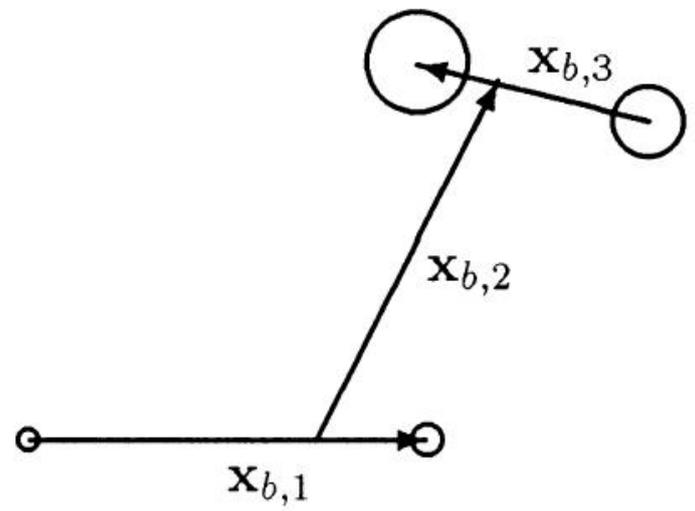
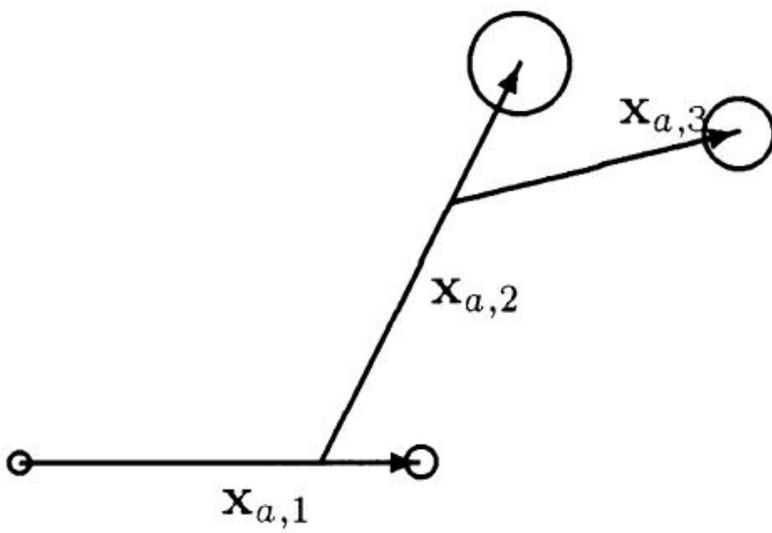


Ab-initio few-body Methods and Nuclear structure

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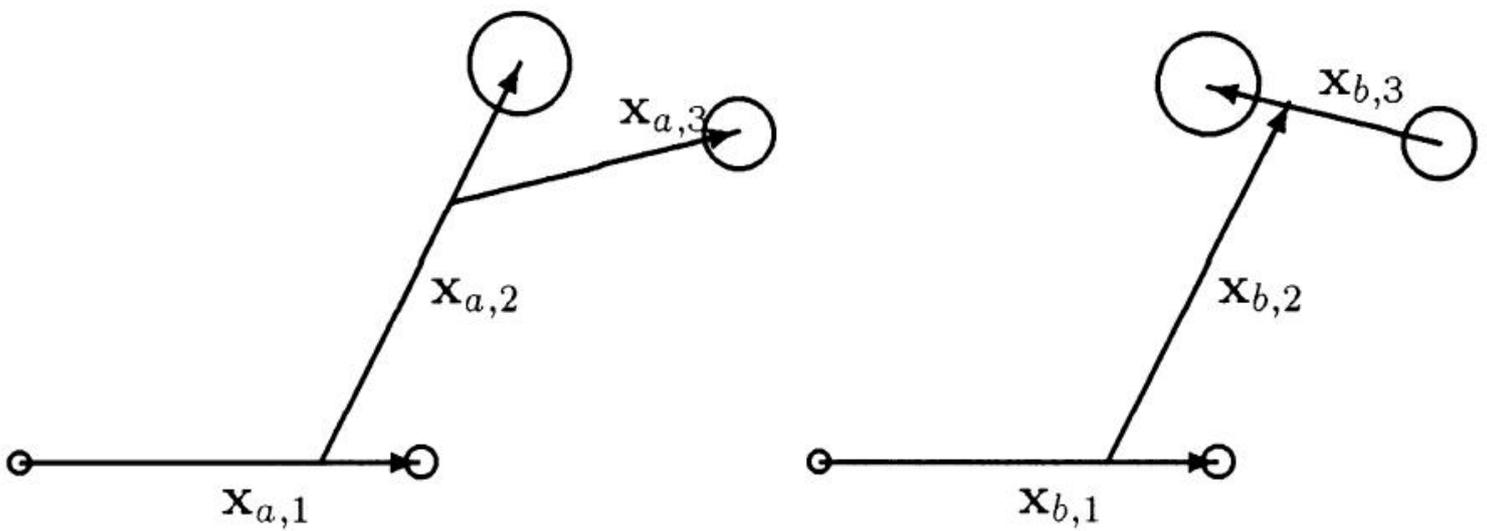
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1. Preliminaries

Definition 1.0.1 — Ab-initio. Ab-initio - from the beginning (Merriam-Webster)

These lectures in few-body physics are meant to present what is often called *ab-initio* techniques, meaning numerical methods that are meant to solve the N -body problem “accurately” without any assumption but the nuclear potential and the currents.

In essence we want to solve the N -body Schroedinger equation

$$(T + V) \Psi = E\Psi \quad (1.1)$$

or the response functions

$$R(\omega) = \int df |\langle \Psi_f | O | \Psi_0 \rangle|^2 \delta(E_f - E_0 - \hbar\omega) \quad (1.2)$$

There are few analytical solutions to these equations, but in most cases we need to rely on numerical work. In the following lectures I’ll present some of the techniques developed over the years to handle the problem. Of course it would be too much to cover all such techniques, therefore the topics covered reflect my personal preferences and experience.

1.1 Notation

Configuration space

$$\langle x | x' \rangle = \delta(x - x') \quad (1.3)$$

$$\langle x | p | x' \rangle = \delta(x - x') \frac{1}{i} \nabla \quad (1.4)$$

Momentum space

$$\langle p | p' \rangle = \delta(p - p') \quad (1.5)$$

Note that people might employ different normalization of momentum states.

Definition 1.1.1 Free wave
Infinite volume normalization

$$\langle \mathbf{x} | \mathbf{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k} \cdot \mathbf{x}} \quad (1.6)$$

in box normalization

$$\langle \mathbf{x} | \mathbf{k} \rangle = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k} \cdot \mathbf{x}} \quad (1.7)$$

Units

- Natural units: $m = \hbar = c = 1$
- Nuclear physics $\hbar c = 197.33 \text{ MeV} \cdot \text{fm}$.
- In Atomic physics $\hbar c = 1973.3 \text{ eV} \cdot \text{\AA}$.

1.2 The 2-Body case

The 2-body wave function, see e.g. [Sak94]

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \langle \mathbf{x}_1 \mathbf{x}_2 | \psi \rangle \quad (1.8)$$

Time dependence

$$i \frac{\partial}{\partial t} \psi = H \psi \quad (1.9)$$

The 2-body Hamiltonian

$$H = -\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(|\mathbf{x}_2 - \mathbf{x}_1|) \quad (1.10)$$

In the 2-body case we separate the center of mass motion from the relative motion through the transformation

$$\begin{aligned} \mathbf{R} &= \frac{1}{M_{12}} (m_1 \mathbf{x}_1 + m_2 \mathbf{x}_2) \\ \mathbf{r} &= (\mathbf{x}_2 - \mathbf{x}_1) \end{aligned} \quad (1.11)$$

The internal Hamiltonian is given by

$$H = -\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \quad ; \quad \mu = \frac{m_1 m_2}{m_1 + m_2} \quad (1.12)$$

Stationary solution

$$H\psi = E\psi \quad \psi(t) = \exp(iE(t - t_0))\psi(t_0) \quad (1.13)$$

The Schroedinger equation

$$\left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (1.14)$$

or

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\hat{l}^2}{r^2} \right) + V(r) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (1.15)$$

Here \hat{l} is the angular momentum operator.

The spherical harmonics

$$\hat{l}^2 Y_{lm}(\hat{\mathbf{r}}) = l(l+1)Y_{lm}(\hat{\mathbf{r}}) \quad \hat{l}_z Y_{lm}(\hat{\mathbf{r}}) = mY_{lm}(\hat{\mathbf{r}}) \quad (1.16)$$

$$\int d\hat{\mathbf{r}} Y_{lm}^*(\hat{\mathbf{r}}) Y_{l'm'}(\hat{\mathbf{r}}) = \delta_{ll'} \delta_{m'm} \quad (1.17)$$

The wave function assumes the form

$$\psi(\mathbf{r}) = Y_{lm}(\hat{\mathbf{r}}) R_l(r) \quad (1.18)$$

Boundary conditions ($E < 0$)

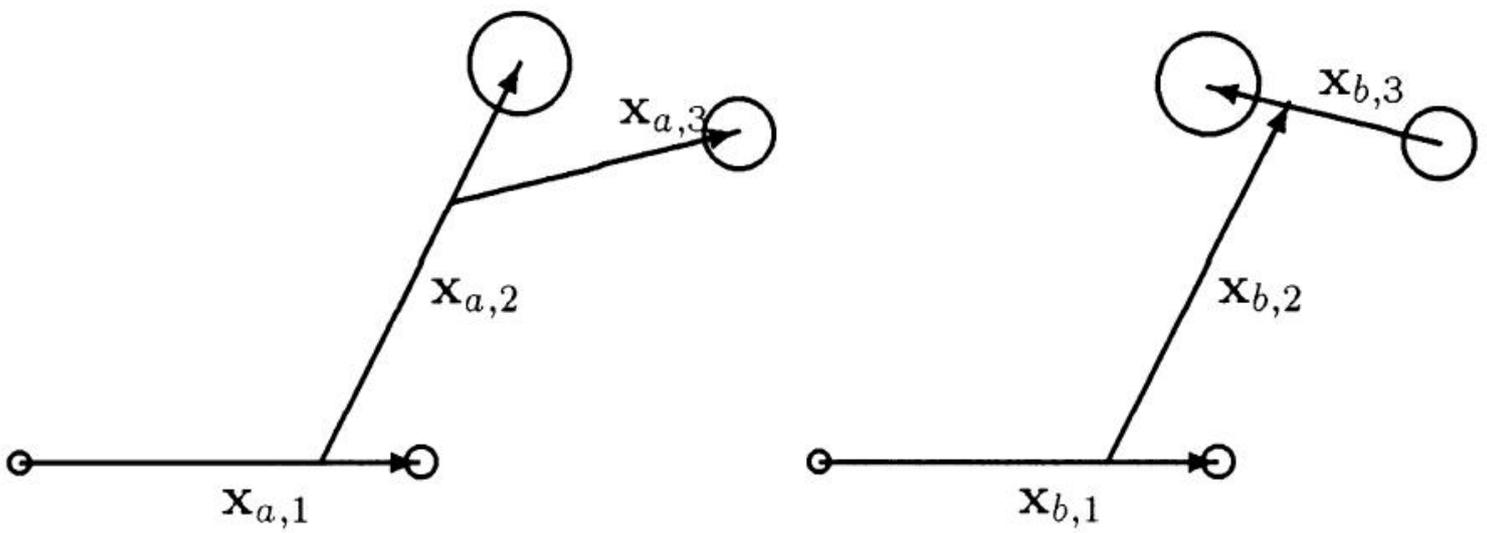
$$\begin{aligned} R_l(r) &\xrightarrow{r \rightarrow 0} Ar^l + Br^{-(l+1)} \\ R_l(r) &\xrightarrow{r \rightarrow \infty} C \frac{\exp(-\kappa r)}{r} + D \frac{\exp(+\kappa r)}{r} \end{aligned} \quad (1.19)$$

$\kappa = \sqrt{-2\mu E}/\hbar, B = D = 0!$

Boundary conditions ($E > 0$)

$$\begin{aligned} R_l(r) &\xrightarrow{r \rightarrow 0} Ar^l + Br^{-(l+1)} \\ R_l(r) &\xrightarrow{r \rightarrow \infty} C \frac{\exp(-ikr)}{r} + D \frac{\exp(+ikr)}{r} \end{aligned} \quad (1.20)$$

$k = \sqrt{2\mu E}/\hbar, B = 0!$



2. Identical particles

2.1 The symmetry principle

Two particles are said to be identical if all their intrinsic properties (mass, spin, charge, etc.) that we shall denote collectively as λ are exactly the same: no experiment can distinguish one from the other.

For such indistinguishable particles, it can make no difference what numbers or names we assign to the position and spin labels of separate individuals. From this perspective, the state vector $\Psi(\mathbf{r}_1, \lambda_1; \mathbf{r}_2, \lambda_2; \dots)$ must represent the same physical state as the state vector $\Psi(\mathbf{r}_2, \lambda_2; \mathbf{r}_1, \lambda_1; \dots)$. This does not mean that these state vectors are equal, only that they are equal up to a constant factor¹

$$\Psi(\mathbf{r}_1, \lambda_1; \mathbf{r}_2, \lambda_2; \dots) = \alpha \Psi(\mathbf{r}_2, \lambda_2; \mathbf{r}_1, \lambda_1; \dots). \quad (2.1)$$

Exchanging the same pair of variables one more time, yields

$$\Psi(\mathbf{r}_1, \lambda_1; \mathbf{r}_2, \lambda_2; \dots) = \alpha^2 \Psi(\mathbf{r}_1, \lambda_1; \mathbf{r}_2, \lambda_2; \dots). \quad (2.2)$$

It follows that

$$\alpha^2 = 1 \quad \text{or} \quad \alpha = \pm 1. \quad (2.3)$$

Particles with $\alpha = 1$ are known as *bosons* and particles with $\alpha = -1$ are known as *fermions*, respectively. One of the most important consequences of special relativity in quantum mechanics is that the spin dictates the permutational properties of the particles:

Half-integers spin particles are fermions;

¹If the states are normalized in the same way, then the constant factor is just a phase, but it is not necessary to assume a particular normalization.

Integer spin particles are bosons.

Even though (2.1) meets our expectations and rests on the intuition about the concept of identical particles, it is actually a demand. If the state does not satisfy (2.1) it cannot describe a system of identical particles. Note that condition (2.1) defines a subspace of the total Hilbert space.

2.2 The two-particle case

Consider a system of two identical particle where particle "1" is in state a , and particle "2" is in state b . With both states properly normalized, the total wave function take the form

$$|\Psi\rangle = |\varphi_a(1)\rangle|\varphi_b(2)\rangle. \quad (2.4)$$

The exchange of variables we have discussed above can be realized now as exchange of the particles 1 and 2 in the wave function. To this end we can define the linear transposition operator P_{12} , that permutes between the particle '1' and particle '2', by

$$P_{12}|\varphi_a(1)\rangle|\varphi_b(2)\rangle = |\varphi_a(2)\rangle|\varphi_b(1)\rangle = |\varphi_b(1)\rangle|\varphi_a(2)\rangle. \quad (2.5)$$

Inspecting the above result we realize that under P_{12} particle 1 moves from state a to state b and the opposite for particle 2. We also realize that

$$P_{21} = P_{12} \quad \text{and} \quad P_{12}^2 = 1. \quad (2.6)$$

Thus the transposition operator is unitary and self adjoint

$$P_{12}^\dagger = P_{12}^{-1} = P_{12}. \quad (2.7)$$

The hermiticity condition follows from the definition of the self adjoint operator.

To understand the permutation properties of operators let O_1 be an hermitian operator acting on the hilbert space of particle 1, and let O_2 be an operator acting on the hilbert space of particle 2. Clearly

$$\begin{aligned} \langle\Psi|O_1|\Psi\rangle &= \langle\varphi_a(1)|O_1|\varphi_a(1)\rangle \\ \langle\Psi|O_2|\Psi\rangle &= \langle\varphi_b(2)|O_2|\varphi_b(2)\rangle \end{aligned} \quad (2.8)$$

Now, using the property $P_{12}^2 = 1$ we see that

$$\begin{aligned} \langle\varphi_a(1)|O_1|\varphi_a(1)\rangle &= \langle\varphi_a(1)\varphi_b(2)|O_1|\varphi_a(1)\varphi_b(2)\rangle \\ &= \langle\varphi_a(1)\varphi_b(2)|P_{12}^2 O_1 P_{12}^2|\varphi_a(1)\varphi_b(2)\rangle \\ &= \langle\varphi_b(1)\varphi_a(2)|P_{12} O_1 P_{12}|\varphi_b(1)\varphi_a(2)\rangle. \end{aligned} \quad (2.9)$$

This equation will be fulfilled only if

$$P_{12} O_1 P_{12} = O_2. \quad (2.10)$$

Looking for eigenstates of P_{12} as we demand for identical particles, there are two possible combinations

$$|\Psi\rangle_+ = \frac{1}{\sqrt{2}} (|\varphi_a(1)\rangle|\varphi_b(2)\rangle + |\varphi_a(1)\rangle|\varphi_b(2)\rangle) \quad (2.11)$$

and

$$|\Psi\rangle_- = \frac{1}{\sqrt{2}} (|\varphi_a(1)\rangle|\varphi_b(2)\rangle - |\varphi_a(1)\rangle|\varphi_b(2)\rangle). \quad (2.12)$$

The upper is for *bosons* and the lower for *fermions*. These states are associated with two operators, the symmetrizer

$$\mathcal{S}_{12} = \frac{1}{2} (1 + P_{12}) \quad (2.13)$$

and the antisymmetrizer

$$\mathcal{A}_{12} = \frac{1}{2} (1 - P_{12}). \quad (2.14)$$

Applying each of these operators to $|\Psi\rangle$ we will get the proper eigenstate of P_{12} .

2.3 The symmetry group

- The size of the group $\dim(S_A) = A!$.
- Each group element $p \in S_A$ can be represented as

$$p = \begin{pmatrix} 1 & 2 & 3 & \dots & A \\ p_1 & p_2 & p_3 & \dots & p_A \end{pmatrix}$$

which reads “The item in box 1 moves to box p_1 , the item in box 2 etc.”

- The product of two group elements $p, q \in S_A$ can be represented as

$$\begin{aligned} pq &= \begin{pmatrix} 1 & 2 & 3 & \dots & A \\ p_1 & p_2 & p_3 & \dots & p_A \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 & \dots & A \\ q_1 & q_2 & q_3 & \dots & q_A \end{pmatrix} \\ &= \begin{pmatrix} 1 & 2 & 3 & \dots & A \\ p_1 & p_2 & p_3 & \dots & p_A \end{pmatrix} \begin{pmatrix} p_1 & p_2 & \dots & p_A \\ q_{p_1} & q_{p_2} & \dots & q_{p_A} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 2 & 3 & \dots & A \\ q_{p_1} & q_{p_2} & \dots & q_{p_A} \end{pmatrix} \end{aligned} \quad (2.15)$$

- A short hand notation is through cycles. An Example

$$p = (1352)(4)$$

which reads “The item in box 1 moves to box 3, the item in box 3 moves to box 5, etc. The item in box 2 moves to box 1. The item in box 4 stays”

- Each permutation can be written as a product of transpositions (i, j) . For example, (acting from right to left)

$$(123) = (13)(12)$$

- Each permutation is associated with a **parity**. The parity of a transposition is (-1) , therefore the parity of a length l cycle is $l - 1$.

2.4 Classes

Definition 2.4.1 Two group elements $c, c' \in S_A$ are conjugate to each other if there is $b \in S_A$ such that $c' = bcb^{-1}$. A class C is an object that contains all the conjugate elements. That is, if $c \in C$ then for any $p \in S_A$ also $pcp^{-1} \in C$. The partition of the group elements into cycles is also a partition into conjugate classes $\{C\}$.

For example the classes of S_4 are

$$(4), (3)(1), (2)(2), (2)(1)(1), (1)(1)(1)(1)$$

Theorem 2.4.1 The class sum operators

$$\hat{C} = \sum_{c \in C} c$$

are Casimir operators of the group, i.e. they commute with all the group elements.

