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Hyperspherical-Harmonics Methods for Few-Body Problems*

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Abstract. A review of hyperspherical-harmonics (HH) methods from the standpoint of their applications is given. In the first lecture, the symmetrized and unsymmetrized HH bases and symmetrization methods are presented. The physical obstacles to the straightforward application of the HH expansion are discussed, and expansion acceleration methods are described. In the second lecture, the main HH methods are described, including the correlation function hyperspherical harmonic method (CFHHM), the potential harmonic (PH) methods, and the correlated HH methods (PHH, CHH). The third lecture discusses the advantages and limitations of different HH methods in applications, and compares the results for specific few-body problems obtained by HH methods as well as non-HH methods.

1 Notation

m_i	mass of particle i	$\hat{\mathbf{x}}_{k,i}, i = 1, \ldots, N$	angular coordinates of Jacobi vectors
μ_k	reduced mass of particles i and j of the triple $\{i, j, k\}$	$\Omega_k = \{\alpha_{k,i}, \hat{\mathbf{x}}_{k,i}\}$	three-body angular coordinates (tree base on k-th pair); $3N-4$ angular coordinates for tree label k
Z_i	charge of particle i		
N	number of particles		
L	total angular momentum		
K	grand total angular momentum (order of harmonic polynomial)	$\mathcal{Y}_{\mathcal{K}}(\Omega)$	generic HH
		$\mathcal{Y}^{\kappa}_{KLM}(\Omega)$	generic HH ($\mathcal{K} = \{\kappa, KLM\}$)
N_e	number of coupled equations		
N_{HH}	number of HH basis states	$\mathcal{Y}^{l_{k,1}l_{k,2}}_{KLM}(\Omega_k)$	three-body HH (tree base on k-th pair)
N_c	number of channels		
$\mathbf{x}_{k,i}$, $\mathbf{x}_{a,i}$	i-th weighted Jacobi coordinate (tree labels k, a)	$\mathcal{R}_{\mu\nu}(a_k, \lambda_k)$	Simonov "real" HH ($N = 3$, $L = 0$, pair k)
$\mathbf{r}_{k,i}$, $\mathbf{r}_{a,i}$	i-th Jacobi coordinate	$Y_{\mu\nu}(a_k, \lambda_k)$	Simonov "complex" HH ($N = 3$, $L = 0$, pair k)
ρ	hyperradius		
$\alpha_{k,i}, i = 1, \ldots, N-1$	hyperangles (tree label k)	Y_{lm}	spherical harmonic function

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$\mathcal{D}^j_{mk}$	Wigner $\mathcal{D}$-function	OS	optimal subset
$P_n^{(\alpha,\beta)}$	Jacobi polynomial	PHH	pair-correlated HH
${}^{(2)}P_K^{l_{k,1}l_{k,2}}$	hyperangular polynomial, $N=3$	CHH	Jastrow-correlated HH
		CFHHM	correlation-function hyperspherical harmonics method
$\langle LM\|l_{k,1}m_1l_{k,2}m_2\rangle$	Clebsch-Gordan coefficient		
$\langle\kappa\|\kappa'\rangle_{KL}^{km}$	Raynal-Revai coefficient	HCM	hyperspherical coordinate method
HH	hyperspherical harmonics	ODE	ordinary differential equations
PH	potential harmonics		

2 *Lecture 1*: Hyperspherical Harmonics

2.1 The HH Expansion

The motivation for the introduction of hyperspherical harmonics (HH) is to reduce the N-body, $(3N-3)$-variable, centre-of-mass Schrödinger equation to a system of coupled ordinary differential equations (ODE) in a single variable, which makes possible the application of the existing tools from the theory of Fourier series, orthogonal polynomials, and the solution of systems of ordinary differential equations. In this way many quantities appearing in the HH formulation, such as matrix elements of potentials in the HH basis, are for the most part expressible through closed analytic expressions. Although with the availability of powerful computers this aspect is becoming less important by itself, it has the important consequence that it enables the separation of numerical approximations in different parts of the procedure, thus making it more controllable. Also, the convergence properties of such expansions are known, and a proper expansion should converge to the correct answer. This is by no means guaranteed in variational calculations, for example.

The fact that all save one coordinate can be made cyclic (angular), can be intuitively illustrated by the following insight: Apart from its size (scale), all other transformations of the triangle spanned by three particles can be described by the rotation group. In particular, deformations can be viewed as the shadow (projection) of a rotating triangle.

The history of the HH began in 1935 as they were introduced by Zernike and Brinkman [1]. HH were reintroduced 25 years later by Delves [6] and Smith [7]. However, only in the recent decades methods based on the HH expansion have been developed to their full potential.

The reduction of the Schrödinger equation to a system of coupled ODE begins with the expansion of the N-body wave function

$$\Psi(\rho,\Omega)=\sum_{\mathcal{K}}\phi_{\mathcal{K}}(\rho)\,\mathcal{Y}_{\mathcal{K}}(\Omega), \tag{2.1}$$

where the basic quantities are:

$\mathcal{Y}_{\mathcal{K}}(\Omega)$: HH functions;

ρ : hyperradius;

$$\mathcal{K}: \quad 3N-4 \text{ quantum numbers;}$$
$$\Omega: \quad 3N-4 \text{ angular variables.}$$

$\mathcal{K}$ comprises K and the quantum numbers associated with $3N-5$ angular operators which commute with H and between themselves. The quantum number K is called *quasi*, or *grand total, angular momentum*. In calculations, the HH basis is truncated to a finite size except when it is implicitly summed over (see IDEA and its variants, below). The truncation is defined by $K \leq K_m$; further truncation is sometimes performed, based on physical considerations.

The coupled ODE for the hyperradial functions are

$$\left[\frac{1}{\rho^n}\,\frac{d}{d\rho}\left(\rho^n\,\frac{d}{d\rho}\right) - \frac{K(K+3N-5)}{\rho^2} + E\right]\phi_{\mathcal{K}}(\rho) = \sum_{\mathcal{K}'} V_{\mathcal{K},\mathcal{K}'}(\rho)\phi_{\mathcal{K}'}(\rho), \tag{2.2}$$

where $n = 3N-4$, the matrix elements of the potential are

$$V_{\mathcal{K},\mathcal{K}'}(\rho) = \int \mathcal{Y}_{\mathcal{K}}(\Omega)^* V(\rho,\Omega)\mathcal{Y}_{\mathcal{K}'}(\Omega)\; d\Omega, \tag{2.3}$$

and the eigenvalue of the hyperangular part of the Laplacian operator is

$$\mathcal{K}^2_{3N-3}(\Omega)\mathcal{Y}_{\mathcal{K}}(\Omega) = K(K+3N-5)\mathcal{Y}_{\mathcal{K}}(\Omega). \tag{2.4}$$

Many derivations for the general N will be found in [38]. Certain HH methods are usable also in P-space: See, for example, Kievsky et al. [71].

2.2 Indistinguishability and Cusps

Symmetry under exchange of identical particles and *clustering* (rearrangement) aspects of N-body systems, trivial or absent for $N = 2$, become of major importance in the formalism for $N > 2$.

2.2.1 Jacobi Coordinates

Each Jacobi coordinate connects the centre of mass of a subsystem with one of the remaining particles or with the centre of mass of another subsystem. In the case $N = 3$ they are

$$\begin{aligned}
\mathbf{R} &= \frac{1}{M}(m_i\,\mathbf{R}_i + m_j\,\mathbf{R}_j + m_k\,\mathbf{R}_k),\\
\mathbf{x}_{k,1} &= \sqrt{\frac{m_i m_j}{m_i+m_j}}\;(\mathbf{R}_i - \mathbf{R}_j) = \sqrt{\frac{m_i m_j}{m_i+m_j}}\;\mathbf{r}_k,\\
\mathbf{x}_{k,2} &= \sqrt{\frac{m_k(m_i+m_j)}{M}}\left(\mathbf{R}_k - \frac{m_i\mathbf{R}_i + m_j\mathbf{R}_j}{m_i+m_j}\right),
\end{aligned} \tag{2.5}$$

where $M = m_1 + m_2 + m_3$ and $\mathbf{R}$ is the centre-of-mass coordinate, which is eliminated in what follows. The three choices ($k = 1, 2, 3$ in the spectator notation) are connected by a linear transformation [21, 51] (*kinematic rotation*, see Eq. (2.16)). In the case of indistinguishable particles, the kinematic rotations play a role in the symmetrization of

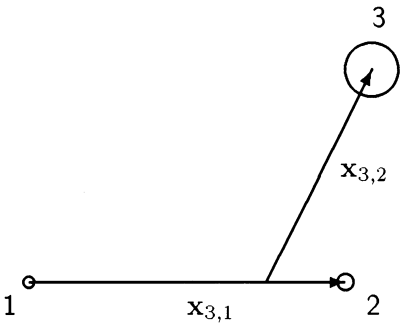

Fig. 1. Relative Jacobi coordinates for a three-body system ($k = 3$)

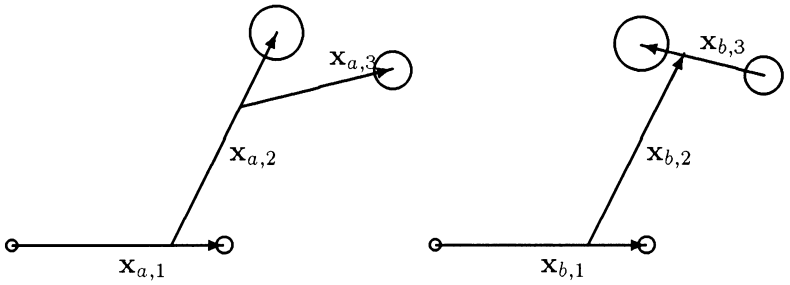

Fig. 2. Two choices of relative Jacobi coordinates for a four-body system. Labels *a* and *b* are not associated with a particular particle

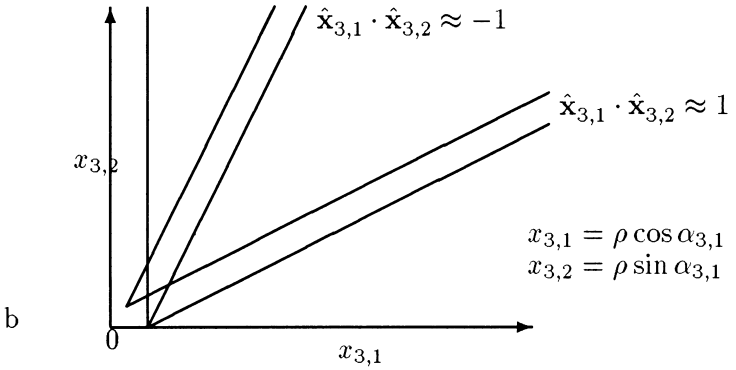

Fig. 3. The regions of strong potential for three particles with $m_1 \neq m_2$, in the coordinates with respect to particle 3. Two regions appear only at special values of the angle between the Jacobi coordinates

the basis. Different sets of Jacobi coordinates are employed, for example, in the case of rearrangement collisions.

The *hyperradius* measuring the overall size of the system is defined as

$$\rho^2 = \sum_{i=1}^{N-1} x_{k,i}^2 \tag{2.6}$$

and is independent of *k*, i.e., of the permutation of the particles.

2.2.2 Cusps

Cusps [4] appear with Coulomb-type potentials at *coalescence points* or *lines*:

$$\lim_{r_k \to 0} \frac{1}{\Psi} \frac{\partial \Psi}{\partial r_k} = Z_i Z_j \frac{m_i m_j}{m_i + m_j}. \tag{2.7}$$

The regions bordering the coalescence lines extend to the channel regions if $\rho \longrightarrow \infty$. This is illustrated in Fig. 3 for the case of a short-range potential.

2.2.3 Asymptotics

The asymptotics of the wave function depend in different ways on ρ in different angular directions. For example, in the $N = 3$ scattering problem above the breakup threshold with short-range potentials, in the *breakup region* which lies far from coalescence lines, Ψ has a $\rho^{-5/2}$ dependence. The regions of strong potential have decreasing *angular* width as the size of the system increases, and therefore require an increasingly large expansion basis in the *angular* variables.

Thus, cusps in the case of bound states and channels in the case of scattering states both represent a major obstacle for a direct application of the HH expansion to Ψ. Figs. 4, 5, and 6 illustrate the appearance of the cusps in two different parametrizations of the angular coordinates, once as lines and once as points.

