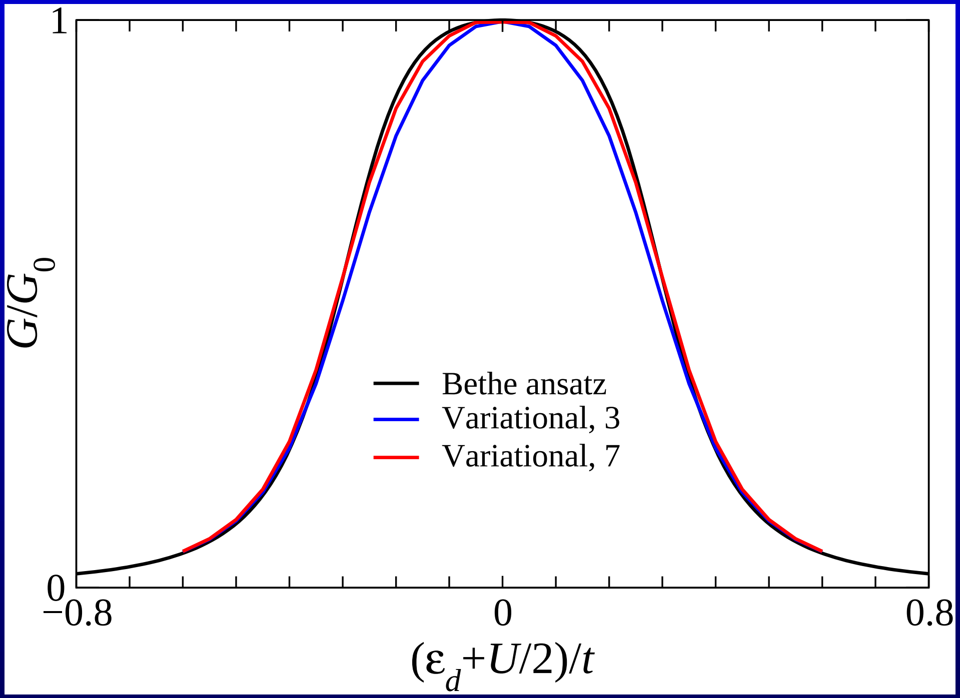


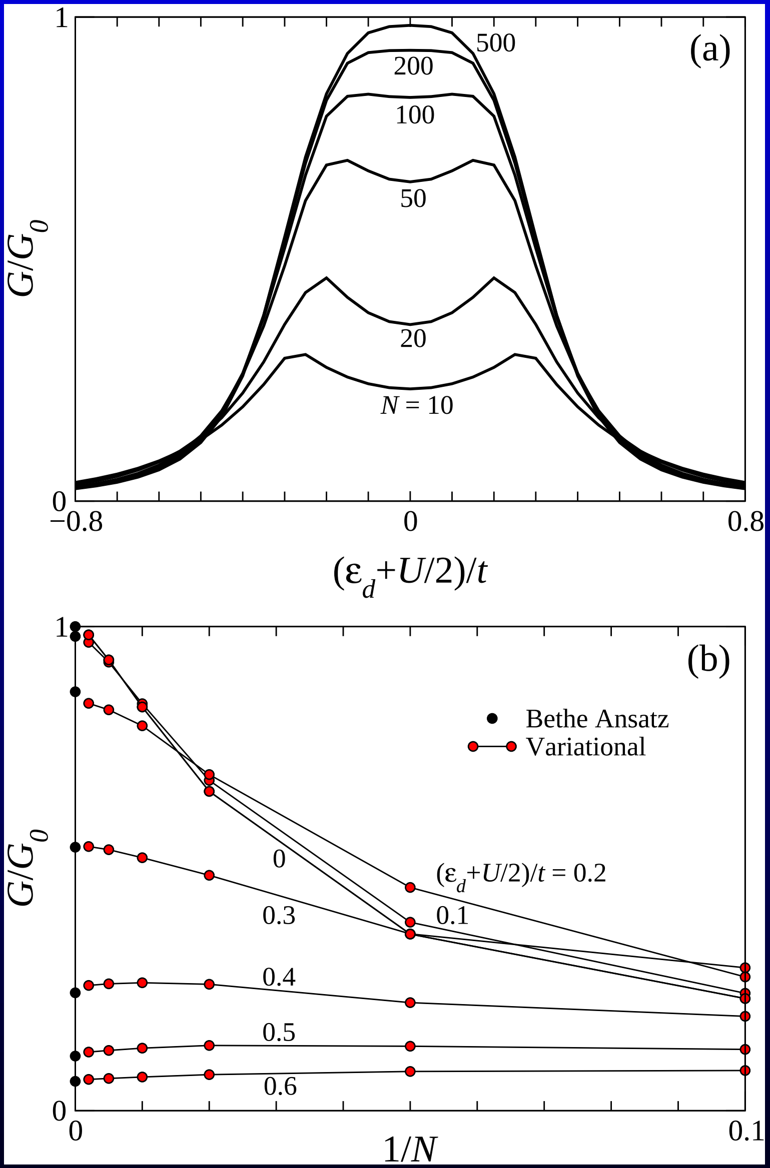
2.0
1.5
1.0
0.5
0.0
G (e²/h)
N even
N + 1
N + 2
N + 3
A
U
-450
-425
-400
-375
Vgl (mV)
T (mK)



(b1) (b2) (b3) (b4)
G/G0
(εd+U/2)/Δ
A(ω)/πΔ
−8 −4 0 4 8

Tests



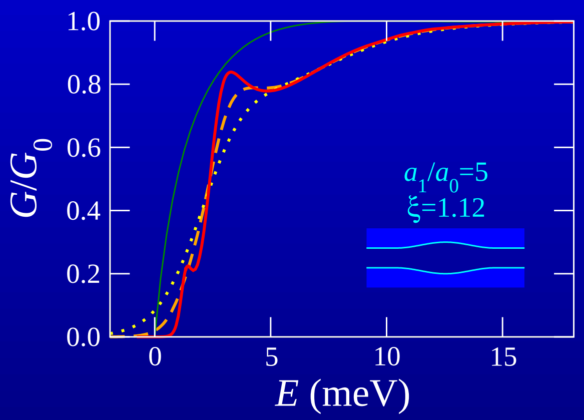


$$G = \frac{2e^2}{h} \left| t\left(\epsilon_F\right) \right|^2$$

$$\left| t\left(\epsilon_F\right) \right| = \sin\left(\frac{\pi}{2} N \rho\left(\epsilon_F\right) \left| E\left(\pi\right) - E\left(0\right) \right| \right)$$

Summary

- weak potential well in a quantum wire gives rise to spin-dependent conductance structures (0.7 and 0.3 anomalies) on the rising edge of the first conductance plateau



- an extended Anderson model could explain the Kondo-like low-temperature behavior of these anomalies

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- $T = 0$ conductance of a Fermi liquid system is related to the ground-state energy of a ring system threaded by a magnetic flux

$$G = \frac{2e^2}{h} \sin^2 \left(\frac{\pi}{2} N \rho \left(\epsilon_F \right) \left| E \left(\pi \right) - E \left(0 \right) \right| \right)$$

- variational methods can be employed to obtain the conductance (no need to calculate the Green's function)