For example

$$\hat{C}_2 = \sum_{i < j}^A (ij)$$

or

$$\hat{C}_3 = \sum_{ijk} (ijk)$$

Proof. For any $p \in S_A$

$$p\hat{C} = p \sum_{c \in C} c = \sum_{c \in C} pc = \sum_{c \in C} pcp^{-1}p = \sum_{c \in C} c'p = \hat{C}p$$

■

A partition is defined by $\lambda_1 \geq \lambda_2 \geq \lambda_3 \dots \geq \lambda_A$, where $\sum_k \lambda_k = A$. Each partition defines a class.

2.5 The IRREPs

The irreducible representations (irreps) of the symmetry group S_A

- For finite symmetry groups there is a one to one correspondance between the irreps and the classes.
- Therefore a partition defined by $\lambda_1 \geq \lambda_2 \geq \lambda_3 \dots \geq \lambda_A$, where $\sum_k \lambda_k = A$ defines not only a class but also an irrep.
- We denote a Young diagram as $\Gamma_A = [\lambda_1, \lambda_2, \dots, \lambda_A]$
- Each young diagram is characterized by a partition and each partition defines an irrep.
- The irreps of the symmetry group S_A are characterized by the Young diagrams.

- A state in an irrep is defined by

$$Y_A = (\Gamma_A, \Gamma_{A-1}, \dots, \Gamma_3, \Gamma_2, \Gamma_1)$$

- The dimension of the irrep is the possible number of writing the numbers $1 \dots A$ such as they increase to the right and down. For example the irreps $[1, 1, 1, 1]$, $[2, 2]$, $[3, 2]$.
- Two important irreps the symmetric (bosonic) irrep $[A]$ and the antisymmetric (fermionic) irrep $[1, 1, 1, \dots, 1]$.

Each irrep is associated with a projection operator, the Young operator. For the symmetric and antisymmetric irreps these operators take a simple form. Symmetric,

$$\mathcal{S} = \frac{1}{A!} \sum_{p \in \mathcal{S}_A} \hat{p} \quad (2.16)$$

Antisymmetric,

$$\mathcal{A} = \frac{1}{A!} \sum_{p \in \mathcal{S}_A} \text{sign}(p) \hat{p} \quad (2.17)$$

2.5.1 The Casimir operators

Thanks to Schor's Lemmas we know that an object that commutes with all the group elements is proportional to the unit operator in any irreducible subspace. Therefore the class sum operators have a one eigenvalue for each irrep. In principle the full set of the class sum operators is needed to uniquely identify an irrep. In practice the transposition class-sum operator is enough to identify all the irreps for $A \leq 5$. The eigenvalues of the class-sum operator \hat{C}_2 are given by

$$\hat{C}_2|\Gamma\rangle = \left(\sum_i \frac{\lambda_i(\lambda_i - 1)}{2} - \sum_j \frac{r_j(r_j - 1)}{2} \right) |\Gamma\rangle \quad (2.18)$$

The first degenerated eigenvalue appears for the S_6 irreps $[411]$, $[33]$, and for their mirror image $[3111]$, $[222]$. The S_7 irreps are uniquely identified, and so on. The symmetric and antisymmetric irreps are largest and smallest eigenvalues of \hat{C}_2 and are always unique.

2.6 Bosons and fermions

For constructing fermionic or bosonic states we can define the two operators

$$\begin{aligned} \mathcal{S} &= \frac{1}{N!} \sum_{g \in \mathcal{S}_N} P_g, \\ \mathcal{A} &= \frac{1}{N!} \sum_{g \in \mathcal{S}_N} \text{sign}(g) P_g, \end{aligned} \quad (2.19)$$

where P_g is a unitary representation of the group element g in our Hilbert space, i.e.

$$P_g^\dagger P_g = P_g P_g^\dagger = I \quad (2.20)$$

and

$$P_{g_1} P_{g_2} = P_{g_1 g_2}. \quad (2.21)$$

In other words, we arrived at the unitary representation of the permutation group S_N . This is another realization of the Wigner's theorem in the special case of permutation symmetry.

We recall that $\text{sign}(g) = 1$ if g is even and $\text{sign}(g) = -1$ for odd g , and that any operator $g \in S_N$ can be written as a product of 2-particle transpositions such as (26), or (13). An even operator is a product of even number of transpositions, an odd operator is a product of an odd number of transpositions.

Theorem 2.6.1 The operators \mathcal{S} and \mathcal{A} satisfy the following properties:

- (a) \mathcal{S} and \mathcal{A} are Hermitian operators: $\mathcal{S}^\dagger = \mathcal{S}$, $\mathcal{A}^\dagger = \mathcal{A}$.
 (b) \mathcal{S} and \mathcal{A} commute with P_g for all $g \in S_N$,

$$\begin{aligned} P_g \mathcal{S} &= \mathcal{S} P_g = \mathcal{S}, \\ P_g \mathcal{A} &= \mathcal{A} P_g = \text{sign}(g) \mathcal{A}. \end{aligned} \quad (2.22)$$

- (c) \mathcal{S} and \mathcal{A} are projectors to orthogonal subspaces of \mathcal{H}_{tot} , i.e.

$$\mathcal{S}^2 = \mathcal{S}, \quad \mathcal{A}^2 = \mathcal{A}, \quad \mathcal{S}\mathcal{A} = \mathcal{A}\mathcal{S} = 0. \quad (2.23)$$

Proof. (a) By definition

$$\mathcal{S}^\dagger = \frac{1}{N!} \sum_{g \in S_N} P_g^\dagger = \frac{1}{N!} \sum_{g \in S_N} P_g^{-1} = \frac{1}{N!} \sum_{g \in S_N} P_{g^{-1}} = \mathcal{S}, \quad (2.24)$$

where 2nd equality follows from unitarity of representation $P_g^\dagger = P_g^{-1}$, the 3rd equality rests on $P_g^{-1} = P_{g^{-1}}$ which follows from P_g being a representation of the group. Finally, the last equality is true because inverse operation is a bijection from S_N to itself. The proof of $\mathcal{A}^\dagger = \mathcal{A}$ is almost identical. We only need to note that since $g^{-1}g = I$ and $\text{sign}(I) = 1$ we must have $\text{sign}(g^{-1}) = \text{sign}(g)$.

- (b) We have

$$\begin{aligned} P_g \mathcal{A} &= \frac{1}{N!} \sum_{g' \in S_N} \text{sign}(g') P_g P_{g'} = \frac{1}{N!} \sum_{g' \in S_N} \text{sign}(g)^2 \text{sign}(g') P_{gg'} \\ &= \frac{\text{sign}(g)}{N!} \sum_{g' \in S_N} \text{sign}(gg') P_{gg'} = \text{sign}(g) \mathcal{A}, \end{aligned} \quad (2.25)$$

where in the 2nd equality we used (2.21) and $\text{sign}(g)^2 = 1$, $\forall g \in S_N$, whereas in the 1st equality of the second line we substituted $\text{sign}(g)\text{sign}(g') = \text{sign}(gg')$. Finally, last equality rests on the bijective nature of the map $g' \rightarrow gg'$. The proof for \mathcal{S} follow suit.

- (c) Using the definition of \mathcal{S} and (b), yields

$$\mathcal{S}^2 = \frac{1}{N!} \sum_{g \in S_N} P_g \mathcal{S} = \frac{1}{N!} \sum_{g \in S_N} \mathcal{S} = \mathcal{S}. \quad (2.26)$$

Similarly,

$$\mathcal{A}^2 = \frac{1}{N!} \sum_{g \in \mathcal{S}_N} \text{sign}(g) P_g \mathcal{A} = \frac{1}{N!} \sum_{g \in \mathcal{S}_N} \text{sign}(g)^2 \mathcal{A} = \mathcal{A}. \quad (2.27)$$

Now for $\mathcal{S}\mathcal{A}$ we see that

$$\mathcal{S}\mathcal{A} = \mathcal{S}(P_g^{-1} P_g) \mathcal{A} = (\mathcal{S} P_g^{-1})(P_g \mathcal{A}) = \mathcal{S} \text{sign}(g) \mathcal{A}, \quad (2.28)$$

and choosing an odd parity g we much have $\mathcal{S}\mathcal{A} = 0$. ■

Exercise 2.1 Show that $\mathcal{A} + \mathcal{S} = I$ iff $N = 2$. ■

2.6.1 Construction of physical states

Tools of the preceding subsection lead directly to the following rule for construction of the *unique* physical state corresponding to a system of N identical particles:

- (a) Enumerate the particles arbitrarily and assign to each particle an individual state in the corresponding Hilbert space $\mathbf{r}_n \lambda_n \in \mathcal{H}_n$. Construct the state $|\Psi(\mathbf{r}_1 \lambda_1; \mathbf{r}_2 \lambda_2; \dots)\rangle \in \mathcal{H}_{\text{tot}}$.
- (b) Apply \mathcal{S} or \mathcal{A} to $|\Psi\rangle$, depending on whether the identical particles are bosons or fermions.
- (c) Normalize the state obtained in this way, *e.g.* the physical state describing N identical fermions is given by $|\Psi\rangle_F = \mathcal{N} \mathcal{A} |\Psi\rangle$, where \mathcal{N} is normalization constant.

Indeed,

$$P_g |\Psi\rangle_F = P_g \mathcal{N} \mathcal{A} |\Psi\rangle = \text{sign}(g) \mathcal{N} \mathcal{A} |\Psi\rangle = \text{sign}(g) |\Psi\rangle_F, \quad (2.29)$$

in full agreement with (2.1), where we used $P_g \mathcal{A} = \text{sign}(g) \mathcal{A}$ proved in the previous section.

2.6.2 Outer product wave functions

We note that if the wave function is an outer product of two different spaces $\Psi \in \mathcal{Y} \otimes \mathcal{X}$ and we managed to construct in each subspace states with well defined symmetry then we can use the Clebsch-Gordan coefficients of the symmetry group and construct states with the desired symmetry. For example we can construct fermionic wave function as a product

$$\Psi_A = \sum_{\gamma_{A-1}} \frac{\Lambda_{\Gamma_A, \gamma_{A-1}}}{\sqrt{|\Gamma_A|}} \mathcal{Y}_{\Gamma_A \gamma_{A-1}} \mathcal{X}_{\tilde{\Gamma}_A, \tilde{\gamma}_{A-1}} \quad (2.30)$$

where in $\tilde{\Gamma}_k$ the row and columns are inverted with respect to Γ_k , $\Lambda_{\Gamma_A, \gamma_{A-1}}$ is a phase factor, and $|\Gamma_A|$ is the dimension of the irrep.

2.7 Slater determinant and the structure of the lightest nuclei

A simple way of obtaining fermionic states rests on the so-called *Slater determinant*. The signs of the various terms in the definition of \mathcal{A} are determined by the same rule as those of a $N \times N$ determinant. Utilizing this observation and choosing a single particle basis $\{|\varphi_a(\mathbf{r}, \lambda)\rangle\}_{a=1}^{\infty}$ it is convenient to write an anti-symmetric state in the form of a Slater determinant

$$\Psi(1, 2, \dots, N) = \begin{vmatrix} \varphi_1(1) & \varphi_2(1) & \cdots & \varphi_N(1) \\ \varphi_1(2) & \varphi_2(2) & \cdots & \varphi_N(2) \\ \vdots & \vdots & \cdots & \vdots \\ \varphi_1(N) & \varphi_2(N) & \cdots & \varphi_N(N) \end{vmatrix}. \quad (2.31)$$

Obviously, $\mathcal{A}|\Psi\rangle$ vanishes if two or more of the states $\{|\varphi_i\rangle\}_{i=1}^N$ coincide. Moreover, the Slater determinant makes it obvious that the full physical state vanishes if one of the states $\{|\varphi_i\rangle\}_{i=1}^N$ is given by a linear combination of the other states.

2.7.1 The lightest nuclei

The simplest picture of the nucleus is the shell model. The nucleons are moving in a mean-field, i.e. the harmonic-potential, produced by the interaction with the other nucleons. The energy levels of the 3-dimensional harmonic-oscillator are

$$E_{nl} = (2n + l + \frac{3}{2})\hbar\omega = (N + \frac{3}{2})\hbar\omega. \quad (2.32)$$

Here n is the radial quantum number and l the angular momentum. The single particle states are given by

$$\varphi_{nlm\lambda}(\mathbf{r}, \lambda) = \langle \mathbf{r}\lambda | nlm\lambda \rangle. \quad (2.33)$$

Constructing an A -body Slater determinant using the lowest HO basis states we see the shell structure:

- $A \leq 4$ - $n = l = m = 0$, the state are defined by the internal degrees of freedom, the spin s and the isospin t .
- $4 < A \leq 16$ - $n = 0$, $l = 1$, and $m = -1, 0, +1$. Here we have a total of 12 states $4 \times (2l + 1)$.
- ...

2.8 The magnetic moment of the nucleon

The constituent quark model provides a simple description of the nucleon N (proton or neutron) as a system composed of 3 interacting quarks, moving in a central confining potential. Each quark q carries 3 internal quantum numbers color c , spin σ , and flavour f . The flavour indicates the type of quark which in our case is either an *up* quark or a *down* quark, i.e. $f = (u, d)$.

$$\Psi_N = \Psi(x_1 c_1 \sigma_1 f_1, x_2 c_2 \sigma_2 f_2, x_3 c_3 \sigma_3 f_3). \quad (2.34)$$

It turns out that the nucleons as well as all other hadrons belong to a color singlet, a phenomena sometimes described as color confinement, as we don't find any free colored object. The 3-quarks color singlet state \mathcal{X}_A^c is antisymmetric, therefore we shall denote it with subscript A . As a consequence, the space-spin-flavour part of the wave function Ψ_{RSF} must be symmetric,

$$\Psi_N = \mathcal{X}_A^c \otimes \Psi_{RSF}(x_1\sigma_1f_1, x_2\sigma_2f_2, x_3\sigma_3f_3). \quad (2.35)$$

Considering now the nucleon as a system of 3 quarks moving in a confining potential (such as the harmonic oscillator), it is clear that in the ground state of the nucleon all 3 quarks will assume the same lowest energy state which we expect to be an $\ell = 0$ state. Denoting this state by φ_0 , the nucleon wave-function takes the form

$$\Psi_N = \mathcal{X}_A^c \otimes \underbrace{\varphi_0(x_1)\varphi_0(x_2)\varphi_0(x_3)}_{\Psi_R(x_1, x_2, x_3)} \otimes \Phi_{SF}(\sigma_1f_1, \sigma_2f_2, \sigma_3f_3). \quad (2.36)$$

Evidently, $\Psi_R(x_1, x_2, x_3)$ is symmetric under particle permutations, hence the spin-flavour part of the wave-function Ψ_{SF} must also be symmetric.

QCD is blind to the flavour of the quark, and as the masses of the u, d quarks are rather similar the hadronic spectrum as well as the nuclear force exhibit an approximate symmetry to the exchange of these quark. This symmetry is an $SU(2)$ symmetry analogous to the spin symmetry and is known as isospin symmetry, i.e. isotopic-spin symmetry. From algebraic point of view isospin states are equivalent to spin states. The proton and the neutron are an example of isospin symmetry as they have the same mass to within 2 permil. They belong to the isospin $I = \frac{1}{2}$ doublet, with the proton corresponding to the $|I = \frac{1}{2}, I_z = \frac{1}{2}\rangle$ state, and the neutron to the $|I = \frac{1}{2}, I_z = -\frac{1}{2}\rangle$ state.

The proton and the neutron are also $S = \frac{1}{2}$ particles. To construct a 3-quark $S = \frac{1}{2}$ we can couple the first two quarks to form an $S = 0$ and couple this state with the single quark $S = \frac{1}{2}$ state, i.e.

$$|S = \frac{1}{2}, M = \frac{1}{2}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle). \quad (2.37)$$

Similarly we can write down an isospin state

$$|I = \frac{1}{2}, I_z = \frac{1}{2}\rangle = \frac{1}{\sqrt{2}}(|udu\rangle - |duu\rangle). \quad (2.38)$$

The proton's spin-isospin state is a symmetrized product of these two states

$$\begin{aligned} |p\uparrow\rangle &= \mathcal{N}\mathcal{S}(|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle)(|udu\rangle - |duu\rangle) \\ &= \mathcal{N}\mathcal{S}(|u\uparrow d\downarrow u\uparrow\rangle + |d\downarrow u\uparrow u\uparrow\rangle - |u\downarrow d\uparrow u\uparrow\rangle - |d\uparrow u\downarrow u\uparrow\rangle) \end{aligned} \quad (2.39)$$

where \mathcal{N} is a normalization constant, and

$$\mathcal{S} = \frac{1}{3!} (e + (12) + (23) + (31) + (123) + (132)) \quad (2.40)$$

is the 3-body symmetrization operator. Applying S we get

$$\begin{aligned}
|p\uparrow\rangle = \frac{1}{\sqrt{18}} & \left(2|d\downarrow u\uparrow u\uparrow\rangle + 2|u\uparrow d\downarrow u\uparrow\rangle + 2|u\uparrow u\uparrow d\downarrow\rangle \right. \\
& - |d\uparrow u\downarrow u\uparrow\rangle - |d\uparrow u\uparrow u\downarrow\rangle - |u\uparrow d\uparrow u\downarrow\rangle \\
& \left. - |u\uparrow d\uparrow u\downarrow\rangle - |u\uparrow u\downarrow d\uparrow\rangle - |u\downarrow u\uparrow d\uparrow\rangle \right) \quad (2.41)
\end{aligned}$$

We are now in position to calculate the proton's magnetic moment. Assuming as we have argued above that the motion of the quarks is predominantly an s -wave motion, we may write the magnetic moment as

$$\boldsymbol{\mu} = 2 \sum_{i=1}^3 (\mu_u P_u(i) + \mu_d P_d(i)) \mathbf{s}_i \quad (2.42)$$

Here P_u, P_d are projections on u, d states, \mathbf{s} is the spin operator and

$$\mu_q = \frac{e_q}{2m_q} \quad (2.43)$$

is the quark magneton, with e_q the charge of the quark, and m_q its mass. Assuming the $m_d = m_u$ and recalling that $e_u = 2/3e$, $e_d = -1/3e$ we see that

$$\frac{\mu_d}{\mu_u} = \frac{-1/3}{2/3} = -\frac{1}{2} \quad (2.44)$$

The proton magnetic moment is given by

$$\mu_p = \langle p\uparrow | \mu_z | p\uparrow \rangle = \frac{1}{18} (4 \times 3 \times (2\mu_u - \mu_d) + 6\mu_d) = \frac{4}{3}\mu_u - \frac{1}{3}\mu_d \quad (2.45)$$

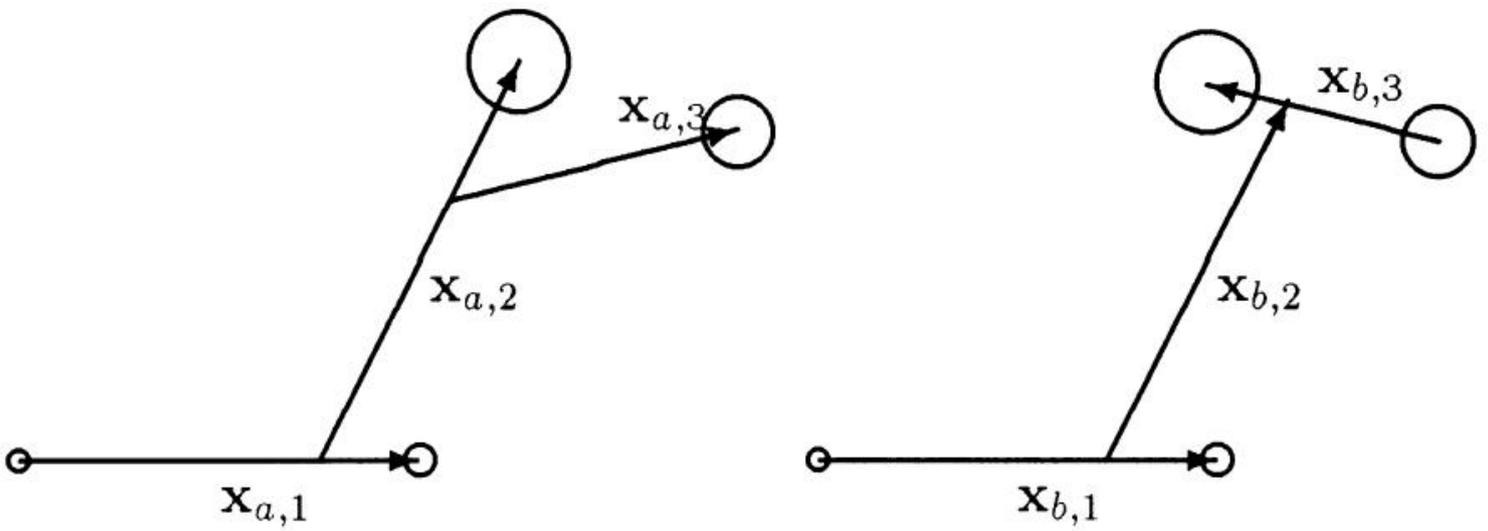
For the neutron we shall get the same result replacing u with d

$$\mu_n = \frac{4}{3}\mu_d - \frac{1}{3}\mu_u \quad (2.46)$$

Calculating now the ratio between the protons's and the neutron's magnetic moments we get

$$\frac{\mu_p}{\mu_n} = \frac{4/3\mu_u - 1/3\mu_d}{4/3\mu_d - 1/3\mu_u} = \frac{4/3 + 1/6}{-2/3 - 1/3} = -\frac{3}{2} \quad (2.47)$$

The proton's magnetic moment is $\mu_p = 2.793\mu_N$ and the neutron's is $\mu_n = -1.913\mu_N$. We see that prediction of the naive quark model, compares well with the experimental ratio $\mu_p/\mu_n \approx -1.46$.