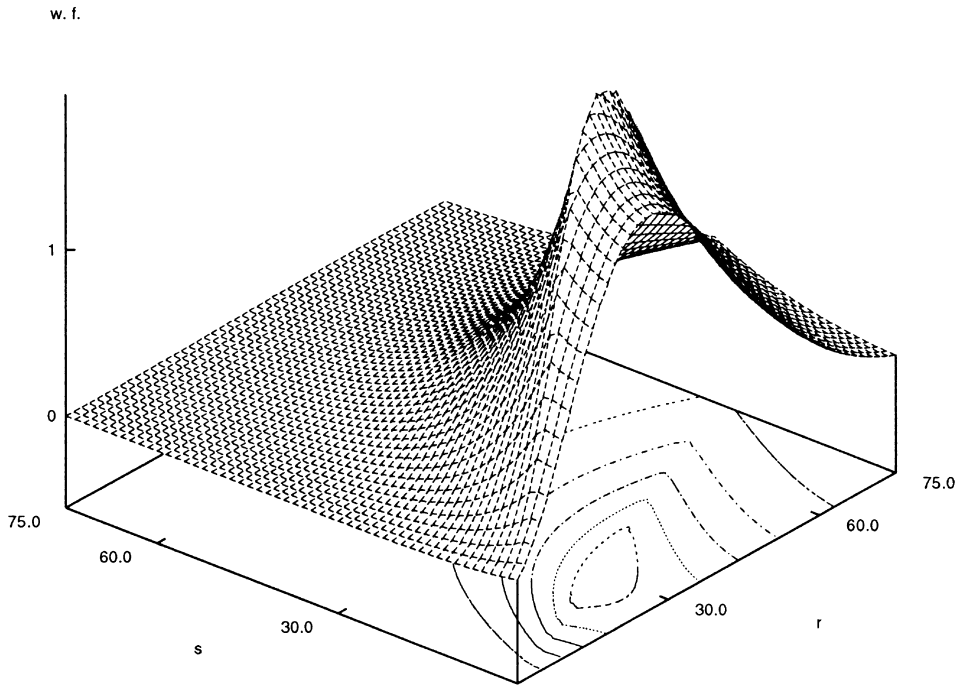

Fig. 4. Unnormalized μdt ground-state wave function. $r = \text{const.} \times x_{3,1}$ is the distance between d and t; $s = \text{const.} \times x_{3,2}$ is the distance between the muon and the centre of mass of d and t; $\arccos(\hat{\mathbf{x}}_{3,1} \cdot \hat{\mathbf{x}}_{3,2}) = 0.001^{\circ}$. $K_m = 40$. Parametrization of f: $a_1 = b_1$, $a_2 = b_2$ (cusp values), $a_3 = -0.29$ d.a.u. (nonlinear); $n_3 = 0.7$. Cusps appear as lines. Only two cusp lines can be seen: the d–t repulsive cusp at $r = 0$ and the μ–t attractive cusp at $s = rm_t/(m_d + m_t)$. From Krivec et al. [97]

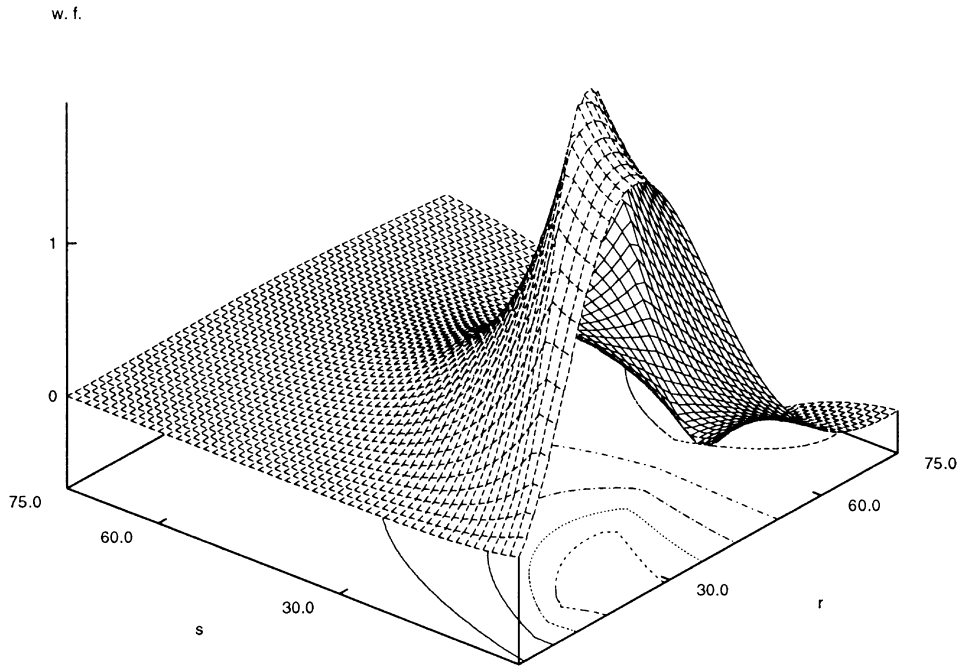

Fig. 5. As in Fig. 4, but for the $(L = 0, v = 1)$ excited state (v is the vibrational quantum number)

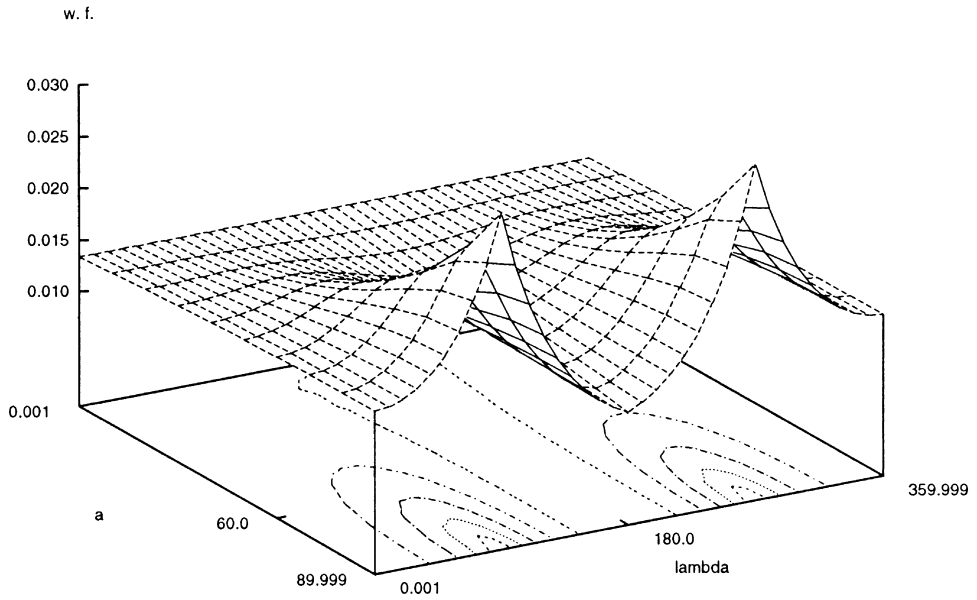

Fig. 6. Unnormalized CFHHM He-atom wave function in a_3, λ_3 coordinates where particle 3 is the He nucleus (degrees). $\rho = 1$, $K_m = 36$. Cusps appear as points at $a_3 = 90°$. Ψ is almost indistinguishable from the correlation factor e^f at this scale

2.3 Parametrizations

There are two basic approaches to the definition of the *angular* coordinates starting from the Jacobi coordinates. One treats all Jacobi coordinates on an equal footing, while the

other involves a separation into Euler and internal angles. The choice of parametrization affects (a) the separation of variables in the Schrödinger equation and (b) the symmetrization and generalization to $N > 3$ and $L > 0$.

2.3.1 Nonsymmetric Parametrization

This was the first type of parametrization, but later proved to be the most suitable one for constructing symmetrized bases in the general case. It was constructed by the **tree method** (Vilenkin et al. [13]); see also Nyiri et al. [22]; Krivec et al. [89]: The basis functions are eigenfunctions of subsystem-angular momenta $l_{k,i}$. This basis has the following advantages:

- has good subsystem-quantum numbers ($l_{k,i}$) and K, L, M;
- is generalizable to any L and any N;
- serves as starting point for symmetrization *with the advent of fast algorithms.*

The hyperspherical angle $\alpha_{k,1}$ for 3 particles is defined as follows:

$$\begin{aligned} x_{k,1} &= \rho \cos \alpha_{k,1}, \\ x_{k,2} &= \rho \sin \alpha_{k,1}. \end{aligned} \tag{2.8}$$

Definition of angles $\alpha_{k,i}, i = 1, \ldots, N-2$ for N particles is:

$$\begin{aligned} x_{k,1} &= \rho \cos \alpha_{k,1}, \\ x_{k,2} &= \rho \sin \alpha_{k,1} \cos \alpha_{k,2}, \\ x_{k,3} &= \rho \sin \alpha_{k,1} \sin \alpha_{k,2} \cos \alpha_{k,3}, \\ &\cdots \\ x_{k,N-1} &= \rho \sin \alpha_{k,1} \sin \alpha_{k,2} \cdots \sin \alpha_{k,N-2}, \\ \alpha_{k,N-1} &= 0, \end{aligned} \tag{2.9}$$

i.e., starting from pair (ij), each "spectator" coordinate becomes in turn a "pair" coordinate. The volume element is

$$d\Omega_k = d\hat{\mathbf{x}}_{k,N-1} \prod_{p=2}^{N-1} d\hat{\mathbf{x}}_{k,N-p} (\sin \alpha_{k,N-p})^{3p-4} \cos^2 \alpha_{k,N-p} d\alpha_{k,N-p}. \tag{2.10}$$

The basis in the three-body case, with eigenvalues $K(K+4)$, $K = 0, 1, 2, \ldots$, by virtue of the weight function determined by the volume element, is composed of Jacobi polynomials:

$$\begin{aligned} \mathcal{Y}^{l_{k,1} l_{k,2}}_{KLM}(\Omega_k) = N^{l_{k,1} l_{k,2}}_K \sum_{m_1 m_2} \langle LM | l_{k,1} m_1 l_{k,2} m_2 \rangle Y_{l_{k,1} m_1}(\hat{\mathbf{x}}_{k,1}) Y_{l_{k,2} m_2}(\hat{\mathbf{x}}_{k,2}) \\ \times (\cos \alpha_{k,1})^{l_{k,1}} (\sin \alpha_{k,1})^{l_{k,2}} P_n^{(l_{k,2}+1/2, l_{k,1}+1/2)}(\cos 2\alpha_{k,1}). \end{aligned} \tag{2.11}$$

The following notation is used:

$$\langle LM | l_{k,1} m_1 l_{k,2} m_2 \rangle : \quad \text{Clebsch-Gordan coefficient;}$$

$P_n^{(\alpha,\beta)}$: Jacobi polynomial;

Y_{lm} : ordinary spherical harmonic function;

$n = \frac{1}{2}(K - l_{k,1} - l_{k,2})$.

The normalization coefficient is

$$N_c^{a,b} = \sqrt{\frac{2(c+2)n!\Gamma(n+a+b+2)}{\Gamma\left(n+a+\frac{3}{2}\right)\Gamma(n+b+\frac{3}{2})}}, \qquad n = \frac{c-a-b}{2}, \tag{2.12}$$

where $\Omega_k = (\alpha_{k,1}, \hat{\mathbf{x}}_{k,1}, \hat{\mathbf{x}}_{k,2})$ denotes the five angular coordinates on the six-dimensional hypersphere; $0 \le \alpha_{k,1} \le \pi/2$; $\hat{\mathbf{x}}_{k,1}$, $\hat{\mathbf{x}}_{k,2}$ are solid angles connected with the vectors $\mathbf{x}_{k,1}$, $\mathbf{x}_{k,2}$, respectively; and the angular volume element is given by

$$d\Omega_k = \tfrac{1}{4} d\hat{\mathbf{x}}_{k,1}\, d\hat{\mathbf{x}}_{k,2} \sin^2 2\alpha_{k,1} d\alpha_{k,1}.$$

Remark on Notation. The function

$$(\cos\alpha_{k,1})^{l_{k,1}} (\sin\alpha_{k,1})^{l_{k,2}} P_n^{(l_{k,2}+1/2, l_{k,1}+1/2)}(\cos 2\alpha_{k,1}) \tag{2.13}$$

up to a normalization factor is denoted ${}^{(2)}P_K^{l_{k,1}l_{k,2}}$ in Ballot et al. [38], but the corresponding notation in Kievsky et al. [71] is ${}^{(2)}P_K^{l_{k,1}l_{k,2}}$, where K is the order of the Jacobi polynomial (n in our notation); our K is denoted by G.