3. The Jacobi Coordinates

3.1 Relative coordinates for the 2,3-body systems

3.1.1 The 2-Body case

In the 2-body case we separate the center of mass motion from the relative motion through the transformation

$$\begin{aligned} R &= \frac{1}{M_{12}} (m_1 r_1 + m_2 r_2) \\ r &= (r_2 - r_1) \end{aligned} \quad (3.1)$$

Here $M_{12} = m_1 + m_2$. It should be noted that this transformation is not orthogonal. Using orthogonal transformation we set

$$\begin{aligned} \eta_0 &= \sqrt{\frac{1}{M_{12}m}} (m_1 r_1 + m_2 r_2) \\ \eta_1 &= \sqrt{\frac{m_1 m_2}{M_{12}m}} (r_2 - r_1) \end{aligned} \quad (3.2)$$

m is an arbitrary mass which we usually take as the nucleon mass $m = m_N$.

3.1.2 The 3-Body case

As it is well known, in order to separate the motion of the center of mass coordinate, $\eta_0 = R_{cm}$, in the 3-body problem one has to work with the Jacobi coordinates [Jac42]

$$\eta_0 = \sqrt{\frac{1}{M_{123}}} (m_1 r_1 + m_2 r_2 + m_3 r_3)$$

$$\begin{aligned}\eta_1 &= \sqrt{\frac{m_1 m_2}{M_{12} m}} (\mathbf{r}_2 - \mathbf{r}_1) \\ \eta_2 &= \sqrt{\frac{M_{12} m_3}{M_{123} m}} \left(\mathbf{r}_3 - \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{M_{12}} \right)\end{aligned}\quad (3.3)$$

where $M_{ij} = m_i + m_j$ and $M_{123} = m_1 + m_2 + m_3$ and m is an arbitrary mass which we usually take as the nucleon mass $m = m_N$.

3.2 The A-body case

3.2.1 General prescription

A general discrete sets of Jacobi coordinates can be written through recursive splitting of the A particles into subgroups. We start writing the A particles in any desired order and then split them in the following way

$$\begin{aligned}&(1234 \dots 789 \dots A) \\ &(1234 \dots 7)(89 \dots A) \\ &(1234)(\dots 7)(89 \dots A) \\ &(12)(34)(\dots 7)(89 \dots A) \\ &\dots \\ &\dots \\ &(1)(2)(3)(4) \dots (7)(8)(9) \dots (A)\end{aligned}\quad (3.4)$$

The splitting continue until all particles reside in a single particle group. Clearly we need $N = A - 1$ steps to complete the split. Now we associate each split with a Jacobi coordinate that connects the center of mass of the two new fragments. Consequently each splitting defines a different set of $A - 1$ relative (Jacobi) coordinates. These coordinates together with the center of mass coordinates completes a set of A coordinates. For example in the 4-body case we may choose the following split

$$\begin{aligned}&(1234) \\ &(12)(34) \\ &(1)(2)(34) \\ &(1)(2)(3)(4)\end{aligned}\quad (3.5)$$

This split is associated with the (H) set of Jacobi vectors

$$\begin{aligned}\eta_1 &= \sqrt{\frac{M_{12} M_{34}}{M_{1234} m}} \left(\frac{M_3 \mathbf{r}_3 + M_4 \mathbf{r}_4}{M_{34}} - \frac{M_1 \mathbf{r}_1 + M_2 \mathbf{r}_2}{M_{12}} \right) \\ \eta_2 &= \sqrt{\frac{m_1 m_2}{M_{12} m}} (\mathbf{r}_2 - \mathbf{r}_1) \\ \eta_3 &= \sqrt{\frac{m_3 m_4}{M_{34} m}} (\mathbf{r}_4 - \mathbf{r}_3),\end{aligned}\quad (3.6)$$

We note again that we may start the procedure with any arbitrary permutation of the particles.

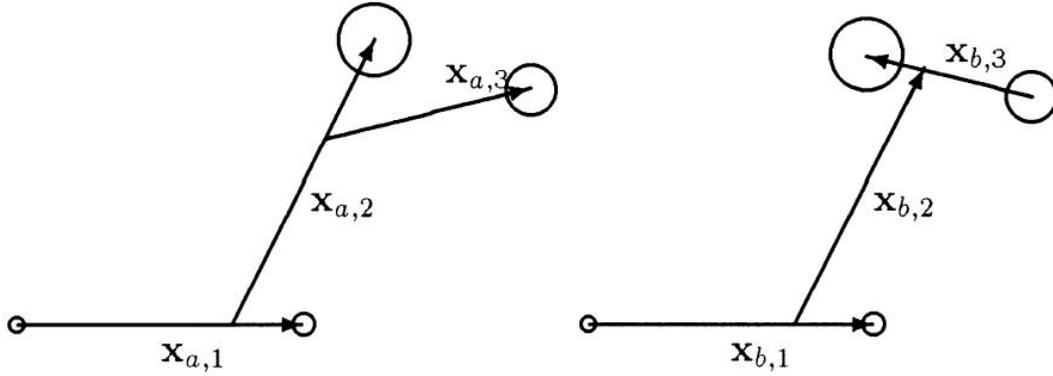


Figure 3.1: The Jacobi coordinates

3.2.2 The A-Body 'K' system

In the general A -body case it is convenient to work with the recursive 'K' splitting

$$\begin{aligned}
 & (1234 \dots 789 \dots A - 2 \ A - 1 \ A) \\
 & (1234 \dots 789 \dots A - 2 \ A - 1)(A) \\
 & (1234 \dots 789 \dots A - 2)(A - 1)(A) \\
 & \dots \\
 & \dots \\
 & (1234 \dots 7)(8)(9) \dots (A - 2)(A - 1)(A) \\
 & \dots \\
 & \dots \\
 & (12)(3)(4) \dots (7)(8)(9) \dots (A - 2)(A - 1)(A) \\
 & (1)(2)(3)(4) \dots (7)(8)(9) \dots (A - 2)(A - 1)(A) \tag{3.7}
 \end{aligned}$$

This splitting defines the $N = A - 1$ Jacobi coordinates [Jac42] $\eta_1, \eta_2, \dots, \eta_N$. That together with the center of mass coordinate, $\eta_0 = \mathbf{R}_{cm}$, forms a complete new set of coordinates.

For this specific set of coordinates it is useful to look at the splitting (3.7) bottom up, i.e. to assume merging. This way the construction of the Jacobi vectors is done adding one particle at a time. The general expressions for the mass weighted Jacobi coordinates were given by Hirshfelder and Dahler [HD56]

$$\eta_{k-1} = \sqrt{\frac{M_{1\dots k-1} m_k}{M_{1\dots k} m}} \left(\mathbf{r}_k - \frac{1}{M_{1\dots k-1}} (m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2 + \dots + m_{k-1} \mathbf{r}_{k-1}) \right) \quad ; \quad k = 2, 3, \dots, A \tag{3.8}$$

Where $M_{1\dots k} = \sum_{i=1}^k m_i$.

This transformation can be written as an orthogonal transformation U_{ij} ,

$$\eta_{k-1} = \sum_{i=1}^A U_{ki} \sqrt{m_i/m} \mathbf{r}_i \quad , \quad \mathbf{r}_i = \frac{1}{\sqrt{m_i/m}} \sum_{k=1}^A U_{ki} \eta_{k-1} \tag{3.9}$$

Here the matrix U_{ki} has the following form:

$$U_{ij} = \begin{cases} \sqrt{\frac{m_j}{M_{1\dots A}}} & \text{for } i = 1 \\ -\sqrt{\frac{M_{1\dots A}}{m_i m_j}} & \text{for } i > 1 \\ \sqrt{\frac{M_{1\dots i-1}}{M_{1\dots i}}} & \text{for } i = j \\ 0 & \text{for } j > i \end{cases} \quad (3.10)$$

One can easily check that the matrix U_{ij} is orthogonal

$$\sum_{j=1}^N U_{ij} U_{kj} = \delta_{ik} \quad , \quad \det(U) = 1. \quad (3.11)$$

In view of (3.9), the expressions for the gradients are

$$\frac{\partial}{\partial \mathbf{r}_i} = \sum_{k=1}^N U_{ki} \sqrt{m_i/m} \frac{\partial}{\partial \boldsymbol{\eta}_{k-1}} \quad , \quad \frac{\partial}{\partial \boldsymbol{\eta}_{k-1}} = \sum_{i=1}^N U_{ki} \frac{1}{\sqrt{m_i/m}} \frac{\partial}{\partial \mathbf{r}_i} \quad (3.12)$$

The corresponding momentum operators

$$\mathbf{p}_i = -i \frac{\partial}{\partial \mathbf{r}_i} \quad , \quad \mathbf{q}^{k-1} = -i \frac{\partial}{\partial \boldsymbol{\eta}_{k-1}} \quad (3.13)$$

are therefore transformed as

$$\mathbf{p}_i = \sum_{k=1}^N U_{ki} \sqrt{m_i/m} \mathbf{q}^{k-1} \quad , \quad \mathbf{q}^{k-1} = \sum_{i=1}^N U_{ki} \frac{1}{\sqrt{m_i/m}} \mathbf{p}_i \quad (3.14)$$

Because of orthogonality of the matrix U the bilinear combinations are given by:

$$\begin{aligned} \mathcal{I}_{\alpha\beta} &= \sum_{i=1}^A m_i (\mathbf{r}_i)_\alpha (\mathbf{r}_i)_\beta = \sum_{i=1}^A m (\boldsymbol{\eta}_{i-1})_\alpha (\boldsymbol{\eta}_{i-1})_\beta \\ \mathcal{T}_{\alpha\beta} &= \sum_{i=1}^A \frac{1}{2m_i} (\mathbf{p}_i)_\alpha (\mathbf{p}_i)_\beta = \frac{1}{2m} \sum_{i=1}^A (\mathbf{q}^{i-1})_\alpha (\mathbf{q}^{i-1})_\beta \\ \mathcal{L}_{\alpha\beta} &= \sum_{i=1}^A m_i (\mathbf{r}_i)_\alpha (\mathbf{p}_i)_\beta = \sum_{i=1}^A m (\boldsymbol{\eta}_{i-1})_\alpha (\mathbf{q}_{i-1})_\beta \end{aligned} \quad (3.15)$$

for $\alpha, \beta = 1, 2, 3$, which defines the inertia tensor $\mathcal{I}_{\alpha\beta}$, the kinetic energy operator $\mathcal{T}_{\alpha\beta}$ and the angular momentum operator $\mathcal{L}_{\alpha\beta}$, respectively, in the new variables. One can check that in view of Eqs. (3.9) and (3.15) the moment of inertia around the center of motion could be expressed through the relative particle distances

$$\mathcal{I} = \sum_{i=1}^N (\boldsymbol{\eta}_{i-1})^2 = \frac{1}{2M_{1\dots A}m} \sum_{i,j=1}^A m_i m_j r_{ij}^2 \quad (3.16)$$

The moment of inertia is thus expressed through sum of squares of mass weighted inter-particle distances $\sqrt{m_i m_j} r_{ij}$ and therefore is usually denoted as ρ^2 . The variable ρ is called the hyperspherical radius. Finally using Eqs. (3.9), and (3.11) one obtains the expressions for volume elements in the coordinate and momentum spaces

$$\prod_{i=1}^N dx_i = \frac{1}{\mu} \prod_{i=1}^N d\eta_{i-1} \quad , \quad \prod_{i=1}^N d\mathbf{p}_i = \mu \prod_{i=1}^N dq_{i-1} \quad (3.17)$$

where $\mu = \prod_{i=1}^N \sqrt{m_i/m}$.

3.3 The normalized equal mass Jacobi coordinates

$$\begin{aligned} \eta_1 &= \sqrt{\frac{1}{2}}(r_2 - r_1) \\ \eta_2 &= \sqrt{\frac{2}{3}}\left(r_3 - \frac{1}{2}(r_1 + r_2)\right) \\ &\dots \\ \eta_{A-2} &= \sqrt{\frac{A-2}{A-1}}\left(r_{A-1} - \frac{1}{A-2}(r_1 + r_2 + \dots + r_{A-2})\right) \\ \eta_{A-1} &= \sqrt{\frac{A-1}{A}}\left(r_A - \frac{1}{A-1}(r_1 + r_2 + \dots + r_{A-1})\right) \end{aligned}$$

This transformation can be written as

$$\boxed{\begin{aligned} \eta_{k-1} &= \sum_{i=1}^A U_{ki} r_i \quad k = 1, \dots, A \\ r_i &= \sum_{k=1}^A U_{ki} \eta_{k-1} \end{aligned}}$$

Where U is the orthogonal matrix

$$U = \begin{pmatrix} \sqrt{\frac{1}{A}} & \sqrt{\frac{1}{A}} & \sqrt{\frac{1}{A}} & \dots & \sqrt{\frac{1}{A}} \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 & \dots & 0 \\ -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} & \sqrt{\frac{2}{3}} & \dots & 0 \\ \vdots & & & & \\ -\sqrt{\frac{1}{A(A-1)}} & -\sqrt{\frac{1}{A(A-1)}} & -\sqrt{\frac{1}{A(A-1)}} & \dots & \sqrt{\frac{A-1}{A}} \end{pmatrix}$$

In this case the internal kinetic energy is just

$$T_{\text{int}} = \frac{1}{2m} \sum_{i=1}^{A-1} \pi_i^2, \quad (3.18)$$

with $\pi_k = -i\hbar \frac{\partial}{\partial \eta_k}$.

3.4 Non normalized Jacobi coordinates

In many application people use non normalized Jacobi vecotrs. The most popular set is defined by the transformation rules

$$\boldsymbol{\eta}_i = \sum_{j=1}^A U_{ij} \mathbf{r}_j \quad ; \quad \mathbf{r}_i = \sum_{j=1}^A U_{ij}^{-1} \boldsymbol{\eta}_j, \quad (3.19)$$

and

$$\mathbf{p}_i = \sum_{j=1}^A U_{ji} \boldsymbol{\pi}_j \quad ; \quad \boldsymbol{\pi}_i = \sum_{j=1}^A U_{ji}^{-1} \mathbf{p}_j, \quad (3.20)$$

with

$$U = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ \frac{m_1}{M_{12}} & \frac{m_2}{M_{12}} & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{m_1}{M_{12\dots A-1}} & \frac{m_2}{M_{12\dots A-1}} & \cdots & \cdots & -1 \\ \frac{m_1}{M_{12\dots A}} & \frac{m_2}{M_{12\dots A}} & \cdots & \cdots & \frac{m_A}{M_{12\dots A}} \end{pmatrix}. \quad (3.21)$$

Here $M_{12\dots n} = m_1 + m_2 + \dots + m_n$. We note that in this system $\boldsymbol{\eta}_A$ is the center of mass coordinate, and $\boldsymbol{\pi}_A = \sum \mathbf{p}_i$ is the center of mass momentum.

The intrinsic kinetic energy now takes the form

$$\begin{aligned} T_{int} &= T - T_{\text{cm}} = \sum_i \frac{\mathbf{p}_i^2}{2m_i} - \frac{1}{2M_{12\dots A}} (\mathbf{p}_1 + \mathbf{p}_2 + \dots + \mathbf{p}_A)^2 \\ &= \frac{1}{2} \sum_{i,j} \left(\frac{1}{m_i} \delta_{ij} - \frac{1}{M_{12\dots A}} \right) \mathbf{p}_i \cdot \mathbf{p}_j \\ &= \frac{1}{2} \sum_{i',j'} \left(\frac{1}{m_i} \delta_{ij} - \frac{1}{M_{12\dots A}} \right) U_{i'i} U_{j'j} \boldsymbol{\pi}_{i'} \cdot \boldsymbol{\pi}_{j'} = \\ &= \frac{1}{2} \sum_{i,j} \Lambda_{ij} \boldsymbol{\pi}_i \cdot \boldsymbol{\pi}_j \end{aligned} \quad (3.22)$$

with Λ an $(A-1) \times (A-1)$ dimensional matrix given by

$$\Lambda_{ij} = \sum_{k=1}^A U_{ik} U_{jk} \frac{1}{m_k}. \quad (3.23)$$

The CM contribution vanishes since

$$\sum_{ij} \left(\frac{1}{m_i} \delta_{ij} - \frac{1}{M_{12\dots A}} \right) U_{Ni} U_{Nj} = \sum_i \frac{m_i}{M_{12\dots A}^2} - \frac{1}{M_{12\dots A}} = 0. \quad (3.24)$$

3.5 Kinematic Rotations and Some Group Structure

Note that we can easily generalize the Jacobi coordinates. In fact any orthogonal transformation $O \in O_N$ will define a new set of coordinates through the transformation

$$\eta'_k = \sum_{k'=1}^N O_{kk'} \eta_{k'} \quad (3.25)$$

The infinitesimal generators of this rotation group are given by,

$$\hat{X}_{m,n} = i(\eta_m \cdot \nabla_n - \eta_n \cdot \nabla_m) . \quad (3.26)$$

It should be noted that the group $O_N = SO_N \otimes Z_2$, where Z_2 is the parity or reflection group, contains the permutation group of $A = N + 1$ particles, i.e. $S_A \in O_{A-1}$. The generators of the angular momentum rotations are given by

$$\hat{L}_{a,b} = i \sum_k (\eta_{k,a} \nabla_{k,b} - \eta_{k,b} \nabla_{k,a}) . \quad (3.27)$$

Comparing (3.26) with (3.27) we can easily see that

$$[\hat{X}_{m,n}, \hat{L}_{a,b}] = 0 \quad (3.28)$$

i.e. the groups O_N of kinematic rotations and $O(3)$ of angular rotations commute.

3.6 Symmetrization of the wave-function

Using the Jacobi coordinates to describe the wave-function, i.e. $\Psi = \Psi(\eta_1, \eta, \dots)$ we would like to know that action of a permutation operator $p \in S_N$ on Ψ .

The permutation operator

$$p = \begin{pmatrix} 1 & 2 & 3 & \dots & A \\ p_1 & p_2 & p_3 & \dots & p_A \end{pmatrix} \quad (3.29)$$

acts on the particle indices and transforms the single-particle coordinates as $\mathbf{r}_i \rightarrow \mathbf{r}_{p_i}$. Using the short hand notation $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$, this transformation can be written as a matrix operation:

$$P\mathbf{r} = T_p \mathbf{r} \quad (3.30)$$

where the matrix elements of T_p are given by

$$(T_p)_{ij} = \delta_{j,p_i} \quad i, j = 1, \dots, N. \quad (3.31)$$

The matrices for the 3-body problem are given in Fig. 3.2.

With the help of these matrices it is easy to transform the single particle coordinates.