2.3.2 Symmetric Parametrization

In this approach symmetry is imposed by construction (Simonov et al. [14], Barnea et al. [54]): HH simultaneously realize irreps of "kinematic rotations" $O(N-1)$ together with irreps of the permutation group S_N and the rotation group. The first construction by Simonov [14] was spawned by the interest in the nuclear three-body problem. The Dalitz-Fabri coordinates (see the Redish lectures [169]) were used to accomplish the separation of motion in Euler and internal coordinates. The explicit expression for $L = 0$ is:

$$\sin a_k \sin\lambda_k = \frac{2}{\rho^2} \mathbf{x}_{k,1} \cdot \mathbf{x}_{k,2}$$

$$\sin a_k \cos\lambda_k = \frac{1}{\rho^2}\left(x_{k,1}^2 - x_{k,2}^2\right),$$

$$\mathcal{R}_{\mu\nu}(a_k, \lambda_k) = \sqrt{\frac{2\mu+2}{\pi^3(1+\delta_{\nu 0})}} \cos(\nu\lambda_k)(\sin a_k)^{\nu} P_{(\mu-\nu)/2}^{(\nu,0)}(\cos 2a_k), \qquad \nu \ge 0,$$

$$\mu = \frac{K}{2} = 0, 1, 2, 3, \ldots, \qquad \nu = -\mu, -\mu+2, \ldots, \mu.$$

This is symmetric for particles 1 and 2. (Note that λ_k is the coordinate of kinematic rotations, and ν is the label of the kinematic rotation group $O(2)$.) K is the order of the harmonic polynomial, therefore each HH limits the subsystem angular momenta to at most K. (In the Sommerfeld approach, a part of the Laplacian operator is rewritten as the equation for the Wigner functions $\mathcal{D}^j_{mk}$; the counting of possible eigenvalues and polynomial orders gives the set of K, ν pairs.)

The problem with this parametrization is that it is very difficult to generalize the basis to large L and N. Works [9–37] were devoted to finding expressions for symmetrized HH realizing irreducible representations of the permutation group S_N. This presents a very difficult problem even for the three-particle case (Smith et al. [7, 9–37]). Simple expressions in closed form were found only for $L = 0$ (Smith et al. [7], Whitten et al. [17]), and $L = 1$ (Barnea et al. [44, 46]) (see also Zickendraht [9], Nyiri et al. [22], Whitten [20]). For $L \geq 2$, the difficulties were in finding the proper "fifth" operator of the complete set (containing $\mathcal{K}^2_6(\Omega)$, $\mathbf{L}^2$, L_z and the generator of $SO(2)$) which would have equally spaced, easily calculable, and nonirrational eigenvalues (Racah [8]).

2.3.3 Symmetrization Algorithms

Symmetrization algorithms are necessary in order to keep the dimension of the HH basis manageable if one goes beyond $N = 4$. Up to $N = 4$, several different prescriptions are used in practice to reduce the basis.

The basic property of the HH employed is the fact that HH for different choices $(k, m, \ldots; a, b, \ldots)$ of Jacobi coordinates are connected via the so-called Raynal-Revai coefficients [21]

$$\mathcal{Y}^{\kappa}_{KLM}(\Omega_k) = \sum_{\kappa'} \mathcal{Y}^{\kappa'}_{KLM}(\Omega_m) \langle \kappa | \kappa' \rangle^{km}_{KL}, \tag{2.15}$$

$$\begin{pmatrix} \mathbf{x}_{k,1} \\ \mathbf{x}_{k,2} \\ \cdots \\ \mathbf{x}_{k,N-1} \end{pmatrix} = c^{(km)} \begin{pmatrix} \mathbf{x}_{m,1} \\ \mathbf{x}_{m,2} \\ \cdots \\ \mathbf{x}_{m,N-1} \end{pmatrix}, \tag{2.16}$$

where the *kinematic rotation* matrix $c^{(km)}$ depends on masses.

In a variational setting, symmetry can be imposed by Faddeev decomposition and reduction of resulting linearly dependent HH (Efros [26], Kievsky et al. [71]), which, however, is tractable mainly in nuclear physics with a limited number of channels, as well as relatively low accuracy requirements as compared with atomic physics.

Useful algebraic generalizations of the symmetrization algorithms and fast implementations of these algorithms for larger N have been obtained only recently.

The work by Efros [55] first obtains the Raynal-Revai coefficients [51, 52] as solutions of a linear system generated by writing Eq. (2.15) for a (random) set of coordinate vectors $\Omega^{(i)}_k$, where i takes as many values as κ. The coefficients of the symmetrized linear combinations of HH can be expressed with $\langle \kappa | \kappa' \rangle^{km}_{KL}$.

A completely general, even faster algorithm, especially for $N > 4$, is constructed by recursion in Novoselsky et al. [53, 54] and Barnea et al. [56]. Most of the work from the 1970's up to now was devoted to the problem of symmetrizing the *tree-method* basis functions. In most of these works it was attempted to realize analytically (Raynal-Revai [51, 52], Kildyushov [29]) or numerically (Efros [55]) the Young symmetrizer. The new idea of Novoselsky [53] was to improve the symmetrization process by a recursive method rather than to improve the realization of the Young operator. In [54] this approach is further improved using the kinematic group.

2.4 Convergence and Its Acceleration

2.4.1 The Simple HH Method

It was recognized rather early that the simple HH method has very limited accuracy:

- Banville [57] found in the three-nucleon problem, using a Gaussian potential, that with 35 HH states it was possible to come within 0.03 MeV to the correct result, but that 65 HH states were needed for 4-digit accuracy.
- Erens et al. [23] discuss their result that the number of Simonov HH was too large for use with realistic nuclear potentials.

The reasons for slow convergence are as follows:

- In atomic physics (Coulomb potential) or nuclear physics (realistic potentials) Ψ converges as K_m^{-2} (coefficients as K_m^{-3}); E converges as K_m^{-4} (Gaussian potentials: e^{-cK_m}), see Schneider [28], and [38, 84, 27]. (See also Ballot et al. [34], Haftel et al. [87].)
- A finite number of HH cannot describe Ψ at the origin in the case of Coulomb-type singularities (the wave function in this case contains the well-known Bartlett or Fock logarithmic terms).
- N_{HH} (basis size) grows very fast with K and N: see Table 1.

2.4.2 Reduction of the Degeneracy

Reducing the degeneracy of HH states is an approximate method for selecting only the most important basis functions. This method entails a numerical error which usually proves tolerable only in nuclear physics.

Table 1. Rounded power of 10 of the degeneracy of unsymmetrized HH as function of N and K. The second part of the table shows N_{HH} (the sum of degeneracies up to K). Degeneracy grows exponentially with N

	K				
N	20	40	60	80	100
	Degeneracy				
3	4	5	6	7	7
4	6	8	9	10	11
5	8	10	12	13	14
6	9	12	14	16	17
	Number of HH				
3	5	6	7	8	8
4	7	9	10	11	12
5	8	11	13	14	15
6	9	13	15	17	18

The potential harmonics (**PH**) method (also called the optimal subset (OS) method) expands Ψ on the subset of HH needed to expand the interparticle potentials V_k. This OS truncation means that only two-body correlations are included in the wave function. Permutational symmetry is usually included in the construction of the OS (Ballot et al. [38]). For modifications of PH like the full-set PH see Fabre et al. [121].

The **IDEA** (integro-differential equation approach) is derived from PH. It is based on the approximation that Ψ depends only on $x_{k,1}, k = 1, \ldots, N-1$ and ρ. This leads to an integro-differential equation representing an infinite, untruncated sum over the PH basis, i.e., IDEA contains only two-body correlations but a complete sum over the PH.

Ordering and elimination of linearly dependent HH is another method of reducing the number of HH in nuclear physics. This approach, after several years of the development of sophisticated correlated schemes, resurrects, by virtue of more computer power being available, the simple HH method in nuclear physics (Kievsky et al. [71], see also Efros [26]).

2.4.3 Removing the Singularities: Correlated HH Methods

Typical problems, where correlation factors are called for, is atomic physics and nuclear physics using realistic potentials. Inserting correlation factors by itself does not entail numerical approximations. Mathematically, it represents a method of accelerating the convergence of the HH expansion. The modified Ψ converges one power of K_m faster for each derivative smoothened. It should be noted that in a non-variational setting, the *factorization* of the singularities is only possible in a simple way for the Schrödinger equation, despite the fact that in the Faddeev formulation each pair-correlation factor appears in a single Faddeev component.

The idea of using the hyperspherical expansion together with the correlation functions originated in the works by Zakharyev et al. [18], Raynal [31], and Revai et al. [32] in scattering, and to works by Fenin et al. [58] and Gorbatov et al. [41] is bound-state nuclear problems.

The **PHH** and **CHH** methods have been developed by the Pisa group. They have been used in and adapted for nuclear-physics problems. In order to facilitate the use of correlation factors in bound as well as scattering problems, the Kohn-type variational method is used to determine the hyperradial dependence of Ψ. Partly, these methods employ both correlation functions and the PH (OS) basis (Kievsky et al. [67]). Lately the group switched back to *uncorrelated*, full HH expansions, where the necessary basis sizes for $N \leq 4$ reach several thousand functions.

The correlation function hyperspherical harmonic method (**CFHHM**) addresses the problem of precise nonvariational calculations primarily in atomic physics. The complete HH basis is used, and the cusps are factored out of Ψ: This is a favourable tradeoff despite the non-self-adjointness of the resulting effective H. The Fock terms at the origin are included completely by construction. (HH basis truncation may also be used for larger N.) The method is used for bound states.

2.4.4 Adjusting the Angular Scale

A method which strictly speaking cannot be counted as a HH method is interesting from the physical viewpoint because it addresses directly the problem of clustering: the

hyperspherical coordinate method (**HCM**). In this method the angular basis depends on ρ (adiabatic approach) [104, 73]. In this property it is similar to the Born-Oppenheimer approach. The precision of the method is limited compared with the state-of-the-art variational or correlated HH methods; however, it is applicable to a large set of problems, and it can provide good insight into the structure of spectra. It can also be used for scattering.

3 *Lecture 2*: HH Methods

In this lecture we shall give a more detailed overview of the basic formalism of the HH methods. Most formulas given are not limited to specific methods.

3.1 Introduction

The basic advantages of HH methods are as follows:

- **Analytic expressions for matrix elements** are available in most cases. This was one of the original motivations for the introduction of the HH methods.
- **Knowledge of the radial solutions at the origin** (Bartlett-Fock type expansions, etc.) is available. The behaviour at the coalescence points is also known. These points are not ''natural'' in a HH setting.
- **Convergence properties** of the HH expansion are known.

3.2 CFHHM

One of the most important properties of the CFHHM is that it solves the Schrödinger equation directly (i.e., it is not a variational method). This means that the wave function will have uniform precision over a finite region of the configuration space, and that observables will have almost uniform precision, whether they correspond to singular or nonsingular operators. This is not the case in variational calculations where the variational functional emphasizes the regions important for the optimization of the energy.

Details of the CFHHM will give insight into analytic expressions for the matrix elements of interparticle potentials, and into how the correlations are included in order to eliminate singularities.

Equations. The correlation function f in the factor e^f should make ϕ smooth and therefore expandable in HH:

$$\Psi = e^f \phi, \tag{3.1}$$

$$\tfrac{1}{2}\nabla^2\phi + (E - W)\phi = 0, \tag{3.2}$$

$$W = V - (\nabla f, \nabla) - \tfrac{1}{2}\nabla^2 f - \tfrac{1}{2}(\nabla f)^2, \tag{3.3}$$

$$\phi = \frac{\chi}{\rho^2}, \tag{3.4}$$

$$\chi''_{\mu\nu} + \frac{1}{\rho}\chi'_{\mu\nu} + \left[2E - \frac{(2\mu+2)^2}{\rho^2}\right]\chi_{\mu\nu} = 2\sum_{\mu'\nu'} \overline{W}_{\mu\nu,\mu'\nu'}\chi_{\mu'\nu'}, \tag{3.5}$$

$$\overline{W} = W + \frac{2}{\rho^2}\frac{\partial f}{\partial \rho}. \tag{3.6}$$

Matrix elements (I). As an example of expansion in the *symmetrical basis*, we give the expressions in the Simonov ''complex'' basis for $L = 0$ [87]:

$$g(\rho, a_k, \lambda_k) = \sum_{\mu\nu} g_{k,\mu\nu}(\rho) Y_{\mu\nu}(a_k, \lambda_k), \tag{3.7}$$

$$\langle \mu\nu | g | \mu'\nu' \rangle = \sum_{\mu''=|\mu'-\mu|}^{\mu'+\mu} \gamma^{\mu''}_{\mu\nu,\mu'\nu'} g_{\mu''\nu-\nu'}(\rho), \tag{3.8}$$

$$\gamma^{\mu''}_{\mu\nu,\mu'\nu'} = (-1)^{(\mu'-\mu-3\mu'')/2} \left(\frac{\mu'}{2}\ \frac{\nu'}{2}\ \frac{\mu''}{2}\ \frac{\nu-\nu'}{2} \middle| \frac{\mu}{2}\ \frac{\nu}{2} \right) \sqrt{\frac{(\mu''+1)(\mu'+1)}{\pi^3(\mu+1)}}, \tag{3.9}$$

and if $g(\rho, a_k, \lambda_k)$ is a series in powers of $r_m(\rho, a_k, \lambda_k)$, $m = 1, 2, 3$ (like a pair potential), then

$$g(\rho, a_k, \lambda_k) = \sum_{p=p_0}^{\infty} g_{km,p} r_m^p, \tag{3.10}$$

$$r_k = \sqrt{2\kappa_k(1 + \sin a_k \cos(\lambda_k + \omega_k))}, \tag{3.11}$$

$$(r_m^p)_{\mu\nu} = \exp\left[i\left(\omega_m - \frac{\pi}{2} \right) \nu \right] \left[4\pi\rho^p (2\kappa_m)^{p/2} (-1)^{3\mu/2} \frac{\Gamma\left(\frac{p+3}{2}\right) \sqrt{\mu+1} (-\frac{p}{2})_\mu}{\Gamma\left(\mu + \frac{p}{2} + 3\right)} \right]. \tag{3.12}$$