In order to find the transformation of the Jacobi vector we write $\eta = (\eta_1, \eta_2, \dots, \eta_N)$, and use the relation $\eta = U\mathbf{r}$, to get

$$P\eta = T'_p \eta = UT_p U^{-1} \eta. \quad (3.32)$$

$$\begin{aligned}
T_{\begin{pmatrix} 123 \\ 123 \end{pmatrix}} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & T_{\begin{pmatrix} 123 \\ 213 \end{pmatrix}} &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\
T_{\begin{pmatrix} 123 \\ 321 \end{pmatrix}} &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & T_{\begin{pmatrix} 123 \\ 132 \end{pmatrix}} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\
T_{\begin{pmatrix} 123 \\ 231 \end{pmatrix}} &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, & T_{\begin{pmatrix} 123 \\ 312 \end{pmatrix}} &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.
\end{aligned}$$

Figure 3.2: The permutation matrices for the group S_3 .

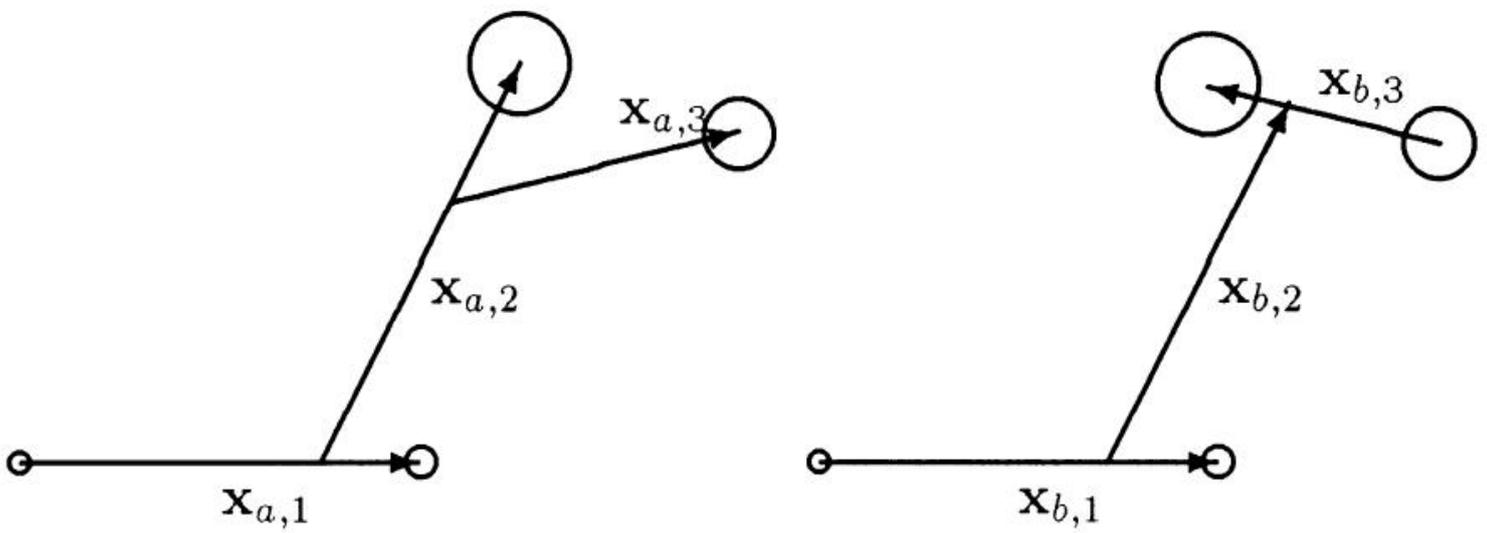
The matrix elements of T'_p are given by

$$\left(T'_p\right)_{ij} = \sum_{k=1}^N U_{ik}(U^{-1})_{pkj} \quad i, j = 1, \dots, N. \quad (3.33)$$

We note that T'_p is splitted into two matrices the unit operator acting on the symmetric center of mass coordinate and an $(N-1) \times (N-1)$ dimensional matrices that carry the $[N-1, 1]$ irrep of S_N .

Last comment. The action of a group element on the wave-function is given by

$$P\Psi(\boldsymbol{\eta}) = \Psi(P^{-1}\boldsymbol{\eta}) = \Psi(T'_{P^{-1}}\boldsymbol{\eta}). \quad (3.34)$$



4. The variational principle and friends

Here we mostly follow chapter 3 in the Suzuki–Varga book [SV98] presenting several theorems on the properties of the energy and wave-function approximations.

4.1 Variational principles

In the following we assume that the Hamiltonian H is a bounded time-independent Hermitian operator. To simplify the discussion we further assume that our system is confined in a big box so the spectrum of the Hamiltonian is discrete. We denote by Φ_n the eigenstates of H and by E_n the eigenvalues,

$$H\Phi_n = E_n\Phi_n, \quad n = 0, 1, \dots \quad (4.1)$$

The eigenvalues, i.e. the energies, are real and are ordered in an increasing order $E_n \leq E_{n+1}$. The ground state is assumed to be unique, i.e. non-degenerated.

Theorem 4.1.1 — Ritz Theorem. For an arbitrary function Ψ in our Hilbert space, the expectation value of H fulfills the relation

$$E \equiv \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_1. \quad (4.2)$$

The equality holds if and only if Ψ is the ground state wave-function of H .

The proof of the Ritz theorem is standard and can be found in almost any quantum-mechanics text book.

Proof. As the eigenstates of H form a complete basis of the Hilbert space, Ψ may be expanded as

$$\Psi = \sum_k c_k \Phi_k. \quad (4.3)$$

It follows that for any integer n

$$\frac{\langle \Psi | H^n - E_1^n | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\sum_{k=1}^{\infty} (E_k^n - E_1^n) |c_k|^2}{\sum_{k=0}^{\infty} |c_k|^2} \geq 0. \quad (4.4)$$

The last relation is due to the ordering of the energies. Clearly the case $n = 1$ proves Ritz's theorem. ■

Theorem 4.1.2 — Generalized Ritz Theorem. The expectation value of the Hamiltonian H is stationary in the neighborhood of its eigenvalues.

Proof. To prove this theorem we induce a small variation in the wave function Ψ , thus if $E \langle \Psi | \Psi \rangle = \langle \Psi | H | \Psi \rangle$ then

$$\begin{aligned} \delta E \langle \Psi | \Psi \rangle &= \delta(\langle \Psi | H | \Psi \rangle) - E \delta(\langle \Psi | \Psi \rangle) \\ &= \langle \delta \Psi | H - E | \Psi \rangle + \langle \Psi | H - E | \delta \Psi \rangle \end{aligned} \quad (4.5)$$

If we choose $\delta \Psi = \epsilon(H - E)\Psi$, then on the right hand side we get the norm of the function $\epsilon(H - E)\Psi$. It follows that E is stationary iff $(H - E)\Psi = 0$, i.e. Ψ is an exact eigenstate of H . ■

Let us assume that $\Psi = \Phi_n + \delta\Phi$, with $\langle \Phi_n | \delta\Phi \rangle = 0$. In this case

$$E = \frac{\langle \Phi_n + \delta\Phi | H | \Phi_n + \delta\Phi \rangle}{\langle \Phi_n + \delta\Phi | \Phi_n + \delta\Phi \rangle} = \frac{E_n \langle \Phi_n | \Phi_n \rangle + \langle \delta\Phi | H | \delta\Phi \rangle}{\langle \Phi_n | \Phi_n \rangle + \langle \delta\Phi | \delta\Phi \rangle} = E_n + O(\delta\Phi^2). \quad (4.6)$$

Thus, we conclude that the energy converge as $O(\delta\Phi^2)$. We note that all other observables converge as $O(\delta\Phi)$.

Theorem 4.1.3 Given the variance of the energy expectation value

$$\sigma^2 \equiv \frac{\langle \Psi | (H - E)^2 | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi | H^2 | \Psi \rangle}{\langle \Psi | \Psi \rangle} - E^2, \quad (4.7)$$

there is at least one exact eigenvalue of H in the interval $[E - \sigma, E + \sigma]$.

Proof. Expanding the wave-function Ψ using the normalized eigenstates of H we can rewrite the variance as

$$\sigma^2 = \sum_{i=1}^{\infty} (E_i - E)^2 |c_i|^2. \quad (4.8)$$

Now let E_K be the eigenstates closest to E , then

$$\sum_{i=1}^{\infty} (E_i - E)^2 |c_i|^2 \geq (E_K - E)^2 \sum_{i=1}^{\infty} |c_i|^2 = (E_K - E)^2. \quad (4.9)$$

Thus $\sigma^2 \geq (E_K - E)^2$, QED. ■

4.2 Basis states

The most straight forward way to solve the Schroedinger equation is to expand the wave function Ψ using a finite set of independent basis functions $\{B_i; i = 1 \dots K\}$. These basis states define a linear vector space \mathcal{V}_K . An approximation of the wave-function on \mathcal{V}_K takes the form

$$\Psi = \sum_k^K c_k B_k \quad (4.10)$$

The energy expectation value E associated with this state is given by

$$E = \frac{\mathbf{c}^\dagger \mathcal{H} \mathbf{c}}{\mathbf{c}^\dagger \mathcal{N} \mathbf{c}} \quad (4.11)$$

with

$$\mathcal{H}_{ij} = \langle B_i | H | B_j \rangle \quad (4.12)$$

the $K \times K$ Hamiltonian matrix in \mathcal{V}_K , and

$$\mathcal{N}_{ij} = \langle B_i | B_j \rangle \quad (4.13)$$

the normalization matrix. Of course, if $\{B_i\}$ is an orthonormal basis $\mathcal{N}_{ij} = \delta_{ij}$.

The linear parameters can be determined applying generalized variational theorem. Variation of (4.11) with respect to c_i^* leads to the generalized eigenvalue problem

$$\sum_j (\mathcal{H}_{ij} - E \mathcal{N}_{ij}) c_j = 0 \quad (i = 1, \dots, K), \quad (4.14)$$

or

$$\mathcal{H} \mathbf{c} = E \mathcal{N} \mathbf{c}. \quad (4.15)$$

The matrix \mathcal{N} requires some attention. We first note that if the basis states are not independent \mathcal{N} is a singular matrix. To this point we note that if $\{B_i\}$ are dependent then there is a vector $\mathbf{c} \neq 0$ such that $\sum c_i B_i = 0$. It follows that $\sum_i c_i \langle B_k | B_i \rangle = \sum_i \mathcal{N}_{ki} c_i = 0$.

Being an Hermitian matrix we can diagonalize \mathcal{N} ,

$$\mathcal{N} \mathbf{c}^{(\mu)} = \mu \mathbf{c}^{(\mu)}. \quad (4.16)$$

The normalized eigenvectors $\mathbf{c}^{(\mu)}$ with $\mathbf{c}^{(\mu)\dagger} \mathbf{c}^{(\mu)} = 1$ give us an orthonormal basis to \mathcal{V}_K

$$\tilde{B}_\mu = \frac{1}{\sqrt{\mu}} \sum_i c_i^{(\mu)} B_i. \quad (4.17)$$

It may happen that \mathcal{N} has a very small eigenvalue μ . If this occurs, then the expansion coefficients $c_i^{(\mu)} / \sqrt{\mu}$ of the corresponding basis state become very large, and the solution of (4.15) may run into serious numerical problems.

When the normalization matrix \mathcal{N} is not ill conditioned we can safely solve the generalized eigenvalue problem (4.15),

$$\mathcal{H} \mathbf{c}^{(i)} = \epsilon_i \mathcal{N} \mathbf{c}^{(i)}. \quad (4.18)$$

Here again we assume that the eigenvalues are ordered. To normalize the state $\Psi^{(i)} = \sum_k c_k^{(i)} B_k$, $\mathbf{c}^{(i)}$ has to be normalized to $\mathbf{c}^{(i)\dagger} \mathcal{N} \mathbf{c}^{(i)} = 1$. It is also not too difficult to prove that

$$\langle \Psi^{(i)} | \Psi^{(j)} \rangle = \mathbf{c}^{(i)\dagger} \mathcal{N} \mathbf{c}^{(j)} = \delta_{ij}. \quad (4.19)$$

Theorem 4.2.1 — Mini-Max Theorem. Let H be a Hermitian operator with discrete eigenvalues $E_1 \leq E_2 \leq \dots$ and let $\epsilon_1 \leq \epsilon_2 \leq \dots \leq \epsilon_K$ be the eigenvalues of H in the subspace \mathcal{V}_K , then

$$E_1 \leq \epsilon_1, \quad E_2 \leq \epsilon_2, \quad \dots \quad E_K \leq \epsilon_K. \quad (4.20)$$

Proof. We start this proof showing that there is at least one normalized state $\Psi \in \mathcal{V}_K$ such that

$$\langle \Psi | H | \Psi \rangle \geq E_K. \quad (4.21)$$

To this end let $\mathcal{W}_K = \text{span}(\Phi_1, \Phi_2, \dots, \Phi_K)$, and define the projection operator into \mathcal{W}_K $P_K = \sum_{i=1}^K |\Phi_i\rangle\langle\Phi_i|$. There are two options:

1. There exists a function $\Psi_0 \in \mathcal{V}_K$ such that $P_K \Psi_0 = 0$.
2. $P_K \Psi \neq 0$ for all $\Psi \in \mathcal{V}_K$.

In the first case, Ψ_0 is a combination of $\Phi_{K+1}, \Phi_{K+2}, \dots$. It follows that $\langle \Psi | H | \Psi \rangle \geq E_{K+1} \geq E_K$. In the second case P_K is a non-singular mapping between \mathcal{V}_K and \mathcal{W}_K , and we can find a vector $\Psi_K \in \mathcal{V}_K$ such that $P_K \Psi_K = a \Phi_K$ with $a \neq 0$. This state is therefore orthogonal to $\Phi_1, \Phi_2, \dots, \Phi_{K-1}$. The latter observation implies that

$$\epsilon_K = \langle \Psi_K | H | \Psi_K \rangle = \sum_{j=1}^{\infty} E_j \langle \Psi_K | \Phi_j \rangle \langle \Phi_j | \Psi_K \rangle = \sum_{j=K}^{\infty} E_j |\langle \Psi_K | \Phi_j \rangle|^2 \geq E_K. \quad (4.22)$$

In view of this success we would like to repeat the process with $(K-1)$ basis states. To this end we can define the $(K-1)$ dimensional linear vector space \mathcal{V}_{K-1} as the subspace of \mathcal{V}_K orthogonal to Ψ_K . Clearly, following the argument above there must be an eigenstate $\Psi_{K-1} \in \mathcal{V}_{K-1}$ with energy expectation value ϵ_{K-1} such that $\epsilon_{K-1} \geq E_{K-1}$, and so on. ■

Theorem 4.2.2 Let $\epsilon_1 \leq \epsilon_2 \leq \dots \leq \epsilon_K$ be the eigenvalues of H restricted to $\mathcal{V}_K = \text{span}(B_1, \dots, B_K)$, and let $\epsilon'_1 \leq \epsilon'_2 \leq \dots \leq \epsilon'_{K+1}$ be the eigenvalues of H restricted to $\mathcal{V}_{K+1} = \text{span}(B_1, \dots, B_K, B_{K+1})$. Then

$$\epsilon'_1 \leq \epsilon_1 \leq \epsilon'_2 \leq \dots \leq \epsilon'_K \leq \epsilon_K \leq \epsilon'_{K+1} \quad (4.23)$$

The proof of this theorem is given in [SV98].

Proof. To prove this theorem let us analyze in some detail the calculation of the energy eigenvalues adding the new basis states B_{K+1} . After diagonalizing H in the subspace \mathcal{V}_K we get K eigenvectors and eigenvalue $\{\Psi_j\}, \{\epsilon_j\}$ such that

$$H|\Psi_j\rangle = \epsilon_j|\Psi_j\rangle \quad (4.24)$$

Adding the new basis state $|B_{K+1}\rangle$, the eigenvalue problem takes now a very simple form

$$\begin{pmatrix} \epsilon_1 & 0 & \cdots & 0 & \langle \Psi_1 | H | B_{K+1} \rangle \\ 0 & \epsilon_2 & \cdots & 0 & \langle \Psi_2 | H | B_{K+1} \rangle \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & \epsilon_K & \langle \Psi_K | H | B_{K+1} \rangle \\ \langle B_{K+1} | H | \Psi_1 \rangle & \cdots & \langle B_{K+1} | H | \Psi_K \rangle & \langle B_{K+1} | H | B_{K+1} \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ \vdots \\ c_K \\ c_{K+1} \end{pmatrix} \\ = E \begin{pmatrix} 1 & 0 & \cdots & 0 & \langle \Psi_1 | B_{K+1} \rangle \\ 0 & 1 & \cdots & 0 & \langle \Psi_2 | B_{K+1} \rangle \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & 1 & \langle \Psi_K | B_{K+1} \rangle \\ \langle B_{K+1} | \Psi_1 \rangle & \cdots & \langle B_{K+1} | \Psi_K \rangle & \langle B_{K+1} | B_{K+1} \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ \vdots \\ c_K \\ c_{K+1} \end{pmatrix}$$

Using the Gram-Schmidt orthogonalization

$$|\tilde{B}_{K+1}\rangle = \mathcal{N} \left(|B_{K+1}\rangle - \sum_k |\Psi_k\rangle \langle \Psi_k | B_{K+1} \rangle \right) \quad (4.25)$$

The eigenvalue problem is reduced to the conventional form

$$\begin{pmatrix} \epsilon_1 & \cdots & 0 & q_1 \\ 0 & & 0 & q_2 \\ \vdots & \ddots & & \vdots \\ 0 & \cdots & \epsilon_K & q_K \\ q_1 & \cdots & q_K & a \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ \vdots \\ c_K \\ c_{K+1} \end{pmatrix} = E \begin{pmatrix} c_1 \\ \vdots \\ \vdots \\ c_K \\ c_{K+1} \end{pmatrix} \quad (4.26)$$

where $q_i = \langle \Psi_i | H | \tilde{B}_{K+1} \rangle$ and $a = \langle \tilde{B}_{K+1} | H | \tilde{B}_{K+1} \rangle$. The eigenvalues are the roots of the secular equation

$$\lambda(E) = \prod_{i=1}^K (\epsilon_i - E) \left(a - E - \sum_{j=1}^K \frac{q_j^2}{\epsilon_j - E} \right) = 0. \quad (4.27)$$

It is not too difficult to convince one self that $E = \epsilon_j$, $j = 1, \dots, K$ is not a root of this equation, thus we must have

$$E - a = \sum_{j=1}^K \frac{q_j^2}{E - \epsilon_j}. \quad (4.28)$$

As can be inferred from Fig. 4.1, this equation have $K + 1$ roots ϵ'_j such that

$$\epsilon'_1 \leq \epsilon_1 \leq \epsilon'_2 \leq \epsilon_2 \dots \leq \epsilon_K \leq \epsilon'_{K+1} \quad (4.29)$$

This concludes our proof. ■

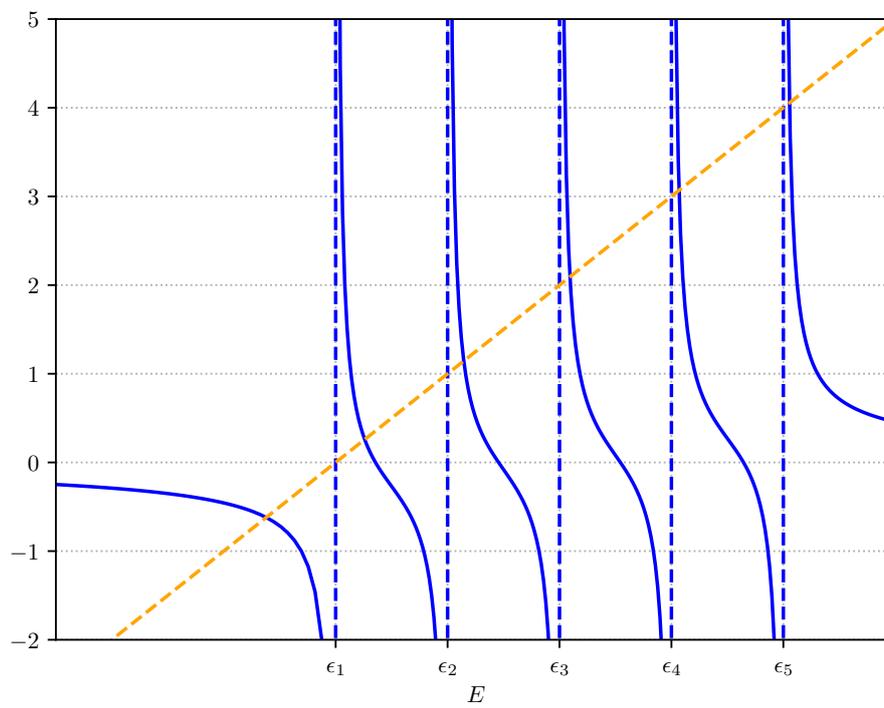
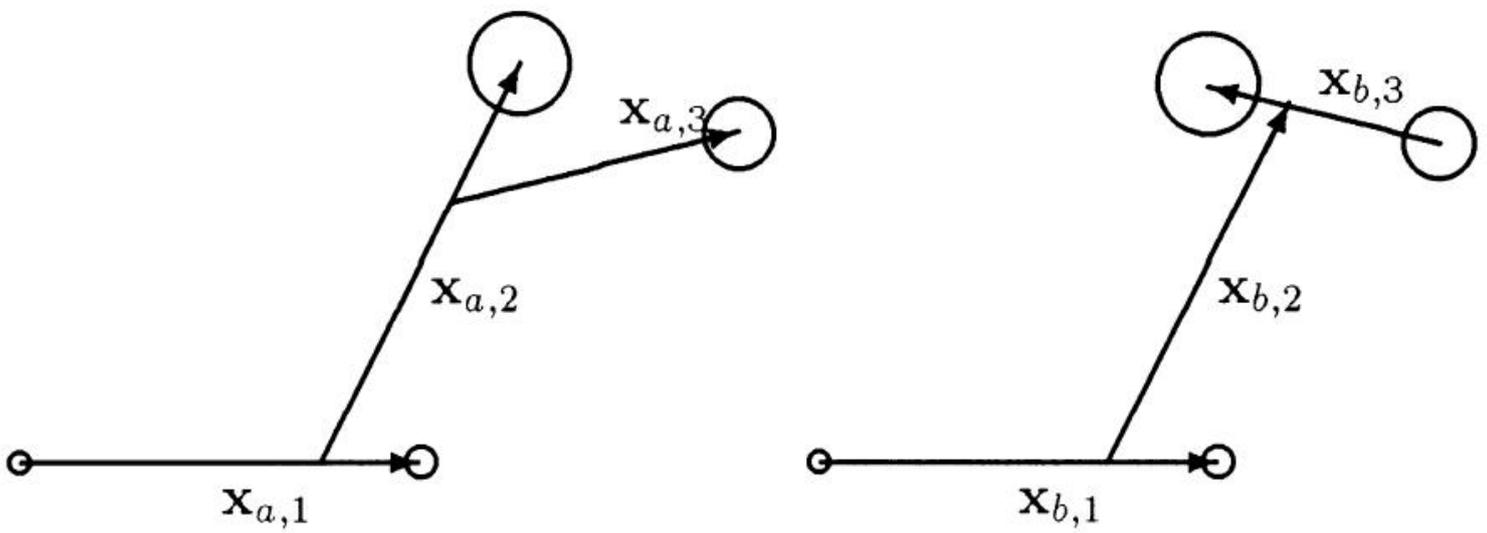


Figure 4.1: Graphical representation of Eq. (4.28). Orange line - $E - a$, blue line $\sum_{j=1}^K \frac{q_j^2}{E - \epsilon_j}$.



5. The Correlated Gaussian Basis

5.1 References

- [SV98] Y. Suzuki and K. Varga, "Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems", Springer (1998).
- [VS95] K. Varga and Y. Suzuki. "Precise solution of few-body problems with the stochastic variational method on a correlated Gaussian basis". In: *Phys. Rev. C* 52 (6 Dec. 1995), pages 2885–2905. DOI: 10.1103/PhysRevC.52.2885. URL: <https://link.aps.org/doi/10.1103/PhysRevC.52.2885>.
- K. Varga, and Y. Suzuki, *J. Comp. Phys.*

5.2 Gaussian basis

In the correlated Gaussians approach the wave function is expanded through basis states of the form

$$\Phi_k(\eta_1, \eta_2, \dots, \eta_N) = \mathcal{A} \left(e^{-\eta^T A \eta / 2} \chi_{ST}^k \right)$$

where A is a symmetric positive definite $N \times N$ matrix, $\eta \equiv (\eta_1, \eta_2, \dots, \eta_N)$ is a $3N$ -dimensional vector, and χ_{ST} is the spin-isospin basis state. The bilinear form is

$$\eta^T A \eta \equiv \sum_{ij} \eta_i A_{ij} \eta_j = \sum_{ij} A_{ij} \eta_i \cdot \eta_j$$

The gaussian basis states are not orthogonal to each other, therefore to obtain the energy spectrum one needs solving the generalized eigenvalue problem

$$H\Psi = EN\Psi \quad (5.1)$$

where the matrix elements of the norm matrix N is the overlap of the basis states.

Why Gaussians?

- Correlated Gaussians basis is an overcomplete and therefore flexible basis.
- A good choice for a variational calculation.
- It allows the description of 2-body correlations through the transformation

$$\prod e^{-\alpha(\mathbf{r}_i - \mathbf{r}_j)^2} = e^{-\sum \alpha(\mathbf{r}_i - \mathbf{r}_j)^2} = e^{-\boldsymbol{\eta}^T A \boldsymbol{\eta}}$$

- Gaussian basis functions allow for analytic evaluation of many integrals.
- Specifically the evaluation of overlaps and kinetic-energy matrix elements.
- The matrix-elements of 2-body potentials can be reduced into one dimensional integrals. Many of which can be evaluated analytically.
- Gaussian basis states are very popular in quantum chemistry. For the atomic and molecular problems the convergence is suggested to go as $e^{-c\sqrt{N}}$ with N the number of Gaussians.
- The explicit anti-symmetrization implies $A!$ permutations.
- The number of actual permutations can be reduced dramatically due to the spin-isospin factor.
- Generalization to $L \neq 0$ leads to rather cumbersome equations.

5.2.1 Completeness

The condition of completeness of the Gaussian basis functions us given by the followig Lemma [KB77],[Sha20], based on the Muntz theorem:

Theorem 5.2.1 Let $\{\alpha_n\}_{n=1}^{\infty}$ be a sequence of real positive numbers. Then, the set of functions $\exp(-\alpha_n r^2)$ are complete in the L_2 norm, (a) if the sequence has a monotonically increasing subsequence α_{n_i} whose elements tend to infinity, such that $\sum 1/\alpha_{n_i} \rightarrow \infty$. (b) if the sequence has a monotonically decreasing subsequence α_{n_i} whose elements tend to zero, such that $\sum \alpha_{n_i} \rightarrow \infty$.

For example, sequences of the form n or $1/n$ lead to complete basis, but it is not possible to determine whether this is true for n^2 or $1/n^2$, although the lemma suggests they may not be. Moreover, this condition implies over-completeness of the basis, as an arbitrary, countable subset of the functions can be removed without affecting the criteria given above.

5.3 Some important integrals

5.3.1 1D integrals

What makes Gaussians an attractive basis for few and many-body calculations is the following analytic result

$$\int_{-\infty}^{+\infty} dx e^{-ax^2/2} = \sqrt{\frac{2\pi}{a}} \quad (5.2)$$

which can be proven using the following trick

$$\left(\int_{-\infty}^{+\infty} dx e^{-ax^2/2} \right)^2 = \int_{-\infty}^{+\infty} dx dy e^{-ax^2/2} e^{-ay^2/2}$$

$$\begin{aligned}
&= \int_0^{+\infty} \int_0^{2\pi} r dr d\theta e^{-ar^2/2} \\
&= \frac{2\pi}{a}
\end{aligned} \tag{5.3}$$

This result can be extended to

$$\begin{aligned}
\int_{-\infty}^{+\infty} dx e^{-ax^2/2+bx} &= \int_{-\infty}^{+\infty} dx e^{-a(x-b/a)^2/2+b^2/2a} \\
&= \int_{-\infty}^{+\infty} dx' e^{-a(x')^2/2+b^2/2a} \\
&= \sqrt{\frac{2\pi}{a}} e^{b^2/2a}
\end{aligned} \tag{5.4}$$

where in the second line we have substituted $x' = x - b/a$. The combination of polynomials with gaussians is an easy integral. For odd powers of x the integral is zero due to symmetry. For even powers of x we can use the following trick

$$\begin{aligned}
\int_{-\infty}^{+\infty} x^2 dx e^{-ax^2/2} &= \left(-2\frac{d}{da}\right) \int_{-\infty}^{+\infty} e^{-ax^2/2} \\
&= \left(-2\frac{d}{da}\right) \sqrt{\frac{2\pi}{a}} = \sqrt{\frac{2\pi}{a}} \frac{1}{a}
\end{aligned} \tag{5.5}$$

which for general even monomial $n > 0$ yield the result

$$\begin{aligned}
\int_{-\infty}^{+\infty} x^{2n} dx e^{-ax^2/2} &= \left(-2\frac{d}{da}\right)^n \int_{-\infty}^{+\infty} e^{-ax^2/2} \\
&= \sqrt{\frac{2\pi}{a}} \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{a^n} = \sqrt{\frac{2\pi}{a}} \frac{(2n-1)!!}{a^n}
\end{aligned} \tag{5.6}$$

5.3.2 Multi dimensional integrals

These 1D results can be easily generalized to multi-dimensional integrals. Consider the diagonal positive definite $n \times n$ matrix

$$\mathbf{D} = \begin{pmatrix} d_1 & 0 & 0 & \cdots & 0 \\ 0 & d_2 & 0 & \cdots & 0 \\ 0 & 0 & d_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ 0 & 0 & 0 & \cdots & d_n \end{pmatrix} \tag{5.7}$$

For this matrix the gaussian $e^{-x\mathbf{D}x/2}$ is just a product of n independent gaussians $\prod_i e^{-d_i x_i^2/2}$ and the n -dimensional gaussian integral is a product of n one-dimensional integrals,

$$\int dx e^{-x\mathbf{D}x/2} = \int dx e^{-\sum d_i x_i^2/2} = \prod_i \sqrt{\frac{2\pi}{d_i}} = \sqrt{\frac{(2\pi)^n}{\det \mathbf{D}}} \tag{5.8}$$

This result holds for a general symmetric matrix A . Using an orthogonal transformations we can diagonalize A , $A = U^{-1}DU$ $x' = Ux$ and obtain

$$\int dx e^{-xAx/2} = \sqrt{\frac{(2\pi)^n}{\det A}} \quad (5.9)$$

When having a linear term

$$\begin{aligned} \int_{-\infty}^{+\infty} dx e^{-xAx/2+b \cdot x} &= \int_{-\infty}^{+\infty} dx e^{-(x-bA^{-1})A(x-A^{-1}b)/2+bA^{-1}b/2} \\ &= \sqrt{\frac{(2\pi)^n}{\det A}} e^{bA^{-1}b/2} \end{aligned} \quad (5.10)$$

An integral of a gaussian with a polynomial can also evaluated. For example

$$\begin{aligned} \int_{-\infty}^{+\infty} dx x_i^2 e^{-xAx/2+b \cdot x} &= \int_{-\infty}^{+\infty} dx \frac{\partial^2}{\partial b_i^2} e^{-xAx/2+b \cdot x} \\ &= \frac{\partial^2}{\partial b_i^2} \left(\sqrt{\frac{(2\pi)^n}{\det A}} \right) e^{bA^{-1}b/2} = \sqrt{\frac{(2\pi)^n}{\det A}} \frac{\partial}{\partial b_i} \left(e^{bA^{-1}b/2} \underbrace{\sum A_{ij}^{-1} b_j}_{(A^{-1}b)_i} \right) \\ &= \sqrt{\frac{(2\pi)^n}{\det A}} e^{bA^{-1}b/2} \left((A^{-1}b)_i^2 + A_{ii}^{-1} \right) \end{aligned} \quad (5.11)$$

Or

$$\begin{aligned} \int_{-\infty}^{+\infty} dx x_i x_j e^{-xAx/2+b \cdot x} &= \int_{-\infty}^{+\infty} dx \frac{\partial}{\partial b_i} \frac{\partial}{\partial b_j} e^{-xAx/2+b \cdot x} \\ &= \frac{\partial}{\partial b_i} \frac{\partial}{\partial b_j} \left(\sqrt{\frac{(2\pi)^n}{\det A}} \right) e^{bA^{-1}b/2} = \sqrt{\frac{(2\pi)^n}{\det A}} \frac{\partial}{\partial b_i} \left(e^{bA^{-1}b/2} \underbrace{\sum A_{jk}^{-1} b_k}_{(A^{-1}b)_j} \right) \\ &= \sqrt{\frac{(2\pi)^n}{\det A}} e^{bA^{-1}b/2} \left((A^{-1}b)_i (A^{-1}b)_j + A_{ij}^{-1} \right) \end{aligned} \quad (5.12)$$

Another integral of interest is the integral of a Dirac delta, which will be useful evaluating potential matrix elements. The best way to evaluate this integral is to use the fourier representation of the delta function,

$$\begin{aligned} \int_{-\infty}^{+\infty} dx e^{-xAx/2} \delta(c \cdot x - y) &= \int_{-\infty}^{+\infty} dx \frac{dk}{2\pi} e^{-xAx/2} e^{ik(c \cdot x - y)} \\ &= \sqrt{\frac{(2\pi)^n}{\det A}} \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{-iky} e^{-k^2 c A^{-1} c / 2} \\ &= \sqrt{\frac{(2\pi)^n}{\det A}} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{c A^{-1} c}} e^{-\frac{1}{2} \frac{y^2}{c A^{-1} c}} \end{aligned} \quad (5.13)$$

5.4 The Hamiltonian matrix elements

5.4.1 The basis functions

The correlated gaussians basis functions for the few-body nuclear problem with quantum numbers $(LS)JMTM_T$ are given by

$$\Phi_{(LS)JMTM_T}(\boldsymbol{\eta}, \sigma, \tau) = \mathcal{A} \left\{ G_A(\boldsymbol{\eta}) [\theta_L(\boldsymbol{\eta}) \otimes \chi_S(\sigma)]^{JM} \zeta_{TM_T}(\tau) \right\} \quad (5.14)$$

where the gaussian function is given by

$$G_A(\boldsymbol{\eta}) = \langle \boldsymbol{\eta} | G_A \rangle = e^{-\tilde{\eta} A \boldsymbol{\eta} / 2}. \quad (5.15)$$

$\mathcal{A} = \frac{1}{\sqrt{A}} \sum_{p \in S_A} \text{sign}(p) \hat{p}$ is the anti-symmetric projection operator. By construction, the gaussian basis states are rotation scalars since

$$\tilde{\eta} A \boldsymbol{\eta} = \sum_{i,j=1}^{A-1} A_{ij} (\boldsymbol{\eta}_i \cdot \boldsymbol{\eta}_j) \quad (5.16)$$

The angular dependence of the wave function is given by the function $\theta_{LM_L}(\boldsymbol{\eta})$. The angular part of the wave function is traditionally given by the product

$$\theta_{LM_L}(\boldsymbol{\eta}) = \left(\prod \eta_i^{\ell_i} \right) [[[Y_{\ell_1}(\hat{\boldsymbol{\eta}}_1) \otimes Y_{\ell_2}(\hat{\boldsymbol{\eta}}_2)]^{L_2} \otimes Y_{\ell_3}(\hat{\boldsymbol{\eta}}_3)]^{L_3} \dots]^{LM_L} \quad (5.17)$$

However, this form is inconvenient for permutations. Therefore Varga and Suzuki proposed to use the ‘‘global vector’’ representation

$$\theta_{KLM_L}(\mathbf{u}, \boldsymbol{\eta}) = \zeta^{2K+L} Y_{LM_L}(\hat{\boldsymbol{\zeta}}) \quad \text{with} \quad \boldsymbol{\zeta} = \sum u_i \boldsymbol{\eta}_i \quad (5.18)$$

The function $r^L Y_{LM}(\hat{\mathbf{r}})$ being an harmonic polynomial of order L , leads to substantial simplification in evaluation of the matrix elements. The parity of Y_L is $(-)^L$. To construct states with parity $(-)^{L+1}$ a slight change should be made coupling an L function with a vector $[\theta_L \otimes \theta_1]^{LM}$.

It should be noted that the functions defined in Eq. (5.18) form a complete set of normal parity angular states, where by normal parity we mean that a state with angular momentum L has parity $(-)^L$. This results from the following theorem:

Theorem 5.4.1 A vector-coupled product of solid spherical harmonics

$$\left(\prod \eta_i^{\ell_i} \right) [[[Y_{\ell_1}(\hat{\boldsymbol{\eta}}_1) \otimes Y_{\ell_2}(\hat{\boldsymbol{\eta}}_2)]^{L_2} \otimes Y_{\ell_3}(\hat{\boldsymbol{\eta}}_3)]^{L_3} \dots]^{LM_L}, \quad (5.19)$$

fulfilling the recursive natural parity condition $(-)^{L_n} = (-)^{L_{n-1} + \ell_n}$; $n = 1 \dots N$ (here $L_1 = \ell_1$ and $L_n = L$), can be written as a linear combination of the functions

$$\left[\prod_{j \geq i} (\boldsymbol{\eta}_i \cdot \boldsymbol{\eta}_j)^{k_{ij}} \right] \zeta^{2K+L} Y_{LM_L}(\hat{\boldsymbol{\zeta}}) \quad \text{with} \quad \boldsymbol{\zeta} = \sum u_i \boldsymbol{\eta}_i \quad (5.20)$$

with $\sum_{j \geq i} k_{ij} + K = (\sum_i \ell_i - L)/2$ and u_i properly chosen expansion coefficients.

The spin-isospin part of the basis is constructed by successive coupling of the particle spins and isospins to yield an A -body state with well defined total spin and isospin.

$$\begin{aligned}\chi_{SM_S}(\sigma) &= \langle \sigma | SM_S \rangle = \langle \sigma_1 \sigma_2 \cdots \sigma_A | S_2 S_3 \cdots SM_S \rangle \\ \xi_{TM_T}(\tau) &= \langle \tau | TM_T \rangle = \langle \tau_1 \tau_2 \cdots \tau_A | T_2 T_3 \cdots TM_T \rangle\end{aligned}\quad (5.21)$$

here we have used the notation σ_i, τ_i for the single particles spin and isospin projections, and σ/τ for the spin/isospin vector.

Summing up, in the gaussian expansion of the wave function takes the form

$$\Psi = \sum_k c_k \Phi_k(\boldsymbol{\eta}, \sigma, \tau) \quad (5.22)$$

where the basis states Φ_k depends on the variational parameters $\mathbf{A}^{(k)}, \mathbf{u}^{(k)}$ and is a product of a gaussian, an harmonic polynomial with well defined angular momentum, a spin state χ_S^k , and an isospin state ξ_T^k . The full set of variational parameters is composed of the nonlinear parameters $\mathbf{A}^{(k)}, \mathbf{u}^{(k)}$ and the linear parameters c_k .

For simplicity, in the following notes we shall restrict the discussion to the s -wave case, avoiding some of the complications associated with the angular momentum algebra. To this end let us write the basis states as

$$\Phi(\boldsymbol{\eta}, \sigma, \tau) = \langle \boldsymbol{\eta}, \sigma, \tau | \mathcal{A} \{ |G_A\rangle |SM\rangle |TM_T\rangle \} = \mathcal{A} \{ G_A(\boldsymbol{\eta}) \chi_{SM}(\sigma) \xi_{TM_T}(\tau) \} \quad (5.23)$$

and assume that the spin-isospin states are normalized.