Matrix elements (II). In the *nonsymmetrical basis* (see Krivec et al. [89]) one uses the Raynal-Revai coefficients to express a matrix element in the HH basis with respect to pair k with the matrix elements of potentials $V_i(x_{i,1})$ and $V_j(x_{j,1})$ in their respective hyperspherical bases $\mathcal{Y}^{l_{i,1}l_{i,2}}_{KLM}(\Omega_i)$ and $\mathcal{Y}^{l_{j,1}l_{j,2}}_{KLM}(\Omega_j)$,

$$\begin{aligned} &\langle K l_{k,1} l_{k,2} LM | V | K' l'_{k,1} l'_{k,2} L' M' \rangle \\ &\quad = \delta_{LL'} \delta_{MM'} \sum_{k'=i,j,k} \sum_{l_{k',1} l_{k',2}} \langle l_{k,1} l_{k,2} | l_{k',1} l_{k',2} \rangle_{KL} \\ &\qquad \times \langle K | V_{k'} | K' \rangle_{l_{k',1} l_{k',2}} \langle l_{k',1} l_{k',2} | l'_{k,1} l'_{k,2} \rangle_{K'L'}, \end{aligned} \tag{3.13}$$

which, as far as the radial dependence of the potentials is concerned, requires only the calculation of the integrals

$$\langle K | V_k | K' \rangle_{l_{k,1} l_{k,2}} = \sum_{p=-2}^{\infty} V_{kp} \langle K | (\cos \alpha_{k,1})^p | K' \rangle_{l_{k,1} l_{k,2}} \rho^p. \tag{3.14}$$

These integrals usually depend on k in a trivial way (via masses and charges), and reduce to the calculation of matrix elements between functions (2.13). In CFHHM, additional matrix elements from velocity-dependent terms must be calculated. This is usually done partly numerically because of the slow convergence of the matrix product in the $-\frac{1}{2}(\nabla f)^2$ matrix element [92].

Solution of equations. The method developed by Haftel et al. [100] expresses, in the variable $z = 2\kappa\rho$ on the interval $[0, z_U]$, the hyperradial vector solution $\chi(z)$ as a $N_e \times N_e$ matrix, as required by the, in general, $N_e \times N_e$ boundary conditions. The matrix solution

is propagated from $z = 0$ to $z = z_M$ and from $z = z_U$ to $z = z_M$. The latter is the stable direction of the system of coupled ODE (self-stabilization). In matrix notation,

$$\chi'' + P\chi' + Q\chi = 0, \tag{3.15}$$

$$P = \frac{1}{z} - \frac{1}{\kappa}\overline{W}^{(D)}, \tag{3.16}$$

$$Q = -\frac{1}{4} - \frac{\Lambda^2}{z^2} - \frac{1}{2\kappa^2}\overline{W}^{(S)}, \tag{3.17}$$

$$\overline{W} = \overline{W}^{(S)} + \overline{W}^{(D)}\frac{\partial}{\partial\rho}, \tag{3.18}$$

where $\Lambda_{\sigma\sigma'} = \delta_{\sigma\sigma'}(K_\sigma + 2), \sigma, \sigma' = 1, 2, \ldots, N_e, \kappa = \sqrt{-2E}$. E is prescribed by the iteration (zero-search) algorithm (see below). Because of the self-stabilization, the boundary condition at the maximum value z_U of z can be specified as: $\chi_{\mu\nu}(z_U) = I$, $\chi'_{\mu\nu}(z_U) = (-\alpha z_U - \beta \ln z_U)I$. The Fock-type terms at $z = 0$ are calculated *exactly* on $0 < z < z_F$ (S: upper triangular):

$$X_1 = z^S z^\Lambda \sum_{n=0}^{n_F} C_{1n} z^n, \qquad C_{10} = I, \tag{3.19}$$

$$\Lambda^2 + (P_{-1} - I)\Lambda + Q_{-2} = 0. \tag{3.20}$$

χ is expanded in matrix power series on small z subintervals, yielding matrix recursion formulas for coefficients. The reexpansion of $\overline{W}_{\mu\nu,\mu'\nu'}$ (i.e., P, Q) in local power series is necessary:

$$\chi_i(z) = X_i(z)\,\mathcal{V}_i, \tag{3.21}$$

$$X_i = \sum_{n=0}^{n_w} C_{in}(z - z_i)^n, \tag{3.22}$$

$$C_{i0} = I, \tag{3.23}$$

$$C_{i1} = X'_{i-1}(z_i)X^{-1}_{i-1}(z_i). \tag{3.24}$$

The renormalization of the solution on subintervals according to Eq. (3.23) helps to maintain numerical stability.

The method reduces to the search for the zero of the determinant of Eq. (3.25). Only about 7 steps are needed for E to converge to precision required in atomic physics. In the final pass the vectors $\mathcal{V}_i$ are constructed in order to generate the solution. At $z = z_M$, after propagation of $\mathcal{V}_i$ from both sides of $z = z_M$, a homogeneous linear system must be solved as follows:

$$[R_+(z_M) - R_-(z_M)]X_+(z_M)\,\mathcal{V}_+ = 0, \tag{3.25}$$

$$(\mathcal{V}_+)_1 = 1, \tag{3.26}$$

$$\text{discard } N_e\text{-th equation.} \tag{3.27}$$

Wave function. Ψ is expressed, on z subintervals, by coefficients calculated from X_i and $\mathcal{V}_i$,

$$\Psi(\rho, a_k, \lambda_k) = \frac{e^f}{\rho^2} \sum_{p=-1}^{n_w} (z - z_i)^p \sum_{\mu\nu} (C_{ip}\, \mathcal{V}_i)_{\mu\nu} \mathcal{R}_{\mu\nu}(a_k, \lambda_k), \qquad z_i < z < z_{i+1} \tag{3.28}$$

and correspondingly on $[0, z_F]$. Observables are calculated by numerical quadrature directly from Ψ.

In special systems like $e\mu^4\mathrm{He}^{++}$ because of its two-scale nature, it is necessary to use quadruple precision in the calculation of the matrix elements but not the solution of the radial equations. Quadrature accuracy needed in the calculation of the expectation values is smaller than that for the matrix elements. Because W is velocity-dependent, the energy is obtained as $\langle H \rangle$; this expression in contrast to the eigenvalue E has a variational property with respect to quadrature parameters.

Correlation function. The general form suitable for atomic physics problems, which describes exactly the cusp structure, and can also partly control the asymptotics of the solution, is

$$f = \sum_{k=1}^{3} [a_k + (b_k - a_k) e^{-r_k/n_k \langle r_k \rangle}] r_k, \tag{3.29}$$

$$b_k = Z_i Z_j \frac{m_i m_j}{m_i + m_j}. \tag{3.30}$$

In the linear f, $f = \Sigma_{k=1}^{3} c_k r_k$, $c_k = b_k$, if $b_k > 0$, it may be necessary to use $c_k < 0$ instead to enable convergence, thus violating the cusp condition. Nonlinear f eliminates this need, and improves convergence as well as the values of the deviation of the local

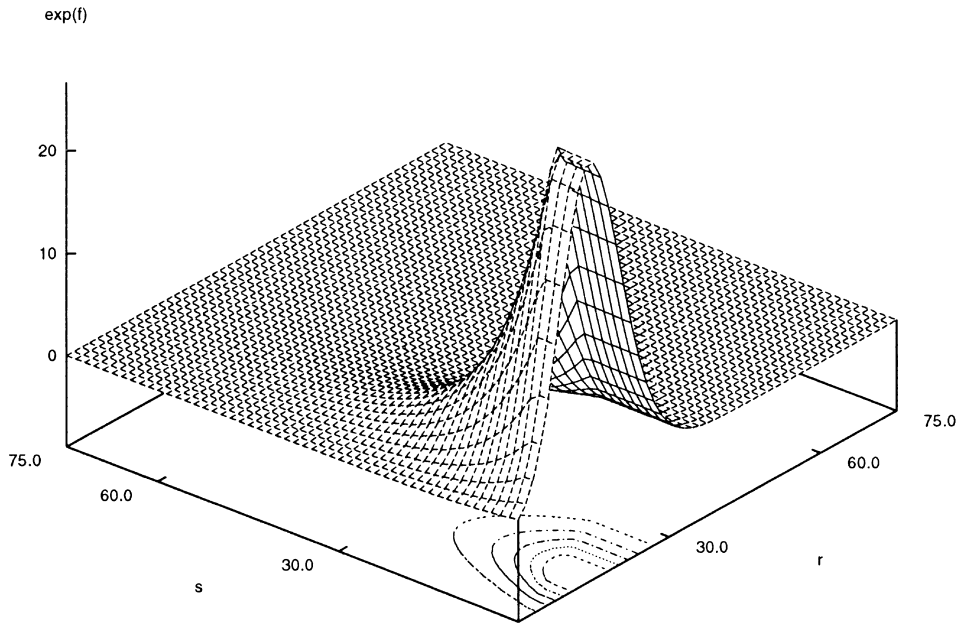

Fig. 7. As in Fig. 4, but the correlation factor e^f

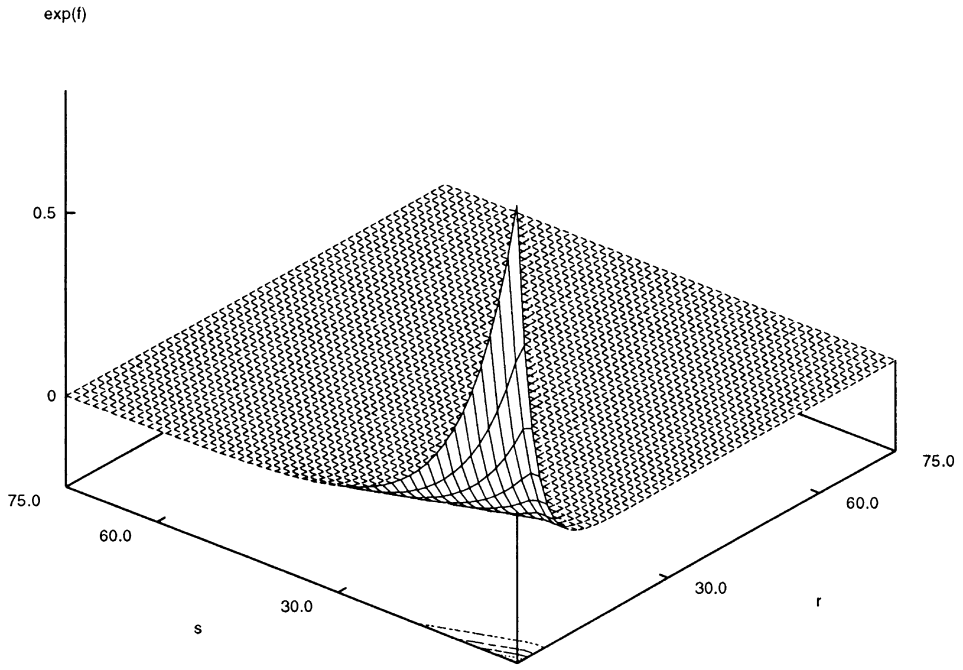

Fig. 8. As in Fig. 7, but for the modified-cusp linear correlation function $f = \Sigma_k\ c_k r_k$ with $c_1 = b_1$, $c_2 = b_2$, and $c_3 = -0.282$ d.a.u. ($c_3 < 0$ replaces the repulsive cusp $c_3 = b_3 > 0$ to prevent f from increasing as $r_k \to \infty$)

energy from the true energy as measured by the operator $\langle H\rangle/E - 1$, by at least an order of magnitude [99] compared to the linear f. The forms of various correlation functions are shown in Figs. 7 and 8 (see also Fig. 6). The convergence of operators can be improved by several orders of magnitude [102].

Numerical parameters. These are of two types:

- *Intrinsic* (for the solution of equations): $(n_F, n_w; T_z, T_w; z_F, z_M, z_U)$ (numbers of terms in the expansion of the solution; lengths of z-intervals; boundary/joining z-points).
- *Free* (to optimize the form of f): (a_k, n_k), $k = 1, 2, 3$.