5.4.2 The norm matrix

The overlap of the different basis states forms the norm or the overlap matrix. Before we evaluate the overlap matrix elements we notice that

$$\begin{aligned}\mathcal{A}\mathcal{A} &= \left(\frac{1}{\sqrt{A!}} \sum_{p \in S_A} \text{sign}(p) \hat{p} \right) \left(\frac{1}{\sqrt{A!}} \sum_{p' \in S_A} \text{sign}(p') \hat{p}' \right) \\ &= \frac{1}{A!} \sum_{p p' \in S_A} \text{sign}(p p') \hat{p} \hat{p}' = \sum_{p'' \in S_A} \text{sign}(p'') \hat{p}''.\end{aligned}\quad (5.24)$$

Where the last equation follows from the group property that $pS_A = S_A$ for any group element $p \in S_A$. Consequently, evaluating the overlap of two basis states one summation over the permuation suffices.

$$\begin{aligned}\langle \Phi | \Phi' \rangle &= \sum_{p \in S_A} \text{sign}(p) \langle G_A | \langle SM | \langle TM_T | \hat{p} \{ |G_{A'}\rangle |S'M'\rangle |T'M'_T \rangle \} \\ &= \sum_{p \in S_A} \text{sign}(p) \langle G_A | \hat{p} | G_{A'} \rangle \langle SM | \hat{p} | S'M' \rangle \langle TM_T | \hat{p} | T'M'_T \rangle\end{aligned}\quad (5.25)$$

The spin-isospin matrix elements are given by

$$\langle SM | \hat{p} | S'M' \rangle = \chi_{SM}^\dagger(\sigma) \cdot \chi_{S'M'}(\hat{p}\sigma)$$

$$\langle TM_T | \hat{p} | T' M'_T \rangle = \zeta_{TM_T}^\dagger(\tau) \cdot \zeta_{T' M'_T}(\hat{p}\tau) \quad (5.26)$$

expressing these matrix elements in term of the elementary spinor state we simply get

$$\begin{aligned} \langle \sigma | \hat{p} \sigma \rangle &= \langle \sigma_1 \sigma_2 \dots \sigma_A | \sigma_{P_1} \sigma_{P_2} \dots \sigma_{P_A} \rangle = \delta_{\sigma_1 \sigma_{P_1}} \dots \delta_{\sigma_A \sigma_{P_A}} \\ \langle \tau | \hat{p} \tau \rangle &= \langle \tau_1 \tau_2 \dots \tau_A | \tau_{P_1} \tau_{P_2} \dots \tau_{P_A} \rangle = \delta_{\tau_1 \tau_{P_1}} \dots \delta_{\tau_A \tau_{P_A}} \end{aligned} \quad (5.27)$$

Turning now to the coordinates $\hat{p}\eta_i = \sum_j P_{ij}\eta_j$, with P an orthogonal matrix $P^T = P^{-1}$,

$$\begin{aligned} \hat{p}(\eta^T A \eta) &= (\hat{p}\eta)^T A (\hat{p}\eta) \\ &= \sum_{i'i''} P_{i'i''} \eta_{i''} A_{ij} P_{jj'} \eta_{j'} = \sum_{i'i''} P_{i'i''}^{-1} \eta_{i''} A_{ij} P_{jj'} \eta_{j'} \\ &= \sum_{i'i''} \eta_{i''} (P^{-1} A P)_{i'i''} \eta_{j'} = \eta^T (P^{-1} A P) \eta \end{aligned}$$

Using Eq. (5.9), the overlap of two gaussians can be easily evaluated

$$\langle G_A | G_{A'} \rangle = \int d\eta e^{-\eta(A+A')\eta/2} = \left(\frac{(2\pi)^n}{\det(A+A')} \right)^{3/2}. \quad (5.28)$$

The power of 3 emerge as we are integrating over 3 space directions, i.e. x, y, z . It follows that the overlap of permuted gaussians is

$$\langle G_A | \hat{p} | G_{A'} \rangle = \left(\frac{(2\pi)^n}{\det(A + P^{-1} A' P)} \right)^{3/2}. \quad (5.29)$$

5.4.3 The kinetic energy

In our normalized Jacobi coordinates, which differ however from those of Varga and Suzuki, the internal kinetic energy operator takes the simple form

$$T = \frac{1}{2m} \sum_{i=1}^N \mathbf{q}_i^2 \quad (5.30)$$

where m is an arbitrary mass, and

$$\mathbf{q}_k = -i \frac{\partial}{\partial \eta_k} \quad (5.31)$$

The operation of the differential operator on the gaussian is given by

$$\begin{aligned} -i \frac{\partial}{\partial \eta_{k,a}} e^{-\eta A \eta / 2} &= -i e^{-\eta A \eta / 2} \frac{\partial}{\partial \eta_{k,a}} (-\eta A \eta / 2) \\ &= i e^{-\eta A \eta / 2} \frac{\partial}{\partial \eta_{k,a}} \left(\sum_{i,j} A_{ij} \eta_i \cdot \eta_j / 2 \right) \\ &= i e^{-\eta A \eta / 2} \left(\sum_j A_{kj} \eta_{j,a} + \sum_i \underbrace{A_{ik}}_{=A_{ki}} \eta_{i,a} \right) / 2 \end{aligned}$$

$$= ie^{-\eta A \eta / 2} \sum_j A_{kj} \eta_{j,a} \quad (5.32)$$

Using this result together with integration by parts we get

$$\begin{aligned} \langle G_A | T | G_{A'} \rangle &= \frac{1}{2m} \sum_{k,a} \int d\eta \frac{\partial e^{-\eta A \eta / 2}}{\partial \eta_{k,a}} \frac{\partial e^{-\eta A' \eta / 2}}{\partial \eta_{k,a}} \\ &= \frac{1}{2m} \sum_{k,a} \int d\eta \left(e^{-\eta A \eta / 2} \sum_i A_{ki} \eta_{i,a} \right) \left(e^{-\eta A' \eta / 2} \sum_j A'_{kj} \eta_{j,a} \right) \end{aligned} \quad (5.33)$$

Rearranging this result

$$\langle G_A | T | G_{A'} \rangle = \frac{1}{2m} \sum_{k,i,j,a} \int d\eta e^{-\eta(A+A')\eta/2} A_{ki} A'_{kj} \eta_{i,a} \eta_{j,a} \quad (5.34)$$

Using Eq. (5.12) we can evaluate this integral to obtain

$$\begin{aligned} \langle G_A | T | G_{A'} \rangle &= \left(\frac{(2\pi)^n}{\det(\mathbf{A} + \mathbf{A}')} \right)^{3/2} \frac{1}{2m} 3 \sum_{ki} A_{ki} A'_{kj} (\mathbf{A} + \mathbf{A}')_{ij}^{-1} \\ &= \langle G_A | G_{A'} \rangle \frac{1}{2m} 3 \sum_{ki,j} A_{ki} \left(\frac{1}{\mathbf{A} + \mathbf{A}'} \right)_{ij} A'_{jk} \\ &= \langle G_A | G_{A'} \rangle \frac{3}{2m} \text{Tr} \left[\mathbf{A} \left(\frac{1}{\mathbf{A} + \mathbf{A}'} \right) \mathbf{A}' \right] \end{aligned} \quad (5.35)$$

5.4.4 Potential matrix elements

Restricting the discussion to central potentials, the matrix elements of a 2-body potential

$$V = \sum_q V_q(\mathbf{r}) \hat{O}_q^S \hat{O}_q^T \quad (5.36)$$

can be written as product of spatial, spin, and isospin matrix-elements

$$\langle \Phi | V | \Phi' \rangle = \sum_q \sum_{p \in S_A} \langle G_A | V_q(\mathbf{r}) | G_{P^{-1}A'P} \rangle \langle SM | \hat{O}_q^S | \hat{p} SM \rangle \langle TM_T | \hat{O}_q^T | \hat{p} TM_T \rangle. \quad (5.37)$$

The spin-isospin matrix elements can be evaluated through the elementary spinors. For the configuration matrix element, it is advantageous to write the potential in the form

$$V(\mathbf{r}_i - \mathbf{r}_j) = \int d\mathbf{r} V(\mathbf{r}) \delta(\mathbf{r}_i - \mathbf{r}_j - \mathbf{r}). \quad (5.38)$$

The transformation between the Jacobi vectors and the single particle coordinates is given by

$$\mathbf{r}_i = \sum_{k=1}^N U_{ik} \boldsymbol{\eta}_k \quad (5.39)$$

Therefore

$$\mathbf{r}_i - \mathbf{r}_j = \sum_{k=1}^N \underbrace{(U_{ik} - U_{jk})}_{C_k^{ij}} \boldsymbol{\eta}_k = \sum_k C_k^{ij} \boldsymbol{\eta}_k \quad (5.40)$$

Using Eq. (5.13) we see that

$$\langle G_A | \delta(\mathbf{r}_i - \mathbf{r}_j - \mathbf{r}) | G_{A'} \rangle = \langle G_A | G_{A'} \rangle \left(\frac{1}{2\pi p_{ij}} \right)^{3/2} e^{-\frac{1}{2} \frac{r^2}{p_{ij}}} \quad (5.41)$$

where

$$p_{ij} = \sum_{kl} C_k^{ij} \left(\frac{1}{A + A'} \right) C_l^{ij} \quad (5.42)$$

Multiplying Eq. (5.43) by V and integrating over \mathbf{r} we get

$$\langle G_A | V_{ij} | G_{A'} \rangle = \int d\mathbf{r} V(\mathbf{r}) \langle G_A | \delta(\mathbf{r}_i - \mathbf{r}_j - \mathbf{r}) | G_{A'} \rangle = \langle G_A | G_{A'} \rangle \tilde{V}(p_{ij}) \quad (5.43)$$

where

$$\tilde{V}(p_{ij}) = \left(\frac{1}{2\pi p_{ij}} \right)^{3/2} \int d\mathbf{r} V(\mathbf{r}) e^{-\frac{1}{2} \frac{r^2}{p_{ij}}} \quad (5.44)$$

It should be noted that for any potential in the form

$$V(r) = r^n e^{-ar^2 + br} \quad (n \geq -2) \quad (5.45)$$

the integration can be done analytically.

5.5 The Stochastic Variational Method - SVM

So far we have seen that gaussians allow for an elegant evaluation of the Hamiltonian matrix elements. The question to be addressed now is how do we choose the variational parameters? Here the SVM of Suzuki and Varga presents an efficient answer. The secret is to distinguish between the linear parameters, that are relatively simple to fix, and the non-linear parameters, that are more involved. In the following subsection we discuss these two parameter families.

5.5.1 The selection of the linear parameters

In order to calculate the linear parameters, we assume for the moment that n sets of non-linear parameters $\{A^{(k)}\}_{k=1}^n$ have already been chosen. Each of these sets together with an appropriate choice of the spin and isospin states defines the anti-symmetric basis function,

$$\left\{ \Phi_k(\boldsymbol{\eta}, \sigma, \tau) = \mathcal{A} \left[G_{A^k}(\boldsymbol{\eta}) \chi_{SM}^k(\sigma) \zeta_{TM_T}^k(\tau) \right] \right\}_{k=1}^n \quad (5.46)$$

The basis functions $\{\Phi_k\}_{k=1}^n$ span an n -dimensional subspace, the approximation of the wave function within this subspace is given by

$$|\Psi\rangle = \sum_k c_k |\Phi_k\rangle \quad (5.47)$$

Using this basis, the linear parameters c_k are calculated via the Ritz variational principle

$$\frac{\delta}{\delta c_i^*} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0. \quad (5.48)$$

The resulting equation is the generalized eigenvalue problem

$$\sum_{k'=1}^n \mathcal{H}_{kk'} c_{k'} = E \sum_{k'=1}^n \mathcal{N}_{kk'} c_{k'} \quad (5.49)$$

Where

$$\mathcal{H}_{kk'} = \langle \Phi_k | H | \Phi_{k'} \rangle \quad \mathcal{N}_{kk'} = \langle \Phi_k | \Phi_{k'} \rangle \quad (5.50)$$

5.5.2 The Stochastic selection of the non-linear parameters

The Stochastic algorithm of selecting the non-linear parameters can be described by the following steps:

- Select a number of parameter sets $\{A\}$ randomly, and keep the one with lowest energy.
- Generate a new random set of parameters, and calculate the new energy.
- Adding one more basis function lowers the energy. Evaluate the "utility" of this set by the gain $|E'_1 - E_1|$.
- If $|E'_1 - E_1| > \epsilon$ keep the state. Otherwise discard the new state.
- Repeat step (b) until the energy converge, refining ϵ in the process.

Let us analyze in some detail the calculation of the energy eigenvalues adding a new parameter set A . After n steps we have n basis functions $\{\Phi_k\}_{k=1}^n$. Diagonalizing the Hamiltonian within this n -dimensional subspace we get n eigenvectors and eigenvalue $\{\Psi_j\}, \{E_j\}$ such that

$$\mathcal{H}|\Psi_j\rangle = E_j|\Psi_j\rangle \quad (5.51)$$

Adding a new basis state $|\Phi_{n+1}\rangle$, the eigenvalue problem takes now a very simple form

$$\begin{pmatrix} E_1 & 0 & \cdots & 0 & \langle \Psi_1 | H | \Phi_{n+1} \rangle \\ 0 & E_2 & \cdots & 0 & \langle \Psi_2 | H | \Phi_{n+1} \rangle \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & E_n & \langle \Psi_n | H | \Phi_{n+1} \rangle \\ \langle \Phi_{n+1} | H | \Psi_1 \rangle & \cdots & \cdots & \langle \Phi_{n+1} | H | \Psi_n \rangle & \langle \Phi_{n+1} | H | \Phi_{n+1} \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ \vdots \\ c_n \\ c_{n+1} \end{pmatrix} \\ = E \begin{pmatrix} 1 & 0 & \cdots & 0 & \langle \Psi_1 | \Phi_{n+1} \rangle \\ 0 & 1 & \cdots & 0 & \langle \Psi_2 | \Phi_{n+1} \rangle \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & 1 & \langle \Psi_n | \Phi_{n+1} \rangle \\ \langle \Phi_{n+1} | \Psi_1 \rangle & \cdots & \cdots & \langle \Phi_{n+1} | \Psi_n \rangle & \langle \Phi_{n+1} | \Phi_{n+1} \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ \vdots \\ c_n \\ c_{n+1} \end{pmatrix}$$

Using the Gram-Schmidt orthogonalization

$$|\tilde{\Phi}_{n+1}\rangle = \mathcal{N} \left(|\Phi_{n+1}\rangle - \sum_k |\Psi_k\rangle \langle \Psi_k | \Phi_{n+1} \rangle \right) \quad (5.52)$$

The eigenvalue problem is reduced to the conventional form

$$\begin{pmatrix} E_1 & \cdots & 0 & q_1 \\ 0 & & 0 & q_2 \\ \vdots & \ddots & & \\ 0 & \cdots & E_n & q_n \\ q_1 & \cdots & q_n & a \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_n \\ c_{n+1} \end{pmatrix} = E \begin{pmatrix} c_1 \\ \vdots \\ c_n \\ c_{n+1} \end{pmatrix} \quad (5.53)$$

where $q_i = \langle \Psi_i | H | \tilde{\Phi}_{n+1} \rangle$ and $a = \langle \tilde{\Phi}_{n+1} | H | \tilde{\Phi}_{n+1} \rangle$. The eigenvalues are the roots of the secular equation

$$\lambda(E) = \prod_{i=1}^n (E_i - E) \left(a - E - \sum_{j=1}^n \frac{q_j^2}{E_j - E} \right) = 0 \quad (5.54)$$

This equation have $n + 1$ roots E'_j such that

$$E'_1 \leq E_1 \leq E'_2 \leq E_2 \dots \leq E_n \leq E'_{n+1} \quad (5.55)$$

Thus solving for the lowest eigenvalue is a rather easy task.

5.6 Gaussian wave-packets

In the SVM method the derivation of the matrix elememnts goes through single particle gaussian wave-packets. This basis as the advantage of using the well developed technology of Slater deteminants. In short, the calculation process is done in three steps:

- Calculate of the matrix elements between Slater determinants of single-particle gaussian wave-packets.
- Transform the single-particle vectors to relative coordinates.
- Apply an integral transform from the gaussian wave-packets to the correlated Gaussian basis.

In the following we shall present in some details the transformation between the single particle wave-packets and the correlated gaussian basis. A complete description of the method can be found in Suzuki & Varga's book.

Consider the single particle states

$$\varphi_{s_i \sigma_i \tau_i}^v(\mathbf{r}_i) \equiv \varphi_{s_i}^v(\mathbf{r}_i) \chi_{\sigma_i} \bar{\zeta}_{\tau_i} = \left(\frac{v}{2\pi} \right)^{3/4} e^{-v(\mathbf{r}_i - s_i)^2/2} \chi_{\sigma_i} \bar{\zeta}_{\tau_i} \quad (5.56)$$

and construct the Slater determinant

$$\Phi(s_1, s_2, \dots, s_A) = \mathcal{A} \left\{ \prod_{i=1}^A \varphi_{s_i \sigma_i \tau_i}^v(\mathbf{r}_i) \right\} \quad (5.57)$$

It is easy to see that

$$\langle \Phi(s_1, s_2, \dots, s_A) | \Phi(s'_1, s'_2, \dots, s'_A) \rangle = \det\{\mathbf{B}\} \quad B_{ij} = \langle \varphi_{s_i \sigma_i \tau_i}^v | \varphi_{s'_j \sigma'_j \tau'_j}^v \rangle \quad (5.58)$$

The technology of Slater determinants makes the calculation of matrix-elements simple. Notice that if

$$\boldsymbol{\eta}_i = \sum_j U_{ij} \mathbf{r}_j \quad \text{and} \quad \mathbf{s}_i = \sum_j U_{ij} \mathbf{s}_j$$

then

$$\sum_i (\mathbf{r}_i - \mathbf{s}_i)^2 = \sum_j (\boldsymbol{\eta}_j - \mathbf{s}_j)^2 \quad (5.59)$$

So

$$\prod_{i=1}^A \varphi_{\mathbf{s}_i}^v(\mathbf{r}_i) = \prod_{i=0}^{A-1} \varphi_{\mathbf{s}_i}^v(\boldsymbol{\eta}_i) \quad (5.60)$$

Therefore the A -body wave-function can be factorized into a product of intrinsic function and a center of mass term term,

$$\Phi(\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_A) = \varphi_{\mathbf{s}_0}^v(\boldsymbol{\eta}_0) \Psi(\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_{A-1}) \quad (5.61)$$

Now, using the relation

$$\int d\mathbf{y} e^{-\mathbf{y} \mathbf{C} \mathbf{y} / 2 + \mathbf{t} \mathbf{y}} = \left(\frac{(2\pi)^N}{\det \mathbf{C}} \right)^{3/2} e^{\mathbf{t} \mathbf{C}^{-1} \mathbf{t} / 2} \quad (5.62)$$

we can relate the correlated Gaussians to the wave-packet

$$\begin{aligned} \int d\mathbf{S} e^{-\mathbf{S} \mathbf{Q} \mathbf{S} / 2} \left\{ \prod_{i=1}^{A-1} \varphi_{\mathbf{s}_i}^v(\boldsymbol{\eta}_i) \right\} &= \int d\mathbf{S} e^{-\mathbf{S} \mathbf{Q} \mathbf{S} / 2 - \sum_i v (\mathbf{s}_i - \boldsymbol{\eta}_i)^2 / 2} \\ &= \int d\mathbf{S} e^{-\mathbf{S} \mathbf{Q} \mathbf{S} / 2 - v (\mathbf{S} - \boldsymbol{\eta})^2 / 2} \\ &= \int d\mathbf{S} e^{-\mathbf{S} (\mathbf{Q} + v \mathbf{I}) \mathbf{S} / 2 + v \boldsymbol{\eta} \mathbf{S} - v \boldsymbol{\eta}^2 / 2} \\ &= \left(\frac{(2\pi)^N}{\det [\mathbf{Q} + v \mathbf{I}]} \right)^{3/2} e^{-\boldsymbol{\eta} (v \mathbf{I} - v (\mathbf{Q} + v \mathbf{I})^{-1} v) \boldsymbol{\eta} / 2} \end{aligned}$$

Equating the last result to $e^{-\boldsymbol{\eta} \mathbf{A} \boldsymbol{\eta} / 2}$ we identify

$$\boxed{\mathbf{Q} = v \frac{\mathbf{I}}{v \mathbf{I} - \mathbf{A}} v - v \mathbf{I}} \quad (5.63)$$

and obtain the relation

$$e^{-\boldsymbol{\eta} \mathbf{A} \boldsymbol{\eta} / 2} = \left(\frac{(2\pi)^N}{\det [\mathbf{Q} + v \mathbf{I}]} \right)^{-3/2} \int d\mathbf{S} e^{-\mathbf{S} \mathbf{Q} \mathbf{S} / 2} \left\{ \prod_{i=1}^N \varphi_{\mathbf{s}_i}^v(\boldsymbol{\eta}_i) \right\} \quad (5.64)$$

Summing up we can rewrite the anti-symmetric correlated Gaussians as

$$\mathcal{A} \left\{ e^{-\boldsymbol{\eta} \mathbf{A} \boldsymbol{\eta} / 2} \prod_{i=1}^A \chi_{\sigma_i} \xi_{\tau_i} \right\} = \left(\frac{(2\pi)^{A-1}}{\det [\mathbf{Q} + v \mathbf{I}]} \right)^{-3/2} \int d\mathbf{S} e^{-\mathbf{S} \mathbf{Q} \mathbf{S} / 2} \Psi(\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_{A-1}) \quad (5.65)$$