For the optimization of the CFHHM parameters, see Haftel et al. [100]. Generally it suffices to impose cluster asymptotics on f alone, not on Ψ; the latter is a nonlinear problem. This nonlinear problem has been solved in several cases by optimizing the parameters at $N_e = 1$ which turned out to be sufficient. Usually, only two parameters actually remain free after physical considerations are taken into account.

Plateaux may appear in the dependence of the integrals on the upper integration limit in the z variable. The plateau values are used to calculate observables and estimate precision. Usually, the plateaux move towards larger z as K_m is increased. K_m is increased until the dependence on free parameters, on K_m and on plateaux is of the same order of magnitude.

Convergence of observables. This is discussed in Haftel et al. [87]. The naive picture that the observables converge as fast as Ψ surprisingly holds, but convergence rates are

Table 2. Rates of convergence (fitted, rounded) in the simple HH method and in CFHHM for the Helium-atom ground state, using finite and infinite nuclear masses. The entries with and without brackets correspond to the electron-nucleus and electron-electron distances, respectively. From Haftel et al. [87]

Method	Ψ	$\langle H\rangle$	$\langle r_k\rangle$	$\langle r_k^{-1}\rangle$	$\langle r_k^{-2}\rangle$	$\langle\delta(\mathbf{r}_k)\rangle$
Simple HH theoretical	2	5	5	4	3	3
CFHHM (cusp, ∞ mass)	3.3–4	5.5	4 (6)	4 (6)	4 (5)	4 (5)
CFHHM (cusp)	3.3–4	5.5	4 (6)	4 (4)	4 (3)	5.5 (4)

substantially higher than in the simple HH method, as illustrated in Table 2. Convergence rates depend on the physical system, but more importantly, the rate of convergence of singular operators depends strongly on the type of correlations used (see Table 3).

Table 3. Approximate number of correct significant digits in $\langle H\rangle$ and $\langle\delta(\mathbf{r}_3)\rangle$ as function of K_m for the CFHHM calculations of the ground states with systems having none or two indistinguishable particles. r_3 is the distance between the repulsive particles. L: linear correlation function f (cusp or one with repulsive cusp modified). NL: nonlinear f. *Italics:* interpolated values if observables converge with K_m in two separate subsequences

	Symmetric systems					Nonsymmetric systems					
		He	Ps^-		μdd		μdt	μdt	$e\mu^4$He		
		L	L	NL	L		L	NL	L	NL	
K_m	N_e					N_e				Separate K_m	*Interpolated*[d]
						$\langle H\rangle$					
24	49	7	5[a]	**5**	3[b]	91	3	**3**		**7**	*7*
32	81	8	5	**5**	4	153	4	**4**	5	**10**	*10*
40	121	8	5	**6**	5	231	5	**5**	6	**10**	*10*
48	169	8	6	**7**	5	325		**5**	6	**10**	*10*
56	225			**7**		435				**10**	*10*
						$\langle\delta(\mathbf{r}_3)\rangle$					
24	49	5	1[a]	**2**	1[b]	91	1	**1**[c]		**3**	*3*
32	81	5	1	**3**	1	153	1	**1**			*4*
40	121	6	1	**3**	2	231	1	**2**		**3**	*4*
48	169	6	1	**4**	2	325		**3**		**3**	*5*
56	225		1	**5**		435				**3**	*6*

[a] Uncorrelated cusp f

[b] Modified linear cusp f

[c] See Fig. 9

[d] Observables converge in separate subsequences corresponding to $K_m/2$ even and odd

3.3 HHGLF, CFHHGLF

This method is similar to CFHHM in the expansion of V into a matrix-power series, but the hyperradial functions are expanded in generalized Laguerre polynomials (including at $\rho = 0$) and the resulting linear system for coefficients is solved (Zhang et al. [77], Wang et al. [78]). This expansion converges much faster than a single power series on the entire ρ interval, but is less flexible than the CFHHM piecewise series.

3.4 HCM

The expansion

$$\Psi = \rho^{-5/2} \sum_{\mu} F_{\mu}^{(n)}(\rho) \Phi_{\mu}(\Omega, \rho) \tag{3.31}$$

leads to the equation

$$\left[\frac{d^2}{d\rho^2} - \frac{15}{4\rho^2} + E - V_{\mu}(\rho) + W_{\mu\mu}(\rho) \right] F_{\mu}^{(n)}(\rho) = \sum_{\nu \neq \mu} W_{\mu\nu}(\rho) F_{\nu}^{(n)}(\rho), \tag{3.32}$$

where μ is the angular channel label and n is the hyperradial excitation number. $\Phi_{\mu}(\Omega, \rho)$ are generated by

$$\left[\frac{\Lambda^2}{\rho^2} + V \right] \Phi_{\mu}(\Omega, \rho) = V_{\mu}(\rho) \Phi_{\mu}(\Omega, \rho) \tag{3.33}$$

and

$$W_{\mu\nu} = 2\langle \Phi_{\mu} | \frac{d}{d\rho} | \Phi_{\nu} \rangle \frac{d}{d\rho} + \langle \Phi_{\mu} | \frac{d^2}{d\rho^2} | \phi_{\nu} \rangle. \tag{3.34}$$

The uncoupled adiabatic approximation deletes the terms on the right-hand side. This proved valid for two-electron atoms [76, 75]. See also [105–113, 43]. Solving Eq. (3.33) is difficult due to localized solutions for large ρ. Ref. [108] proposes a variational approach.

3.5 PH, IDEA

PH. To illustrate the generation of the optimal subset, we give just a simple example for a spherically-symmetric potential (Erens et al. [25]). The OS is defined as the basis needed for expansion of V: Let $\langle \mathcal{Y}_{KLM}^{\kappa} | V_k \rangle = c_k v_K$; then

$$\begin{aligned} V &= \sum_{k=1}^{3} \sum_{KLM\kappa} c_k v_K \mathcal{Y}_{KLM}^{\kappa}(\Omega_k) \\ &= \sum_{k=1}^{3} c_k \sum_{KLM\kappa} v_K \sum_{\kappa'} \langle \kappa | \kappa' \rangle_{KL}^{k1} \mathcal{Y}_{KLM}^{\kappa'}(\Omega_1) \\ &= \sum_{K} v_K \sum_{k=1}^{3} c_k \sum_{LM\kappa\kappa'} \langle \kappa | \kappa' \rangle_{KL}^{k1} \mathcal{Y}_{KLM}^{\kappa'}(\Omega_1) \\ &= \sum_{K} v_K \mathcal{B}_K(\Omega_1). \end{aligned} \tag{3.35}$$

For the general definitions of the HH basis, the potential multipoles, and the symmetry considerations, the reader is referred to Ballot et al. [38].

IDEA by Fabre et al. [42, 45, 49] is based on the following derivation starting from one

Table 4. Triton binding energy (experimental: 8.48 MeV)

Method	N_c	N_{HH}	N_e	MT(V) all p.w.	AV14	AV18
Uncorr. HH-PH,		6	6	7.128		
Rosati [64]		12	12	8.100		
CHH-PH, ref. [64]		7	7	**8.2526**		
CHH, Kievsky [65]	8	6	48		*7.642*[a]	
PHH, Ref. [65]	8	6	48		*7.660*[a]	
	12	6?	72?		7.678	
Ref. [67]	18	6?	108?		**7.683**[c]	
Uncorr. HH,	18					7.61786
Kievsky [71]	22					7.61809[b]
	26		750			7.61812
IDEA, Fabre [142]				8.25		
VIDE, Braun [50]				**8.2525**		
IDEA (see [50] (?))				8.1924		
SIDE (see [50] (?))				8.0408		
CS/Fadd., Papp [142],						
$l_i \leq 6$				8.25215		
Faddeev, Friar [127]				8.251		
Schellingerhout [135]				**8.2527**3		
Chen [131]	34				7.678	
Glöcke [140]	34				7.680	
Wu [137]	52				7.673	
Tensor,						
Schellingerhout [133]				**8.2527**		
Euler + CHO,						
Kievsky cf. [64]				8.250		
ATMS, Akaishi [129]				8.26(1)		
GFMC,						
Zabolitzky [128]				8.26(1)		
Pudliner [144]					7.670(8)	
SVM, Varga [141]				**8.2527**		
Gauss, var.,						
Kameyana [134]	26				**7.684**	

[a] CHH turns out to be worse than PHH – hindered by angular momentum mixing from Jastrow factors

[b] More channels are required for four-digit accuracy than in CHH (although uncorrelated HH is described as "more accurate")

[c] Agrees with [134] – eliminates doubts about "missing contributions"

of the Faddeev equations:

$$(T-E)\phi_k = -V(\mathbf{x}_{k,1})\Psi. \tag{3.36}$$

Let $V_0(\rho)$ be the projection of $V(\mathbf{x}_{k,1})$ on $\mathcal{Y}_0$. Then

$$\left(T + \frac{N(N-1)}{2}V_0(\rho) - E\right)\phi_k = -[V(\mathbf{x}_{k,1}) - V_0(\rho)]\Psi. \tag{3.37}$$

If ϕ_k were expanded in HH (or PH), one would get a system of equations which would have to be truncated at $K = K_m$. IDEA (here for $L = 0$) [42, 49] is based on the approximation of only two-body correlations, which implies $\phi_k = \mathcal{B}_0 F(x_{k,1}, \rho)/\rho^{-5/2}$, where $\mathcal{B}_0$ is the lowest PH. Projecting on $\mathcal{B}_0$ one gets

$$\left(T + \frac{N(N-1)}{2}V_0(\rho) - E\right)F(x_{k,1}, \rho) = -[V(\mathbf{x}_{k,1}) - V_0(\rho)]\sum_m \int d\Omega\ F(x_{m,1}, \rho), \tag{3.38}$$

where T and the sum of the integrals can be expressed in terms of 2 variables, ρ and $z = z(0) = z(\varphi_k) = \cos 2\alpha_{k,1}$. Here

$$z(\varphi) = 2\frac{\xi_k^2(\varphi)}{\rho^2} - 1, \tag{3.39}$$

$$\xi_k(\varphi) = \mathbf{x}_{k,1}\cos\varphi + \mathbf{x}_{k,2}\sin\varphi, \tag{3.40}$$

where $\xi_k(\varphi)$ is the "kinematic rotation vector" giving all three $\mathbf{x}_{k,1}$, $k = 1, 2, 3$ at special values φ_k of the angle φ. Two variables can describe two-body correlations but in the general case, the HH expansion contains all HH (PH) terms and is exact in the HH (PH) expansion.

SIDE is a special case of IDEA for S-state projected potentials, whereby V_0 is also set to zero (and is generally worse than IDEA).

VIDE is a new version if IDEA based on the Schrödinger equation as opposed to the Faddeev equations in order to eliminate multiple counting of certain contributions which is an artifact of the Faddeev equations (see refs. [50, 65] and Table 4; there is a threefold reduction in the number of equations).

3.6 PHH, CHH (CHH-PH)

The ansatz for Ψ in these combined variational and HH methods is as follows: The channel functions for Faddeev components are

$$\Phi_\alpha^{\mathrm{PHH}}(x_{k,1}, x_{k,2}) = \rho^{\,l_{k,1}+l_{k,2}}\, f_\alpha(x_{k,1}) \sum_{K=l_{k,1}+l_{k,2}}^{K_\alpha} u_K^\alpha(\rho)\ {}^{(2)}P_K^{l_{k,1}l_{k,2}}(\alpha_{k,1}), \tag{3.41}$$

$$\Phi_\alpha^{\mathrm{CHH}}(x_{k,1}, x_{k,2}, \hat{\mathbf{x}}_{k,1}\cdot\hat{\mathbf{x}}_{k,2}) = \rho^{l_{k,1}+l_{k,2}} f_\alpha(x_{k,1}) g_\alpha(x_{j,1}) g_\alpha(x_{i,1}) \sum_{K=l_{k,1}+l_{k,2}}^{K_\alpha} u_K^\alpha(\rho)\ {}^{(2)}P_K^{l_{k,1},l_{k,2}}(\alpha_{k,1}). \tag{3.42}$$

The important difference between PHH and CHH, apparent from the above ansätze, is that CHH is applicable also to hard-core interactions. The expansion basis initially was

PH, while recently the full HH basis has been used, also in the four-nucleon problem [69]. In the four-nucleon problem, both types of Jacobi coordinates (see Fig. 2) are used in order to facilitate the channel truncation. This is one of the benefits of the use of the *Rayleigh-Ritz variational principle*, $\langle \delta_u \Psi | H - E | \Psi \rangle = 0$, to obtain the energy and the wave function. This approach is also used in scattering problems like the *N-d* scattering, where the *internal* part of Ψ is expanded in HH. This is an example of correlations being both *multiplicative* (the pairwise Jastrow-type correlation factors) and *additive* (the channels), as was discussed in the first lecture. However, the approximation involved in the formulation of the Kohn-type functional for the *S*-matrix above the breakup threshold without including the time-reversed final three-body state, which contains single and double rescattering terms [170], is left open.

4 *Lecture 3:* Comparison of HH Methods

4.1 Applications and Accuracy

In this section we present the intrinsic accuracies of individual methods and their applicability to specific physical problems. Methods separate roughly in two classes:

- very precise methods, typically applied in atomic physics with small N, and not in scattering;
- approximate methods, which gain in practical efficiency compared to the ''precise'' methods as N is increased; typically applied in $N > 3$ atomic problems and in nuclear problems, including scattering problems. Already Ballot et al. [34] observed that the first PH term gives increasing percentage of binding with increasing N for the ground states of atoms.

4.1.1 CFHHM

Because of the factorization of correlation factors from Ψ, the applicability of the method at present is limited to bound states. In most cases CFHHM gives better converged results than variational calculations, especially for singular operators. This is especially the case if convergence is improved by interpolating the recently observed double convergence of observables with K_m [102, 103].

Advantages:

- The full HH basis is employed (truncated at $K = K_m$).
- The radial part of the Schrödinger equation is solved directly (precisely); Ψ has the correct analytic form at $\rho = 0$.
- Expectation values of observables are of uniform accuracy, including the singular operators.
- Combined with complex coordinate rotation method (CR), CFHHM can be used for atomic resonance studies [101].

Limitations:

- $1/r$-type singular potentials are the limitation for analyticity of integrals (although numerical integration poses no problems).

– The condition of the system being ''spherical'' (not very $e\mu^4$He-like) does not seem to be a restriction; but in such cases the useful region of the parameter space of nonlinear f is rather small.
– Becomes complicated (large N_e) for $N > 3$.
– Parametrization of correlation function may prove difficult, or state-dependent (e^f must be > 0 in order not to affect the nodes of Ψ).

Applications:

– Muonic molecules like μdt (sticking probability and fusion rate) [99, 97].
– Doubly excited Helium atom [101].
– Ps^- annihilation rate [95].
– $e\mu^{3,4}He^{++}$ hyperfine splitting [102, 103].

In the above applications the values of singular operators were obtained in general to better precision than in the literature. The precision of the value of the energy ($\langle H \rangle$) (even though f is not optimized to get a good $\langle H \rangle$) is shown in Table 3, whence some observations can be extracted:

– To get comparable accuracy in nonsymmetrical as in symmetrical systems, K_m must be the same (N_e larger).
– Nonlinear parametrizations are much better than the linear ones.
– For nonlinear parametrizations, accuracy of noninterpolated observables (and probably interpolated) is quite uniform across different systems, except for $\langle H \rangle$.
– The interpolated values for $\langle H \rangle$ have the same accuracy as the separate $-K_m$ values.
– For other observables, interpolated values are improved by 2 orders of magnitude.

4.1.2 PH, IDEA, VIDE

These methods are used in nuclear physics.

Advantages:

– Their relative efficiency increases for $N > 3$.
– The first PH term gives increasing percentage of binding with increasing N.
– Precision of OS is ''at least as in Faddeev formulations'' (Ballot et al. [38]).
– PH fulfills the Rayleigh-Ritz principle in contrast to the Faddeev formalism.

Limitations:

– Only two-body correlations are included.
– Inadequate in atomic physics for $N = 3$.
– Even in the first excited state of He atom, the first term contributes only 50% of binding.

Applications: As discussed in Fabre et al. [121], an early calculation by Erens et al. [25] showing OS gives trinucleon energy to 0.001% using $K_m = 18$. Ballot et al. [38] found that non-potential terms have small contributions. This was also studied by Erens et al., see also Kievsky et al. [71]. Loss of precision due to OS was studied by Desplanques et al. [47]. Accuracy was studied also by Erens et al. [25] and Ballot et al. [34].

A recent application is the DFM model of the nucleon, based on the PH: Dziembowski et al. [48] claim 99.5% accuracy in the overlap between PH and exact Ψ (see Richard et al. [39], Table I: E converges to 4 SD at $N_e = 3$; $\langle\delta(r_{12})\rangle$ converges to 4 SD at $N_e = 10$). However, wrong $\frac{1}{2}+, \frac{1}{2}-$ state ordering is obtained for the nucleon. In fact, the recalculation of the DFM model in SVM and Faddeev methods gives even worse ordering of these states [145].

4.1.3 PHH, CHH

This method combined with variational principles is used in nuclear bound-state and scattering problems.

Advantages:

- Accommodate most potentials (CHH also hard core).
- Inclusion of Coulomb potential below threshold is easier than in the Faddeev formulation.
- Large HH bases (and the Lanczos method) can be used because of the variational formulation.
- Variational formulation enables the treatment of scattering problems using a trial function of the form $\Psi = \Psi_b + \Psi_s$, where Ψ_b is a quadratic integrable part describing clustered subsystems, and Ψ_s is the long-range part describing channels.

Limitations:

- PHH is sometimes faster converging than CHH due to absence of angular momentum mixing.
- Simple HH eventually turned out to be more accurate than both PHH and CHH, provided a large enough N_e is used.
- Variational principle for radial solutions limits accuracy.
- Study of the importance of single- and double-scattering terms is not possible at present.
- Boundary conditions in the transition region cannot be controlled easily.

Applications: For a list of results see Table 4.

4.1.4 HCM

This method is used primarily in atomic physics.

Advantages:

- Relative ease of extraction of qualitative properties.
- HCM can treat channel regions because of the adaptable angular basis.

Limitations:

- Accuracy (see Tables 9, 10).

Applications: A recent calculation of the binding energies shows errors ranging from 0.001% in H^- to 0.1% in B^{+++} [114]. A recent application in the close-coupling method is [115]. For an application of HCM to muon-catalyzed fusion-related problems, where the relevant states of the different muonic molecules were calculated with

uniform precision of up to 3 digits for the sticking coefficients and the fusion rates, see [116] (also shown in Table 9). A recent development is a two-dimensional HCM basis [117], as well as several further variants of HCM, for example [118]. The application of HCM to the $N = 4$ problem of the lithium atom is discussed in [119].

4.2 Comparisons

In this section, early and modern HH methods are compared with each other and with other methods, for a set of specific physical problems. The quoted E values by CFHHM refer to $\langle H \rangle$. It should be noted that some non-HH methods, notably the finite element method (FE), though they are less precise on the presented examples, are directly applicable to scattering problems, where they may be more successful than HH-based methods. FE can be adapted to the local structure of Ψ without affecting the expansion globally as is the case in other methods (variational and HH) [125].

4.2.1 Trinucleon Ground State

PHH, CHH. In the work by Rosati et al. [64], the PH basis together with Jastrow-type correlation factors is used, without Faddeev-type decomposition (fixed choice of Jacobi coordinates). Correlation factors generate terms not describable by PH, but the effect is found to be small.

In the works by Kievsky et al. [65, 67], Faddeev decomposition and PHH, CHH are compared. In ref. [71], the HH method without correlation factors is reexamined, but a reduction technique originally developed by Efros [26] and first applied in Demin et al. [59] is used. This reduction makes the simple HH method more precise than the correlated version, at the price of larger N_e (but N_e can rather easily be increased because of the variational setting).

In ref. [65], it is shown that only 12 channels are sufficient for an accurate solution. The Faddeev formulation would require 36 components; this was one of the insights leading to VIDE [50] based on the Schrödinger equation.

4.2.2 *nd* Scattering

Table 5. *s*-wave phase shift (degrees) for MT(I–III) compared with the Bochum and Iowa/Los Alamos results. From [68]

Method	Phase shift	E	
		0.75	1.5
PHH	$\delta_{\frac{1}{2}0}$	−12.12	−20.66
Fadd. *P*-space		−12.1	−20.7
Fadd. *R*-space		−12.1	−20.7
PHH	$\delta_{\frac{3}{2}0}$	−42.37	−55.86
Fadd. *P*-space		−42.4	−55.9
Fadd. *R*-space		−42.4	−55.8

Table 6. α particle binding energy

Method	N_c	N_e	AV14	AV14 + Ur.8	MT (V)	MT (V)
CHH, Viviani [69]	23	164	23.93	27.48		
EAA + UAA, Fabre [42]						30.63
EAA + UAA, Fabre [42]					29.34	
SIDE, Oehm [45]					28.47	
IDEA, Oehm [45]					29.37	
FY, Kamada [138]			23.87			
GFMC, Carlson [139]			24.2(2)	28.3(2)		
VMC, Wiringa [136]				27.2(2)		
SVM, Varga [141]						31.360
GFMC, Zabolitzky [128]						31.3(2)
ATMS, Akaishi [130]						31.36

Table 7. Comparison of FE, variational, and CFHHM methods for the ground-state energy and $\langle\delta(\mathbf{r}_2)\rangle$ which is proportional to the annihilation rate, for positronium negative ion (Ps^-)

Reference	K_m	N_e	E	$\langle\delta(\mathbf{r}_2)\rangle$
FE, Hu [123]		1080	0.223 115	
		12096	0.266 880	
		9216	0.262 023 4	
		12096	0.262 021 7	
CFHHM, Krivec [95]	40	121	0.262 004 99	0.020 733 56
	48	169	0.262 005 04	0.020 732 42
	56	225	0.262 005 058	0.020 733 02
CFHHM				**0.0207330(6)**
SVM, Varga [141]		150	0.262004	
Faddeev, Schelli. [135]			0.26202	
Variational				
Ho, see [95]			0.262 004 895	0.020 713
Bhatia, cf. [95]			0.262 005 045	0.020 730
			0.262 005 056	0.020 733
Petelenz, cf. [95]			0.262 005 069	
Ho [168]		744	0.262 005 07023286	0.020 733 1980

4.2.3. Four-Nucleon Ground State

4.2.4 Positronium Negative Ion (Ps^-)

The work by Hu et al. [123] uses the FE method by collocation (like the Los Alamos group), employing quintic splines, and the ρ interval transformed to [0, 1]. The method, though less precise, has the advantage over variational calculations in that it is applicable to scattering problems. See Table 7.

4.2.5 Crandall Model

Table 8. Crandall analytically solvable model. Harmonic and inverse-square potentials, $2Qm/\hbar^2 = 1$; see ref. [120]

m/M	N_e	HH	PH	CFHHM	Exact
1	1	4.88	4.88	4.63	4.46
4	1	7.71	7.71	7.20	6.32
25	1	17.59	17.59	16.27	12.58
	4	13.31	12.89		12.58
	6	12.89			12.58

Table 9. Probability of d and t being at the same point, $\rho_0 = \langle\delta(\mathbf{r}_{dt})\rangle$ (in units of 10^{-13} fm^{-3}), for the ground state of μdt for different parametrizations B, C, and D of the correlation function f, and its comparison with HCM and variational calculations

Source	K_m	N_e	C	B	D
CFHHM (Krivec et al. [99])	32	153	0.5204	0.5250	0.5285
	40	231	0.5250	0.5273	0.5290
	48	325	0.5269	0.5280	0.5287
CFHHM		325	**0.528(1)**		
HCM (Abramov et al. [112])		15	0.582		
HCM (Abramov et al. [116])		15	**0.528**		
Alexander et al. [159]		1200	0.5296		
Szalewicz et al. [160]		≈1000	0.5502 (adiabatic)		
			0.5294 (nonadiabatic)		
Variational (different works)		≈1000	**0.5295(1)**		
Bogdanova et al. [161]			0.594		
Langanke et al. [162]			0.6		

4.2.6 Muonic Molecule μdt

Comparison of CFHHM with the result by Ceperley et al. [158] in Krivec et al. [99] is interesting because of the oscillations observed in the GFMC wave function, as