For the center of mass we utilize the relation

$$\int d\boldsymbol{\eta}_0 \phi_{S_0}^{\nu}(\boldsymbol{\eta}_0) = \left(\frac{\nu}{2\pi}\right)^{3/4} \int d\boldsymbol{\eta}_0 e^{-\nu(\boldsymbol{\eta}_0 - S_0)^2/2} = \left(\frac{2\pi}{\nu}\right)^{3/4} \quad (5.66)$$

To get

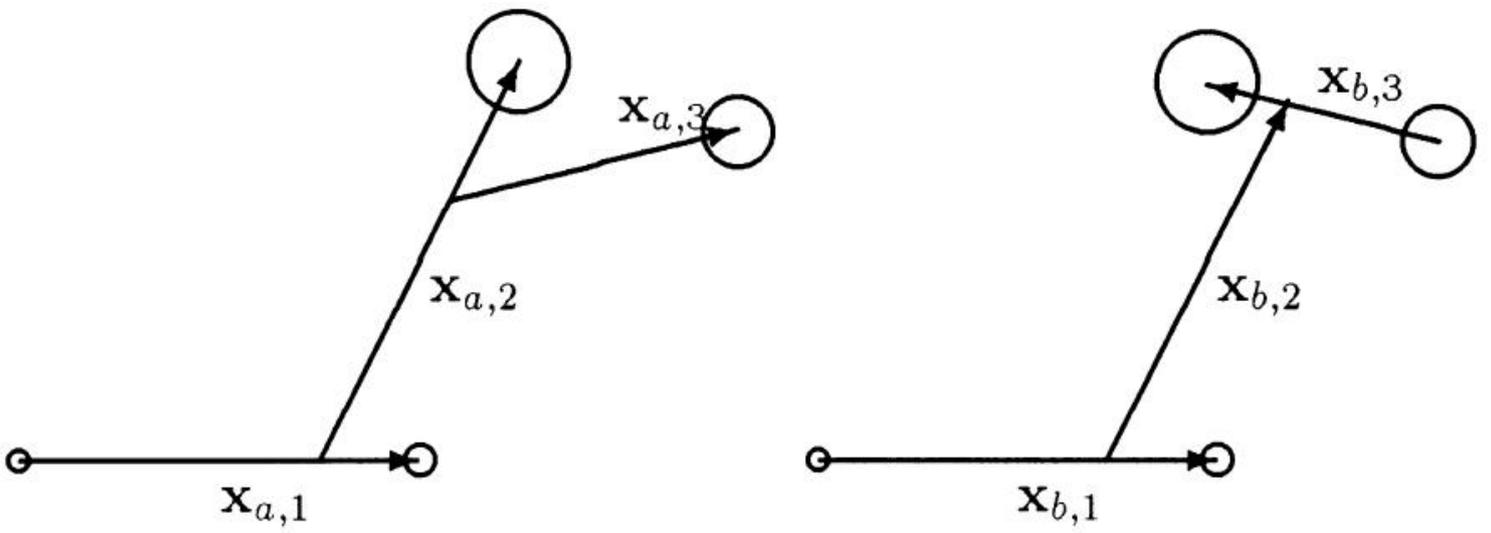
$$\mathcal{A} \left\{ e^{-\boldsymbol{\eta} A \boldsymbol{\eta}/2} \prod_{i=1}^A \chi_{\sigma_i} \xi_{\tau_i} \right\} = \left(\frac{2\pi}{\nu}\right)^{-3/4} \left(\frac{(2\pi)^N}{\det[\mathbf{Q} + \nu \mathbf{I}]}\right)^{-3/2} \times \int d\mathbf{s} e^{-\mathbf{s} \mathbf{U}^{-1} \mathbf{Q} \mathbf{U} \mathbf{s}/2} \Phi(\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_A) \quad (5.67)$$

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- The matrix-elements of the correlated gaussians are simply connected to the matrix-elements of the single-particle wave-packet.
- Although the dS integration looks cumbersome, at the end the matrix-elements are product of gaussians and polynomials that can be evaluated analytically.

5.7 SVM - summary

- Fully analytic calculation, up to 1D integration (for 2-body forces)
- Universality - The scheme can be used for nuclear, atomic, and molecular systems, bosonic or fermionic, with different masses.
- Fast convergence of the energy with small number of states.
- Excited states are also obtained through the diagonalization of the Hamiltonian matrix.
- The wave function is obtained in a compact analytic form.
- The SVM can be easily parallelized. First option: each node check a different set of non-linear parameters. Alternatively, the sum over $A!$ is divided between the different CPUs.



6. The harmonic oscillator basis

The harmonic oscillator based No Core Shell Model (NCSM) method, is one of two few-body methods that have facilitated increasing the domain of the few-body field to nuclear systems with $A > 4$, while working with realistic potentials. The other one Diffusion Monte Carlo techniques and its variants.

The name NCSM is due to the fact that all the nucleons of the nucleus are active and explicitly taken into account as degrees of freedom and thus it is not assumed that there is an inert core. The NCSM couples the traditional SM advantages of working in a harmonic oscillator basis with the rigor of an ab initio approach. To accelerate the convergence of hard potentials the Lee-Suzuki effective interaction was first used, and later the potentials softened by the similarity renormalization group (SRG) transformation.

6.1 The 3-dimensional harmonic oscillator

The harmonic oscillator hamiltonian is given by

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{m\Omega^2}{2}r^2 \quad (6.1)$$

The eigenvalues of the Hamiltonian are given by

$$E_{nl} = (2n + l + \frac{3}{2})\hbar\Omega \quad (6.2)$$

The eigenstates of the Hamiltonian are given by

$$\varphi_{nlm}(\mathbf{r}) = R_{nl}Y_{lm}(\hat{r}), \quad (6.3)$$

with

$$R_{nl}(r) = \frac{1}{r_0^{3/2}} \sqrt{\frac{2n!}{\Gamma(n+l+3/2)}} \left(\frac{r}{r_0}\right)^l \exp\left(-\frac{r^2}{2r_0^2}\right) L_n^{l+1/2}\left(\frac{r^2}{r_0^2}\right). \quad (6.4)$$

Here Y_{lm} are the spherical harmonics, $L_n^a(x)$ are the associated Laguerre polynomials, and $r_0 = \sqrt{\hbar/m\Omega}$.

6.2 The many-body problem

There are two versions of the NCSM, which differ in their treatment of the CM degrees of freedom. In the first version one uses the Jacobi coordinates and the spatial basis states for the A -body problem is a product of harmonic oscillator states associated with the different Jacobi vectors. They are given by

$$\Phi_{[N]} = \prod_j R_{n_j l_j}(\eta_j) [[Y_{\ell_1}(\hat{\eta}_1) \otimes Y_{\ell_2}(\hat{\eta}_2)]^{L_2} \otimes Y_{\ell_3}(\hat{\eta}_3)]^{L_3} \dots]^{LM_L}, \quad (6.5)$$

where $[N]$ is a short hand for the list of quantum numbers

$$[N] = (n_1 \dots n_{A-1}, l_1 \dots l_{A-1}, L_2 \dots L_{A-2} LM).$$

In this case explicit anti-symmetrization of the states is needed.

In the second version one uses single particle coordinates and the Slater determinants to construct anti-symmetric states. In this case, the Hamiltonian is modified by adding a harmonic oscillator CM Hamiltonian H_{CM} to the intrinsic Hamiltonian H

$$\begin{aligned} H_{\Omega}^{[A]} &= H + H_{\text{CM}}^{\text{HO}} = H + \frac{\mathbf{P}_{\text{CM}}^2}{2Am} + \frac{Am}{2} \Omega^2 \mathbf{R}_{\text{CM}}^2 \\ &= \sum_{i=1}^A \left[\frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} m \Omega^2 \mathbf{r}_i^2 \right] + \sum_{i<j=1}^A \left[V_{ij} - \frac{m\Omega^2}{2A} (\mathbf{r}_i - \mathbf{r}_j)^2 \right] \\ &\equiv \sum_{i=1}^A h_i^{\text{HO}} + \sum_{i<j=1}^A \tilde{V}_{ij}. \end{aligned} \quad (6.6)$$

Here \mathbf{R}_{CM} is the CM coordinate, while h_i^{HO} is the single particle harmonic oscillator Hamiltonian, and \tilde{V}_{jk} is a modified potential depending both on the harmonic oscillator frequency Ω and A :

$$\tilde{V}_{ij} = \left[V_{ij} - \frac{m\Omega^2}{2A} (\mathbf{r}_i - \mathbf{r}_j)^2 \right]. \quad (6.7)$$

Naturally, the added CM term has no influence on the internal motion. This means that once the ground-state energy $E_{\Omega}^{[A]}$ of $H_{\Omega}^{[A]}$ is found, then the ground-state energy E of H is obtained by subtraction of the CM ground-state energy $3\hbar\Omega/2$. For excited states one has to avoid CM excitations. This can be achieved by the replacement $H_{\text{CM}}^{\text{HO}} \rightarrow \lambda H_{\text{CM}}^{\text{HO}}$ with sufficiently large λ (Lawson term). A good check on the convergence of E is through the independence of the result on the

HO frequency Ω . On the other hand, one may search for the frequency Ω which exhibits the best convergence pattern.

The calculation of $E_{\Omega}^{[A]}$ is performed in a finite model space P_A . This is the space spanned by all the A -body HO Slater determinants formed by filling the single-particle HO eigenstates with $N \leq N_{\max}$, where N is the total number of single-particle HO quanta. The residual space Q_A , together with P_A , exhausts the full Hilbert space.

6.3 The Lee-Suzuki effective interaction

Let us define P as the subspace described by our basis functions and Q as the complementary space. It would be nice if we could find a transformation $H \rightarrow XHX^{-1}$ such that the resulting Hamiltonian has the form

P	Q
H_{eff}	0
0	$QXHX^{-1}Q$

In such case any eigenvalue $H_{\text{eff}}\Psi_P = E\Psi_P$ is an eigenvalue of the original problem, and any eigenvector $\Psi_P \in P$ is connected to the full space eigenvector through the relation $\Psi_P = X\Psi$.

- Consider the many-body system described by

$$H = H_0 + V$$

- H_0 is the unperturbed Hamiltonian and V is the residual interaction.
- The set of states active in our calculation is called the **model space**, or the P -space.
- The complement of the P -space is called the Q -space.
- We define projection operators P, Q which project respectively into the P -space and the Q -space.

- P, Q are eigenprojectors of H_0

$$[H_0, P] = [H_0, Q] = 0$$

$$QH_0P = PH_0Q = 0$$

- Our aim is to construct H_{eff} which acts only inside the P space and its eigenvalues coincide with the real eigenvalues of H .
- Similarity transformation of H

$$\mathcal{H} = X^{-1}HX = PX^{-1}HXP + PX^{-1}HXQ + QX^{-1}HXP + QX^{-1}HXQ$$

- The condition that $P\mathcal{H}P$ is the P -space effective interaction is

$$Q\mathcal{H}P = Q(X^{-1}\mathcal{H}X)P = 0$$

- Then the effective Hamiltonian is given by

$$H_{eff} = P\mathcal{H}P = P(X^{-1}\mathcal{H}X)P$$

- Consider a similarity transformation

$$X = e^{\omega}$$

$$\mathcal{H} = e^{-\omega}He^{\omega}$$

- Assuming that the ω operator transform a P state into a Q state. Therefore ω has the properties

$$\omega = Q\omega P$$

$$Q\omega Q = P\omega P = P\omega Q = 0$$

- The condition $\omega = Q\omega P$ leads to the property

$$\omega^2 = \omega^3 = \dots = 0$$

- Thus

$$X = e^{\omega} = 1 + \omega$$

- Applying the similarity transformation to H

$$P\mathcal{H}P = PHP + PVQ\omega$$

$$P\mathcal{H}Q = PVQ$$

$$Q\mathcal{H}Q = QHQ - \omega PVQ$$

$$Q\mathcal{H}P = QVP + QHQ\omega - \omega PHP - \omega PVQ\omega$$

- To construct the effective interaction $H_{eff} = P\mathcal{H}P$ we have to solve

$$\boxed{QVP + QHQ\omega - \omega PHP - \omega PVQ\omega = 0}$$

- Suzuki and Lee proposed an iterative method for solving this equation and proved that it convergence.
- Here we will follow a path proposed by Navratil and Barrett.

6.3.1 The Navratil-Barrett solution of the Lee-Suzuki Equation

- Introduce basis sets:
 $P = \text{span}\{|\alpha\rangle\}$ is of dimension d_P
 $Q = \text{span}\{|\beta\rangle\}$ is of dimension d_Q
- There are d_P eigenvectors of H_{eff} , $\{|\phi_\mu\rangle\}$,

$$H_{eff}|\phi_\mu\rangle = E_\mu|\phi_\mu\rangle \quad |\phi_\mu\rangle = \sum_{\alpha=1}^{d_P} \langle\alpha|\phi_\mu\rangle|\alpha\rangle \quad \langle\beta|\phi_\mu\rangle = 0$$

- Each eigenvector $|\phi_\mu\rangle$ corresponds to an eigenvector $|\psi_\mu\rangle$ of H

$$|\psi_\mu\rangle = |\phi_\mu\rangle + \omega|\phi_\mu\rangle \quad |\phi_\mu\rangle = P|\psi_\mu\rangle$$

- Multiplying by $\langle\beta|$ we get the equation

$$\langle\beta|\psi_\mu\rangle = \langle\beta|\omega|\phi_\mu\rangle$$

which holds for all $\{\beta\}_1^{d_Q}$ and all $\{\phi_\mu\}_1^{d_P}$

- Expanding ϕ_μ we get $\langle\beta|\psi_\mu\rangle = \sum_{\alpha=1}^{d_P} \langle\beta|\omega|\alpha\rangle \langle\alpha|\phi_\mu\rangle$
- As $|\phi_\mu\rangle = P|\psi_\mu\rangle$ the last equation can be rewritten as

$$\langle\beta|\psi_\mu\rangle = \sum_{\alpha=1}^{d_P} \langle\beta|\omega|\alpha\rangle \langle\alpha|\psi_\mu\rangle$$

- The matrix $U_{\alpha\mu} = \langle\alpha|\psi_\mu\rangle$ is invertible matrix if $P|\psi_\mu\rangle \neq 0$.
- Applying the inverse of U we can extract the matrix elements of ω

$$\langle\beta|\omega|\alpha\rangle = \sum_{\mu=1}^{d_P} \langle\beta|\psi_\mu\rangle U_{\mu\alpha}^{-1}$$

Few comments

- Note that there are different possible choices of ω , actually $\binom{d_P+d_Q}{d_P}$
- In order to obtain ω we have to solve to full problem !
- The effective interaction $V_{eff} \equiv H_{eff} - H_0$ is an A -body operator.
- V_{eff} is not hermitian.

6.3.2 Hermitian Effective interaction

An hermitian effective interaction can be constructed if we utilize unitary rather similarity transformation

$$\mathcal{H} = e^{-G} H e^G \quad G^\dagger = -G$$

Suzuki (1982) have proven the following connection

$$G = \text{arctanh}(\omega - \omega^\dagger)$$

This complicated expression leads to a simple formula

$$e^G = \frac{1 + \omega - \omega^\dagger}{\sqrt{1 + \omega\omega^\dagger + \omega^\dagger\omega}}$$

To understand this result we note that

$$[(1 + \omega - \omega^\dagger), (1 + \omega\omega^\dagger + \omega^\dagger\omega)] = 0$$

and that

$$Q(e^{-G}He^G)P = \frac{1}{\sqrt{Q + \omega\omega^\dagger}} (QVP + QHQ\omega - \omega PHP - \omega PVQ\omega) \frac{1}{\sqrt{P + \omega^\dagger\omega}}$$

Thus,

$$Q(e^{-G}He^G)P = 0$$

if

$$QVP + QHQ\omega - \omega PHP - \omega PVQ\omega = 0$$

This is just the decoupling equation derived earlier for ω !

The resulting Hermitian effective interaction reads

$$V_{eff} = \frac{1 + \omega^\dagger}{\sqrt{1 + \omega^\dagger\omega}} H \frac{1 + \omega}{\sqrt{1 + \omega^\dagger\omega}} - PH_0P$$

6.4 Effective interaction for NCSM

The approach that is chosen to construct the effective Hamiltonian, appropriate to the finite P_A -space is described above. However, if one applies the unitary transformation to $H_\Omega^{[A]}$ one obtains an effective Hamiltonian that is an A -body operator. To avoid this complication, an approximation is made in the NCSM. It consists in first finding only a two-body effective interaction $\tilde{V}_{ij}^{[2,eff]}$ which is then used to replace the interaction term \tilde{V}_{ij} of Eq. (6.6). The effective interaction $\tilde{V}_{ij}^{[2,eff]}$ is obtained by applying the decoupling condition to a two-nucleon Hamiltonian $H_\Omega^{[2]}$ that arises from $H_\Omega^{[A]}$ by restricting the sums to two nucleons only, keeping however the original mass number A in the interaction term:

$$\begin{aligned} H_\Omega^{[2]} &= \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + \left[\frac{1}{2}m\Omega^2\mathbf{r}_1^2 + \frac{1}{2}m\Omega^2\mathbf{r}_2^2 \right] + \left[V_{12} - \frac{m\Omega^2}{2A}(\mathbf{r}_1 - \mathbf{r}_2)^2 \right] \\ &\equiv H_{HO}^{[2]} + \tilde{V}_{12}. \end{aligned} \quad (6.8)$$

The effective Hamiltonian $H_{eff}^{[2]}$ is determined in a subspace of P , the P_2 -space ($\hat{P}_2 + \hat{Q}_2 = I_2$), via the two-body transformation operator $\omega^{[2]} = \hat{Q}_2\omega^{[2]}\hat{P}_2$. Then

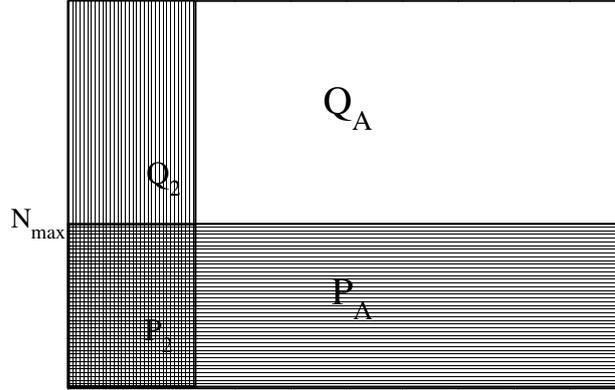


Figure 6.1: The various P and Q spaces relevant for the construction of the two-body effective interaction (see text).

the two-body effective interaction is obtained by subtracting from $H_{\text{eff}}^{[2]}$ the two-body HO Hamiltonian, i.e.

$$\tilde{V}_{12}^{[2,\text{eff}]} = H_{\text{eff}}^{[2]} - H_{\text{HO}}^{[2]}. \quad (6.9)$$

The corresponding $V_{ij}^{[2,\text{eff}]}$ is then used in Eq. (6.6). This procedure is equivalent to the case where **(i)** the similarity operator ω is limited to a two-body operator $\omega^{[2]}$ and **(ii)** the effective Hamiltonian is truncated at the two-body operator level.

Due to the effective interaction the NCSM is not a variational method. The $n > 2$ terms $\omega^{[n]}$ neglected in ω , as well as the n -body terms neglected in the corresponding effective Hamiltonian, could either increase or decrease the binding energy. On the other hand, as the basis space is increased the result converges to the exact solution. This becomes clear from the illustration in Fig. 6.1. At each P_A , the unitary transformation transfers information from a part of the Q_A space, namely the Q_2 space, to the P_2 space. Thus E_{Ω}^A converges much faster when performing a calculation in P_A -space than in a corresponding calculation with the bare interaction. For a sufficiently large P_A , covering practically the whole Hilbert space, the effective interaction coincides with the bare one, and one has the exact result.