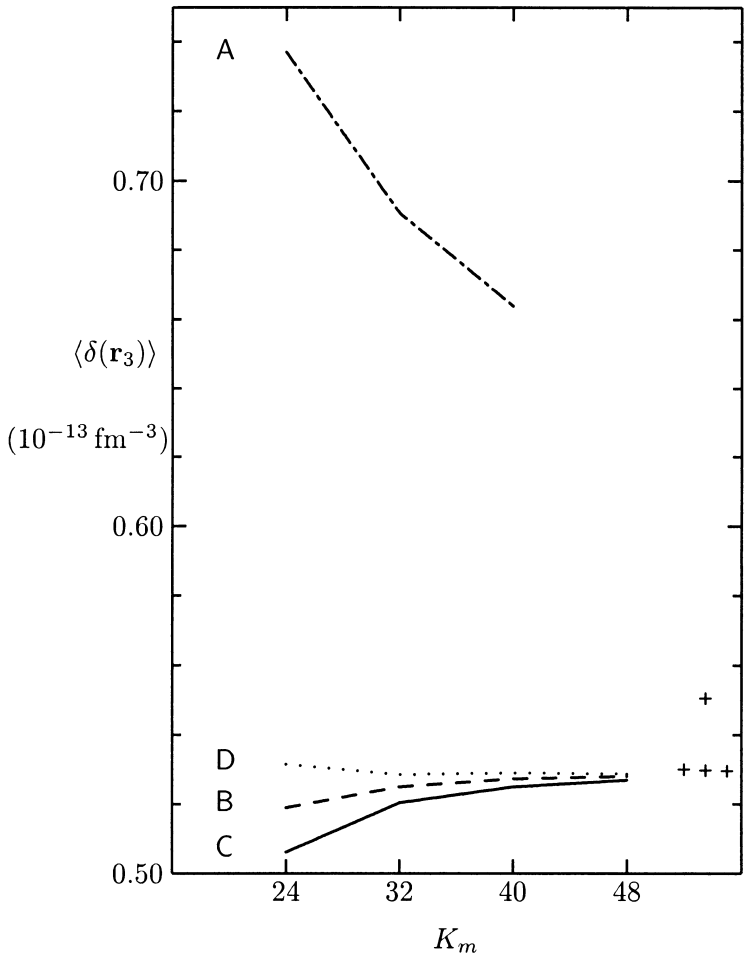

Fig. 9. Expectation values of the delta-function operator of the distance between the deuteron and the triton, proportional to the fusion rate according to the Jackson formula, in units of 10^{-13} fm^{-3}, for the linear (parametrization A) and nonlinear (parametrizations B, C, D) correlation functions. Separate points on the right display the results of variational calculations. The variational results in sequence from left to right on the graph correspond to refs. [159] and [160], respectively, with the upper (lower) points corresponding to the adiabatic (nonadiabatic) values. From Krivec et al. [99]; see Table 9

displayed in Fig. 10. The μdt ground-state fusion rate and sticking probability are examples of CFHHM being more precise than differences in the literature (see Tables 9, 10, and Fig. 9). The difference of sticking probabilities with respect to a recent HCM calculation is up to 0.02 while the CFHHM values are converged within 0.0001. The differences with variational works are substantial. In addition, this system is an example

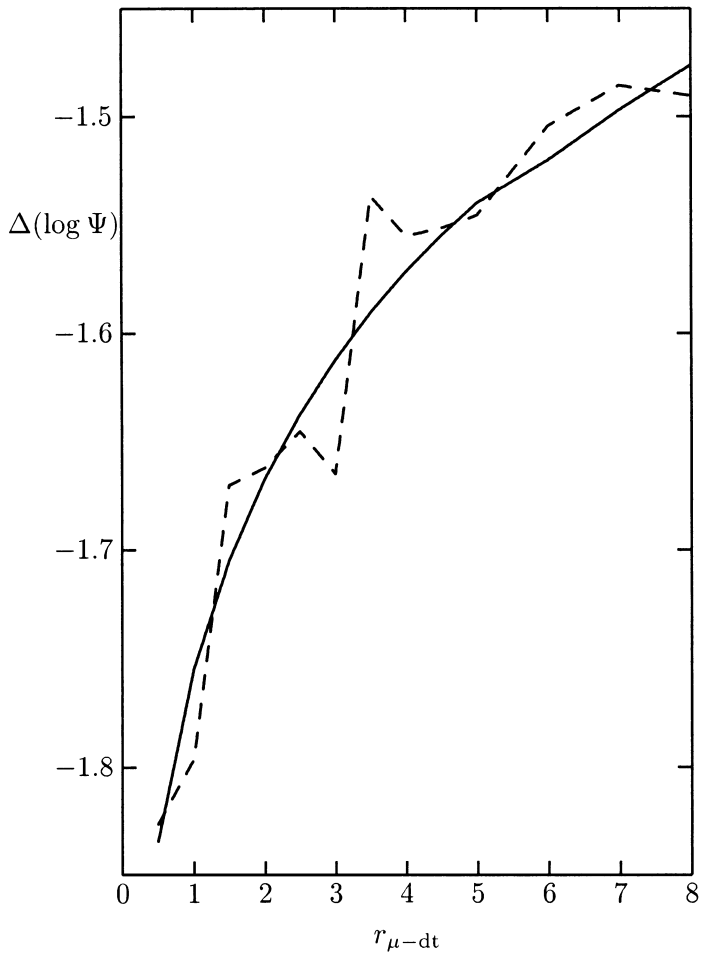

Fig. 10. Divided differences (approximate derivative) of the logarithm of the wave function at the *dt* coalescence point. The differences correspond to intervals of 0.5 for $r_{\mu-dt} \leq 5$ and to intervals of 1 for $r_{\mu-dt} > 5$ (in μ.a.u.). The solid curve is the CFHH wave function calculated with the nonlinear correlation function (parametrization C, $K_m = 40$) while the dashed curve represents the Green-function Monte-Carlo wave function of Ceperley et al. [158]. The Born-Oppenheimer wave function (an exponential) would give a constant value. From Krivec et al. [99]

where wrong convergence of some local observables (sticking probability) was explicitly observed in variational calculations (Haywood et al. [165]).

4.2.7 Helium Atom

Early results by Ballot et al. [34]: The first PH term gives increasing binding with increasing N. However, even for the first excited state, its contribution is only 50%. See Table 11. Newer results are displayed in Table 12.

Table 10. Ground-state sticking probabilities ω_{nl} for $Q = 5.844$ (unless stated otherwise). The CFHHM results are calculated with the nonlinear correlation function f. Parametrizations B, C, and D of f give the same values of ω_{nl} to the number of quoted digits

Method	K_m	1*s*	2*s*	3*s*	4*s*	2*p*
CFHHM,	32	0.6822	0.0978	0.0297	0.0127	0.0238
Krivec [99]	40	0.6820	0.0978	0.0297	0.0127	0.0283
	40	*0.6807*	*0.0976*	*0.0297*	*0.0126*	*0.0237*[a]
	48	0.6819	0.0978	0.0297	0.0126	0.0238
		0.6819(1)				
HCM						
Abramov [112]	15	0.829 (?)				
Abramov [112]	21	0.906 (?)				
Abramov [116]	21	0.7001	0.1004	0.0305	0.0130	0.0245[a]
Variational						
Hu [164]		*0.6932*	0.0992	0.0302	0.0128	0.0241
Haywood [165]		*0.6846*				
GFMC [158]		*0.689*	0.099	0.030	0.013	0.024
Var., Hu [166]		0.6817				
Kamimura [167]		0.6842				
Var., Hu [163]		0.6802	0.0975	0.0296	0.0126	0.0237
Var. (recent)		**0.6802–0.8422**				

[a] $Q = 5.846$

Table 11. Early results for the helium atom, using ordinary HH and PH methods, compared with the correct result, for the finite-mass He-atom ground state. The number of digits quoted shows intrinsic accuracy

Reference	K_m	N_{HH}	N_e	E
HH (Mandelzweig [80])	16	25	25	2.887 54
	20	36	36	2.893 58
HH (Efros [74])	18	30	900	2.887 560
	30	72	2160	2.899 011
	40	121	3630	2.901 775
PH (Ballot [34])	2	1		2.5
	8	4		2.793
	16	8		2.881
	22	11		2.897
CFHHM (Haftel [85])				**2.903 304 5**

Table 12. Comparison of different HH methods and the Hartree-Fock method for the infinite-mass He atom. PH gives better results than HF although equivalent in content (Fabre et al. [121]). CFHH with $N_e = 9$ gives better results than PH with $N_e = 23$. However, at $N_e \approx 20$, full PH is better than ordinary HH because it contains twice the number of K

Reference	K_m	N_{HH}	N_e	E
PH (Fabre [121])	40	10	10	2.877 013 59
	48	12	12	2.877 774 70
	72	18	18	2.878 609 91
Full PH (Fabre [121])	16	7	7	2.887 296 35
	28	13	13	2.898 757 86
	32	15	15	2.900 056 43
	40	19	19	2.901 523 00
	48	**23**	**23**	**2.90***2 259 77*
	72	31	31	2.903 067 40
Faddeev PH (IDEA) (Fabre [121])[a]	28	13	13?	2.930 984 40
Distorted Faddeev PH (Fabre [121])	28	13	13?	2.895 351
HH (FS) (Fabre [121])	16	9	9	2.887 543 91
	28	20	20	*2.899 009 20*
CFHHM (Haftel [85])	0	1	1	2.855 504 862
	8	**9**	**9**	**2.903 7**01 425
	16	**25**	**25**	**2.903 72**3 654
	24	49	49	2.903 724 254
	32	81	81	2.903 724 340
	40	121	121	2.903 724 361
	48	169	169	2.903 724 368
HHGLF (Zhang [77])		256	768	2.902 64
HCM (Frey [105])		196		2.903 73
HCM (Tang [110])		**23**		**2.903** 594 4 (?)
HF (Roothaan), see [121]				2.8617

[a] The work by Fabre et al. [121] compares the results for the ground state of the He atom using the PH, CFHHM and variational methods

Table 13. Comparison of FE, variational, and CFHHM methods for the ground-state energy of the helium atom: Braun et al. [124], Shertzer et al. [122]. The results probably correspond to very roughly the same computational effort. There is apparently no limit on the number of digits obtainable in the variational calculations, but the situation is different for other observables. Infinite-mass He atom; in a.u.

Reference	K_m	N_{HH}	N_e	E
FE, Braun [124]			23652	**2.903** 611 8
Full PH, Fabre [121]	48	23	23	**2.90**2 259 77
CFHHM, Haftel [85]	48	169	169	**2.903 7243**68
Variational				
Drake [147], Baker [146]				**2.903 7243770340(2)**

Table 14. As Table 13, but for the observables of the helium atom 1^1S and 4^1S states (in electron-nucleus separation). From [124]. For the 4^1S state the FE method gives $\langle r_{31}\rangle$ to within 0.002 relative error (ground state: 0.00003), while CFHHM retains its accuracy

Reference	$\langle r_{31}\rangle$	$\langle r_{31}^{-1}\rangle$	$\langle r_{31}^{2}\rangle$	$\langle\delta(\mathbf{r}_{31})\rangle$
		1^1S		
FE, Braun [124]	0.929 50815	1.688 2676	1.193 5886	1.810 2686
CFHHM, Haftel [85]	0.929 47234	1.688 3168	1.193 4831	1.810 42506
Var., Pekeris [148]	0.929 47230	1.688 3168	1.193 4830	1.810 4269
Var., Drake [147]				1.810 429319
		4^1S		
FE, Braun [124]	11.549 239	1.032 4762	281.248 70	1.277 1894
CFHHM, Krivec [92]	11.523 691	1.032 6432	280.230 05	1.277 3070
Var., Accad [149]	11.6		281.5	1.277 21

4.2.8 Double Excited States of He Atom

Table 15. Double excited $^1S^e$ state of He atom

Method	N_{HH}	$-E_r$	$\Gamma/2$
CFHHM [101]	72	0.777 867 6	0.002 270 65
Var. (Ho [150])		0.777 868	0.002 265
HCM (Tang [110])		0.777 35	0.002 2(1)

4.2.9 Lithium Atom

Table 16. Ground state of lithium atom. The "average" correlation factor needs to be improved [78]

Method	N_{HH}	N_{GLF}	E
HHGLF [78]	215	6	*7.339 14*
CFHHGLF [78]	215	6	*7.522 282*
	215	18	7.473 122
Hartree-Fock (Xu et al., see [78])			7.432 7
Experiment (Kusch et al., see [78])			7.478 069

4.2.10 Muonic Helium Atom

In the recent works by Krivec et al. [102,103] the lowest-order hyperfine splitting of the ground states is found to be 4454.206(3) MHz and 4157.691(3) MHz for the muonic ^{4}He and ^{3}He atoms, respectively. The recent variational values from refs. [155, 157] are 0.023 MHz lower and 0.013 MHz higher, respectively, apparently not converging well for the singular operators involved. In particular, the difference $\langle\delta(\mathbf{r}_2)\rangle - \langle\delta(\mathbf{r}_3)\rangle$ is smaller by about 6×10^{-6} a.u. in ref. [157] than in [102, 103], while the effect of different masses used in the literature and of computational errors for these operators are both of the order of only 2×10^{-7} a.u.

4.3 Summary

Milestones

- 1935 HH introduced (Zernike and Brinkman [1]).
- 1965 Nonsymmetric HH (tree method) (Vilenkin et al. [13]).
- 1966 Symmetric HH (Simonov [14], Zickendraht [9]).
- 1969 PH (Fabre de la Ripelle [24]).
- 1969 Slow convergence of HH with realistic nuclear interactions (Erens et al. [23]).
- 1975 The first PH term gives increasing percentage of atomic binding with increasing N (Ballot et al. [34]).
- 1978 CFHHM (Mandelzweig et al. [84]).
- 1988 IDEA (Fabre de la Ripelle et al. [42, 45]).
- 1990 CHH (Rosati et al. [64]).
- 1997 General symmetrization algorithm (Barnea et al. [56]).

Recent developments. In nuclear physics, for $N = 3$ and $N = 4$, the binding energies given by various HH methods (variants of IDEA and PHH/CHH) are of the same accuracy as those by other methods (4–5 digits). The Schrödinger equation as opposed to the Faddeev equations is usually favoured. One of the reasons is the recently found multiple counting of some contributions in the Faddeev formulation (see VIDE, ref. [50]).

PHH and CHH are as good as other methods for $N = 3$ and $N = 4$ observables including scattering parameters [68]. In the *pd* scattering, the discrepancy in forward and backward angles at low E (Coulomb effects) has been confirmed by HH methods [70]. (Inclusion of Coulomb potential below threshold is easier in these methods than in the Faddeev formalism.) Lately the Pisa group has tested the simple HH method without correlation factors again, and found it very accurate in a variational setting where large systems of equations can be used.

In the three-quark system, the work of the Graz group (ref. [145] and references therein) shows that a semirelativistic formalism is necessary and likely sufficient to describe the three-quark system (including the proper flavor operators). The relativistic approach on the other hand favors P-space methods. Some results have also been compared with those by two HH methods; examples of the inadequacy of both the PH method [48] and of the so-called "minimal-K" approximation [143] (see also [66]) in this problem has been found. Both approximations give too good ordering of the $\frac{1}{2}+, \frac{1}{2}-$ states.

The potential accuracy of HHGLF and CFHHGLF is difficult to assess because these methods so far have listed only energy values; it depends on the convergence in the hyperradial basis.

There are examples where HCM obtains better energy values than CFHHM, like in the difficult μdt system, but apparently not better values for singular operators. It should also be noted that in this case the interpolated doubly-convergent values in the CFHHM were not used. Otherwise HCM is in general inferior; however, it can be used for a much larger set of problems including scattering problems.

Conclusion. HH methods have grown up past the phase of constant comparisons with other methods. Two methods, PHH/CHH and CFHHM, flourish in nuclear and atomic physics, respectively. In complicated systems, other methods like FE may eventually overtake them, especially on massively parallel computers.

Acknowledgement. I thank Nir Barnea for clarifying comments on his HH symmetrization algorithm.

5 Exercises

5.1 Analytical

1. Derive the expression for the **Coulomb potential** in the $\mathcal{Y}^{l_{k,1}l_{k,2}}_{KLM}(\Omega_k)$ basis for $L = 0$, using theorems on orthogonal polynomials:

$$\zeta^{(k)} = \sum_{m=1}^{3} \frac{Q_m}{\cos\alpha_k}, \tag{5.1}$$

$$\zeta^{(k)}_{K00ll} = \sum_{m=1}^{3} Q_m \int d\Omega_k \, \mathcal{Y}^{ll}_{K00}(\Omega_k)^* \frac{1}{\cos\alpha_m} \tag{5.2}$$

$$= \sum_{m=1}^{3} Q_m \sum_{\mathcal{K}'} \int d\Omega_m \, \mathcal{Y}^{l'_1 l'_2}_{K'L'M'}(\Omega_m) \frac{1}{\cos\alpha_m} \left[\int d\Omega_m \, \mathcal{Y}^{l'_1 l'_2}_{K'L'M'}(\Omega_m)^* \, \mathcal{Y}^{ll}_{K00}(\Omega_k) \right] \tag{5.3}$$

$$= \sum_{m=1}^{3} Q_m \sum_{K'} \left[\int d\Omega_m \, \mathcal{Y}^{00}_{K'00}(\Omega_m) \frac{1}{\cos\alpha_m} \right] \left[\int d\Omega_m \, \mathcal{Y}^{00}_{K'00}(\Omega_m)^* \, \mathcal{Y}^{ll}_{K00}(\Omega_k) \right]. \tag{5.4}$$

The following is a Raynal-Revai coefficient:

$$\left[\int d\Omega_m \mathcal{Y}^{00}_{K'00}(\Omega_m)^* \mathcal{Y}^{ll}_{K00}(\Omega_k)\right] = \text{const.} \int d\Omega_k {}^{(2)}P^{00}_{K'}(\alpha_m(\alpha_k,\theta_k)) {}^{(2)}P^{ll}_{K}(\alpha_k)P_l(\cos\theta_k) \tag{5.5}$$

$$= \delta_{KK'}(-2\epsilon_{mk}c_{mk}s_{mk})^l C^{(l+1)}_{(K/2)-l}\left(c^2_{mk}-s^2_{mk}\right) \times \frac{\Gamma(2l+2)}{(2l+1)!!}\sqrt{\frac{2(2l+1)\Gamma((K/2)-l+1)}{(K+2)\Gamma((K/2)+l+2)}} \tag{5.6}$$

obtained with the help of the addition theorem for the Gegenbauer polynomials [173]

$$\begin{aligned}\text{const.}{}^{(2)}P^{00}_{K'}(\alpha_m) &= C^{(1)}_{K/2}(-\cos 2\alpha_m)\\ &= C^{(1)}_{K/2}\left(-\left(c^2_{mk}-s^2_{mk}\right)\cos 2\alpha_k + 2\epsilon_{mk}c_{mk}s_{mk}\cos\theta_k\sqrt{1-\cos^2 2\alpha_k}\right)\\ &= \sum_{k=0}^{K/2}\frac{4^k\Gamma((K/2)-k+1)(k!)^2}{\Gamma((K/2)+k+2)}(2k+1)(2\epsilon_{mk}c_{mk}s_{mk})^2(1+\cos^2 2\alpha_k)^{k/2}\\ &\quad\times C^{(k+1)}_{(K/2)-k}\left(c^2_{mk}-s^2_{mk}\right)C^{(k+1)}_{(K/2)-k}\left(-\cos 2\alpha_k\right)P_k(\cos\theta_k).\end{aligned} \tag{5.7}$$

2. Construct **examples of PH bases** (also using the addition theorem for Gegenbauer polynomials): Symmetrical PH basis for *S*-states [49], summed over pairs

$$B^s_K(\Omega) = C_K\sum_k \pi^{-3/2}C^{(1)}_K\left(2\frac{x_k^2}{\rho^2}-1\right). \tag{5.8}$$

This is evaluated using Eqs. (3.39), (3.40) and [49]

$$z(\varphi) = z(0)\cos 2\varphi + \sqrt{1-z(0)^2}\sin 2\varphi\cos\theta, \tag{5.9}$$

$$z(0) = \cos 2\phi, \tag{5.10}$$

to give

$$\begin{aligned}B^s_K(\Omega) &= \pi^{-3/2}C_K\sum_{k=1}^{3}C^{(1)}_K(z(0)\cos 2\varphi_k + \sqrt{1-z(0)^2}\sin 2\varphi_k\cos\theta)\\ &= \frac{C_K}{16\sqrt{\pi}(K+1)}\sum_{k=1}^{3}\sum_{l=0(2)}^{K}(2l+1)\ {}^{(2)}P^{ll}_K(\phi)\,{}^{(2)}P^{ll}_K(\varphi_k)P_l(\cos\theta)\end{aligned} \tag{5.11}$$

using the same theorems as Eq. (5.7).

From Simonov HH for *S*-states, see Eq. (3.12), for pair k:

$$B^{(k)}_\mu(a_k,\lambda_k) = \sum_\nu\left\{\exp\left[i\left(\omega_k-\frac{\pi}{2}\right)\nu\right]\right\}Y_{\mu\nu}(a_k,\lambda_k). \tag{5.12}$$

3. **Check** κ_i, ω_i in Eq. (3.12).

$$\kappa_i = \arccos\frac{m_i(m_k-m_j)-m_j(m_k-m_j)}{(m_i+m_j)(m_j+m_k)}, \tag{5.13}$$

$$\omega_k = \frac{1}{2\mu_k}. \tag{5.14}$$

4. Calculate the V_k **expansion coefficients** (Eq. (3.14)): allowed forms for analytic calculability; power expansion of V_k and limits on allowed powers using the (only similar) known integral

$$\int_{-1}^{1}dx(1-x)^t(1+x)^b P_n^{(a,b)}(x)P_m^{(r,s)}(x) \tag{5.15}$$

which requires Re $b > -1$, Re $t > -1$ ($p > -2-2l_{k,1}$).

5. **Twofold convergence** in CFHHM: Why does it appear (symmetrical basis, nonsymmetrical system)?

6. **CFHHM recursion formulas:** Derive L. Stotland's solution of

$$C_{in} = -\frac{1}{n(n-1)}\left[\sum_{m=-1}^{n-2}(n-m-2)\mathcal{P}_{i,m+1} + \sum_{m=0}^{n-2}\mathcal{Q}_{im}\right]C_{i,n-m-2}, \tag{5.16}$$

where $\mathcal{P}$ and $\mathcal{Q}$ are defined by

$$P = \sum_{m=0}^{\infty}\mathcal{P}_{im}(z-z_i)^m, \tag{5.17}$$

$$Q = \sum_{m=0}^{\infty}\mathcal{Q}_{im}(z-z_i)^m, \tag{5.18}$$

whereby the recurrence formulas are solved (for the case of the Coulomb potential and linear f) such that they need to be calculated only once. Try to generalize this to any potential and any f (i.e., when the effective potential has an infinite expansion). Is the resulting scheme faster than a repeated calculation of the recursion formulas on every interval?

7. $e\mu^4\mathrm{He}^{++}$: Why is linear f in CFHHM not good, although it mimics the asymptotics of the system rather well?

8. **Construction of** f: modified cusp f, nonlinear f. Let us discuss a three-charged particle system where two of the two-particle subsystems have bound states, as is usual in atomic physics. In the leading order, and for $N_e = 1$, the single differential equation gives

$$\chi_1 \sim \exp[(f/\rho + C_{as})\rho] \tag{5.19}$$

as $\rho \longrightarrow \infty$, where we chose the smaller solution

$$C_{as} = \overline{W}_{11}^{D0} - \sqrt{\left(\overline{W}_{11}^{D0}\right)^2 + 2\overline{W}_{11}^{S0} - 2E} \tag{5.20}$$

(see Eqs. (3.16), (3.17)). (This can be generalized to $N_e > 1$.) If particle k is separated from the bound state $\phi_k(\mathbf{x}_k)$ of particles ij (clustering k), χ behaves as

$$\exp\left[-\sqrt{2M_k\epsilon_k}r_i\right]\phi_k(\mathbf{x}_k) \tag{5.21}$$

if $r_i \longrightarrow \infty$, $r_j \longrightarrow \infty$, where $\epsilon_k > 0$ is the particle k separation energy and M_k are the spectator-reduced masses. Then the asymptotic conditions on a_k are

$$a_2 + a_3 + C\sqrt{M_1} = -\sqrt{2M_1\epsilon_1}, \tag{5.22}$$

$$a_3 + a_1 + C\sqrt{M_2} = -\sqrt{2M_2\epsilon_2}, \tag{5.23}$$

$$a_1 + a_2 + C\sqrt{M_3} < 0. \tag{5.24}$$

These equations fix f only in the clustering regions of the hypersphere, and leave one of the a_k as a (partially) free parameter. If $C = 0$, asymptotics are imposed on $\exp(f)$; if $C = C_{as}$, asymptotics are imposed on Ψ. We have $C_{as} = C_{as}(a_1, a_2, a_3, E)$; using an approximate E, the above equations represent a set of nonlinear equations for C. This system does not have to be solved by iteration but by mere tabulation since the results do not depend strongly on C, and the equations are approximate. The third inequality could be replaced by an equation, except that the asymptotics in the "repulsive" clustering is not known. It turned out in the μdt case, however, that the shape of Ψ at $r_3 = r_{dt} = 0$ depends very weakly on a_k, and that good f approximate it well. (The wave function is very small in this region.)

$C = 0$ turned out to be the best choice in the μdt case using nonlinear f [97], as well as in the case of the positronium negative ion [95]. If these systems were calculated with linear f (using $a_k = b_k$), proper asymptotic behavior of the solution would be violated. This would force one to modify the like-charged pair a_k parameter to assume a negative value instead of the positive cusp value. This requirement is

roughly equivalent to applying the constraints on Ψ at $N_e = 1$. Nonlinear f eliminates this necessity [95, 97].

5.2 Computational

1. **CFHHM program package:** Introduction (available at the WWW location http://www−f1.ijs.si/~krivec/dist/pack/).

2. Test the stability of the **Jacobi polynomials** calculation by upward recurrence (see routine M1PJXA).

3. **Precision** in the $e\mu^4$He calculation (routine M1PJQA,…): Why is it sufficient to calculate matrix elements more precisely, but not the hyperradial solution?

4. **Integrals of three Jacobi polynomials** using a recursive method: Enormous efficiency compared to numerical evaluation. Numerical evaluation is avoided if V is expanded in powers of r_k, Eq. (3.14).

5. **The homogeneous system** at $z = z_M$, Eq. (3.25): Test the stability of the solution of such pathological systems by discarding different equations.

6. **The CFHHM "grid":** How it covers the configuration space (do mass weights in $x_{k,i}$ take care of scaling the space, example: $e\mu^4$He)?

7. **Parallelization** of the CFHHM code: For a fine-grained variant, see http://www−f1.ijs.si/~krivec/bench/cfhhoptsppp.txt.

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