From the figure it is also clear that the same exact result could be achieved by enlarging *horizontally* the space where the unitary transformation operates, i.e. considering $\omega^{[n]}$ terms (as well as n -body terms in the effective Hamiltonian) with increasing n up to $n = A$. However, this is much more difficult, since one would need to know the entire n -body spectrum to construct the n -body effective interaction. It is evident that if three-body forces are present in the original Hamiltonian it is expedient to apply the procedure at least up to $n = 3$.

Fig. 6.2 illustrates the convergence pattern of the ground-state energy of ${}^4\text{He}$,

taken from Ref. [NaK00]. The results are obtained with the translationally invariant version of the method and with a realistic potential. It is interesting to note not only the Ω dependence of the convergence but also how rapid the convergence can be for some Ω values. Of course all the results have to converge to the same value.

Concluding this section we would like to mention that momentum space NN potentials can easily be treated by using a HO basis in momentum space (see e.g. [NoN06]). A review on recent developments of the method can be found in [NaQ09].

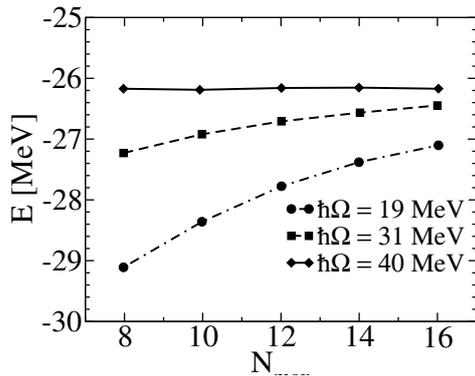


Figure 6.2: N_{\max} dependence of the ${}^4\text{He}$ ground-state energy for a NCSM calculation with the CD-Bonn NN potential [Ma01] and with various values of $\hbar\Omega$ (from Ref. [NaK00]).

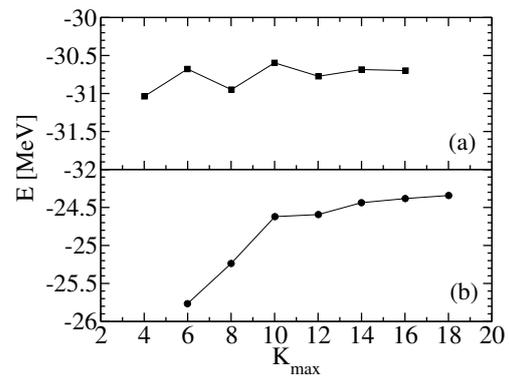
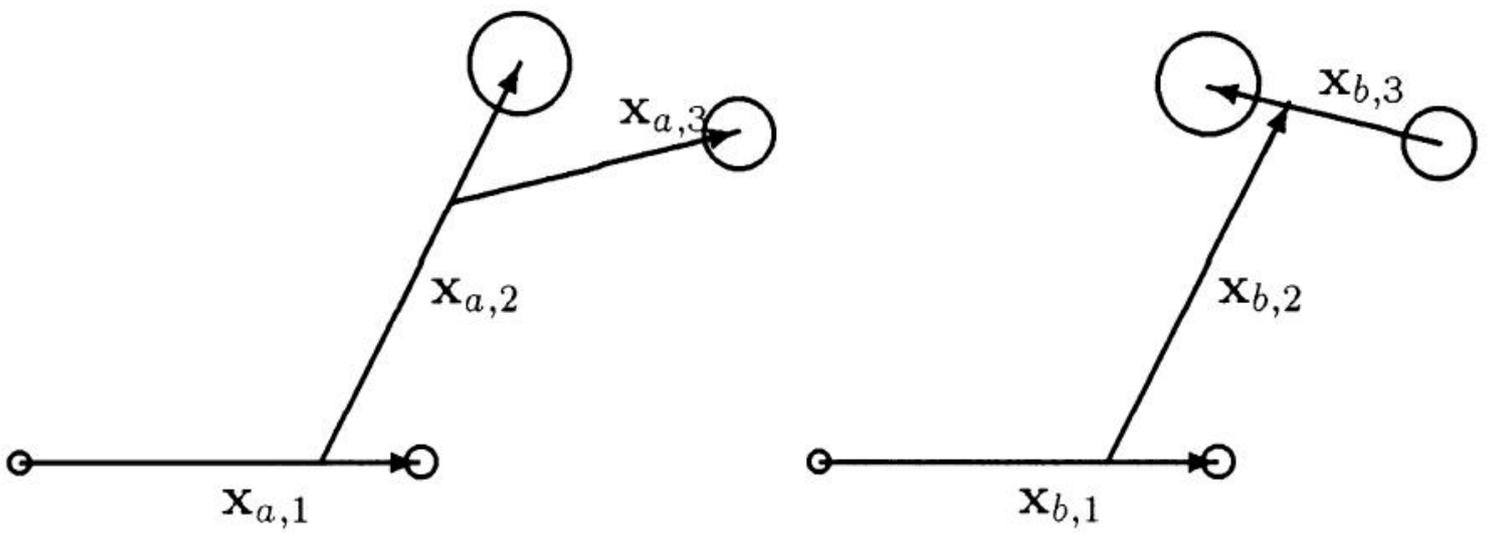


Figure 6.3: K_{\max} dependence of the ${}^4\text{He}$ ground-state energy for a EIHH calculation with the MTI-III [MaT69] (a) and AV14 [WiS84] (b) NN potentials (from Ref. [BaL01]).



7. The Hyperspherical Harmonics

7.1 Overview

7.1.1 Short history

- The study of nuclear systems composed of N nucleons have led to the construction of the hyperspherical harmonics, which are harmonic polynomials in $3(N - 1)$ dimensional space.
- The hyperspherical coordinates and the hyperspherical harmonics are generalization of the spherical harmonics from 3D space into the general case.
- The HH were introduced in 1935 by Zernike and Brinkman.
- They were reintroduced 25 years later by Delves and Smith.
- The hyperspherical harmonics can be constructed in various ways, nevertheless the only general method I know of to construct N -body hyperspherical functions which belong to definite irreducible representation of the group $O(3)$ of spatial rotations, is the “tree” method proposed by Vilenkin *et al.* [Vilenkin65; Vilenkin68] in 1965.
- In the 1970 Raynal and Revai derived the HH transformation coefficients.
- and in 1972 Kil’dushov derives the HH recoupling coefficients.
- All the rest of us ...

7.1.2 Hyperspherical harmonics in a nutshell

- Hyperspherical coordinates $x_1, x_2, x_3, \dots, x_D \rightarrow \rho = \sqrt{\sum x_i^2}, \Omega$.
- In the “tree” method, each hyperspherical coordinate system is set in correspondence to a definite “tree” diagram. For example

$$\begin{aligned} x_1 &= \rho \cos(\alpha) \cos(\beta) \cos(\delta) \\ x_2 &= \rho \cos(\alpha) \cos(\beta) \sin(\delta) \\ x_3 &= \rho \cos(\alpha) \sin(\beta) \end{aligned}$$

$$\begin{aligned}x_4 &= \rho \sin(\alpha) \cos(\gamma) \\x_5 &= \rho \sin(\alpha) \sin(\gamma)\end{aligned}\quad (7.1)$$

correspond to the “tree” diagram in Fig. 7.1.2.

- The “tree” diagram have the following interpretation, segments joining “tree” nodes or a node with a coordinate are called propagators. With each node we associate a certain angle θ ; propagator extending to the right (left) upward from a node is set in accordance with the cosine (sine) of the angle θ . Each coordinate x_i is represented by the product of all the propagators from the vertex of the diagram to the coordinate x_i .
- It is well known that the n -dimensional Laplace operator admits the separation of variables in polyspherical coordinates. Therefore the hyperspherical functions associated with each node and with the “tree” expanding from that node upwards can be written as a product of left “tree” hyperspherical function, right “tree” hyperspherical function and a function of ϕ the angle associated with that node. The rules for obtaining the hyperspherical functions from the “tree” are given in Ref. [Vilenkin65].
- In hyperspherical coordinates

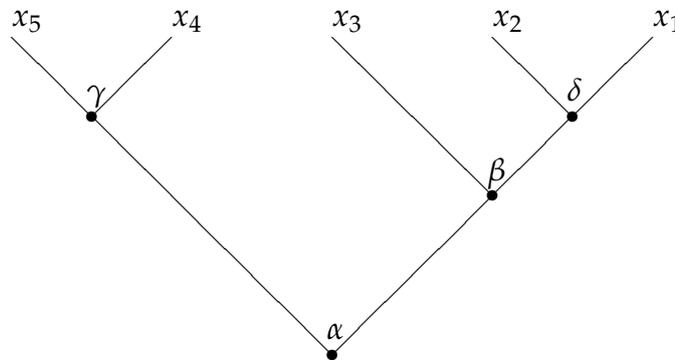
$$\Delta = \frac{\partial^2}{\partial \rho^2} + \frac{D-1}{\rho} \frac{\partial}{\partial \rho} - \frac{\hat{K}^2}{\rho^2}$$

- $\rho^K \mathcal{Y}_{[K]}(\Omega)$ is a Harmonic polynomial.
- The HH are eigenstates of \hat{K}^2

$$\hat{K}^2 \mathcal{Y}(\Omega) = K(K+D-2) \mathcal{Y}(\Omega)$$

- Using the tree structure one can easily construct HH starting from the leafs and uniting branches.
- Each junction is associated with a quantum number.
- Each junction adds a factor $N \cos^{K_R}(\theta) \sin^{K_L}(\theta) P_{(K-K_R-K_L)/2}^{(\alpha_R, \alpha_L)}(\cos(2\theta))$

Figure 7.1: “Tree” diagram



7.1.3 The merits of the HH expansion

- The hyperspherical harmonics are eigenstates of the kinetic energy operator.

- Exhibit separation between “slow” hyperradial coordinate and “fast” hyperangular coordinates.
- A complete set of basis functions.

$$\sum_{[K]} \mathcal{Y}_{[K]}^*(\Omega') \mathcal{Y}_{[K]}(\Omega) \frac{\delta(\rho - \rho')}{\rho^{D-1}} = \prod_{i=1}^N \delta(\eta_i - \eta'_i)$$

- Easy transformation between configuration and momentum space

$$e^{i \sum \eta_j q_j} = \frac{(2\pi)^{D/2}}{(Q\rho)^{D/2-1}} \sum_{[K]} i^K \mathcal{Y}_{[K]}^*(\Omega_q) \mathcal{Y}_{[K]}(\Omega) J_{K+D/2-1}(Q\rho)$$

- Good asymptotics.
- With appropriate choice of Jacobi coordinates and states clusterization can be "easily" treated.

7.2 Mathematical introduction

7.2.1 A 2D example

We begin with the simple 2D transformation

$$\begin{aligned} x &= r \cos \phi \\ y &= r \sin \phi \end{aligned} \quad (7.2)$$

and consider a small translation

$$\begin{aligned} dx &= dr \cos \phi - r \sin \phi d\phi \\ dy &= dr \sin \phi + r \cos \phi d\phi \end{aligned} \quad (7.3)$$

The distance between the original and the new points is given by

$$\begin{aligned} ds^2 = dx^2 + dy^2 &= (dr \cos \phi - r \sin \phi d\phi)^2 + (dr \sin \phi + r \cos \phi d\phi)^2 \\ &= dr^2 + r^2 d\phi^2 = g_{ij} d\zeta_i d\zeta_j \end{aligned} \quad (7.4)$$

here g is the metric matrix

$$\mathbf{g} = \begin{pmatrix} 1 & \\ & r^2 \end{pmatrix} \quad (7.5)$$

$$\mathbf{g}^{-1} = \begin{pmatrix} 1 & \\ & \frac{1}{r^2} \end{pmatrix} \quad (7.6)$$

$$g = \det \mathbf{g} = r^2 \quad (7.7)$$

The volume element in the new (spherical) coordinate set is given by

$$dV = \sqrt{g} d\zeta_1 d\zeta_2 = r dr d\phi. \quad (7.8)$$

The Laplacian is calculated utilizing the inverse matrix $g^{ij} = g_{ij}^{-1}$,

$$\Delta = \sum_{ij} \frac{1}{\sqrt{g}} \frac{\partial}{\partial \zeta_i} \sqrt{g} g^{ij} \frac{\partial}{\partial \zeta_j} \quad (7.9)$$

$$\begin{aligned}\Delta &= \frac{1}{r} \frac{\partial}{\partial r} (r \cdot 1) \frac{\partial}{\partial r} + \frac{1}{r} \frac{\partial}{\partial \phi} \left(r \cdot \frac{1}{r^2} \right) \frac{\partial}{\partial \phi} \\ &= \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2}\end{aligned}\quad (7.10)$$

7.2.2 The n-dimensional case

Consider a simple tree node with ν_L leafs on the left branch and ν_R leafs on the right branch. The total number of leafs being $\nu = \nu_L + \nu_R$ let $\rho_{L/R}$ the hyper radius on each branch, and defined the transformation

$$\begin{aligned}\rho_L &= \rho \sin \alpha \\ \rho_R &= \rho \cos \alpha\end{aligned}\quad (7.11)$$

we look at a small distance in the ν dimensional space

$$ds^2 = ds_L^2 + ds_R^2 \quad (7.12)$$

$$ds_L^2 = d\rho_L^2 + \rho_L^2 \sum_{ij}^{v_L-1} h_{ij}^L d\theta_i^L d\theta_j^L \quad ; \quad ds_R^2 = d\rho_R^2 + \rho_R^2 \sum_{ij}^{v_R-1} h_{ij}^R d\theta_i^R d\theta_j^R \quad (7.13)$$

Here $h_{ij}^{L/R}$ are the $\nu_{L/R} - 1$ dimensional L/R hyperangular metric tensors. I used the notation $\theta_j^{L/R}$ to denote the hyperangular coordinates. In matrix form we can write the metric tensors as

$$\mathbf{g}^L = \begin{pmatrix} 1 & 0 \\ 0 & \rho_L^2 \mathbf{h}^L \end{pmatrix} \quad \mathbf{g}^R = \begin{pmatrix} 1 & 0 \\ 0 & \rho_R^2 \mathbf{h}^R \end{pmatrix} \quad (7.14)$$

Now

$$\begin{aligned}ds^2 &= d\rho_L^2 + \rho_L^2 \sum_{ij} g_{ij}^L d\theta_i^L d\theta_j^L + d\rho_R^2 + \rho_R^2 \sum_{ij} g_{ij}^R d\theta_i^R d\theta_j^R \\ &= d\rho + \rho^2 d\alpha^2 + \rho^2 \sin^2 \alpha \sum_{ij} g_{ij}^L d\theta_i^L d\theta_j^L + \rho^2 \cos^2 \alpha \sum_{ij} g_{ij}^R d\theta_i^R d\theta_j^R\end{aligned}\quad (7.15)$$

$$\mathbf{g} = \begin{pmatrix} 1 & & & \\ & \rho^2 & & \\ & & \rho^2 \sin^2 \alpha \mathbf{h}^L & \\ & & & \rho^2 \cos^2 \alpha \mathbf{h}^R \end{pmatrix} \quad (7.16)$$

$$\begin{aligned}h^L &= \det \mathbf{h}^L \\ h^R &= \det \mathbf{h}^R \\ g &= \det \mathbf{g} = \rho^2 (\rho^2 \sin^2 \alpha)^{\nu_L-1} h^L (\rho^2 \cos^2 \alpha)^{\nu_R-1} h^R \\ &= (\rho^2)^{n-1} (\sin^2 \alpha)^{\nu_L-1} (\cos^2 \alpha)^{\nu_R-1} h^L h^R\end{aligned}\quad (7.17)$$

The volume element

$$dV = \sqrt{g} \Pi d\zeta_i$$

$$\begin{aligned}
&= \rho^{\nu-1} d\rho (\sin \alpha)^{\nu_L-1} (\cos \alpha)^{\nu_R-1} d\alpha \underbrace{\sqrt{h^L} \Pi d\theta_i^L}_{d\Omega_L} \underbrace{\sqrt{h^R} \Pi d\theta_j^R}_{d\Omega_R} \\
&= \rho^{\nu-1} d\rho \underbrace{(\sin \alpha)^{\nu_L-1} (\cos \alpha)^{\nu_R-1} d\alpha d\Omega_L d\Omega_R}_{d\Omega}
\end{aligned} \tag{7.18}$$

$$\mathbf{g}^{-1} = \begin{pmatrix} 1 & & \\ & \frac{1}{\rho^2} & \\ & \frac{1}{\rho^2 \sin^2 \alpha} (\mathbf{h}^L)^{-1} & \\ & & \frac{1}{\rho^2 \cos^2 \alpha} (\mathbf{h}^R)^{-1} \end{pmatrix} \tag{7.19}$$

$$g^{ij} = g_{ij}^{-1}$$

$$\Delta = \sum_{ij} \frac{1}{\sqrt{g}} \frac{\partial}{\partial d\zeta_i} \sqrt{g} g^{ij} \frac{\partial}{\partial d\zeta_j} \tag{7.20}$$

$$\begin{aligned}
\Delta &= \frac{\partial^2}{\partial \rho^2} + \frac{\nu-1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \left(\frac{\partial^2}{\partial \alpha^2} + (\nu_L-1) \frac{\cos \alpha}{\sin \alpha} \frac{\partial}{\partial \alpha} - (\nu_R-1) \frac{\sin \alpha}{\cos \alpha} \frac{\partial}{\partial \alpha} \right) \\
&\quad + \frac{1}{\rho^2 \sin^2 \alpha} \sum_{ij}^{v_L-1} \frac{1}{\sqrt{h^L}} \frac{\partial}{\partial d\theta_i^L} \sqrt{h^L} h_L^{ij} \frac{\partial}{\partial d\theta_j^L} + \frac{1}{\rho^2 \cos^2 \alpha} \sum_{ij}^{v_R-1} \frac{1}{\sqrt{h^R}} \frac{\partial}{\partial d\theta_i^R} \sqrt{h^R} h_R^{ij} \frac{\partial}{\partial d\theta_j^R} \\
&= \frac{\partial^2}{\partial \rho^2} + \frac{\nu-1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \left(\frac{\partial^2}{\partial \alpha^2} + ((\nu_L-1) \cot \alpha - (\nu_R-1) \tan \alpha) \frac{\partial}{\partial \alpha} \right) \\
&\quad - \frac{1}{\rho^2 \sin^2 \alpha} \Lambda_L^2 - \frac{1}{\rho^2 \cos^2 \alpha} \Lambda_R^2
\end{aligned} \tag{7.21}$$

$$\Delta = \frac{\partial^2}{\partial \rho^2} + \frac{\nu-1}{\rho} \frac{\partial}{\partial \rho} - \frac{1}{\rho^2} \Lambda^2 \tag{7.22}$$

$$\Lambda^2 = -\frac{\partial^2}{\partial \alpha^2} + \frac{(\nu_R - \nu_L) - (\nu - 2) \cos 2\alpha}{\sin 2\alpha} \frac{\partial}{\partial \alpha} + \frac{1}{\sin^2 \alpha} \Lambda_L^2 + \frac{1}{\cos^2 \alpha} \Lambda_R^2 \tag{7.23}$$

7.2.3 Hyperspherical harmonics

To get an harmonic polynomial

$$\Delta \rho^K \Psi(\Omega) = 0 \implies \Lambda^2 \Psi(\Omega) = K(K + \nu - 2) \Psi(\Omega) \tag{7.24}$$

Assume $\Psi(\alpha, \Omega_L, \Omega_R) = \Psi(\alpha) \Psi_L(\Omega_L) \Psi_R(\Omega_R)$

$$\begin{aligned}
\Lambda_L^2 \Psi_L(\Omega_L) &= K_L(K_L + \nu_L - 2) \Psi_L(\Omega_L) \\
\Lambda_R^2 \Psi_R(\Omega_R) &= K_R(K_R + \nu_R - 2) \Psi_R(\Omega_R)
\end{aligned} \tag{7.25}$$

$$\begin{aligned}
\left[\frac{\partial^2}{\partial \alpha^2} - \frac{(\nu_R - \nu_L) - (\nu - 2) \cos 2\alpha}{\sin 2\alpha} \frac{\partial}{\partial \alpha} - \frac{K_L(K_L + \nu_L - 2)}{\rho^2 \sin^2 \alpha} - \frac{K_R(K_R + \nu_R - 2)}{\rho^2 \cos^2 \alpha} \right] \Psi(\alpha) \\
= -K(K + n - 2) \Psi(\alpha)
\end{aligned} \tag{7.26}$$

After some algebra we get

$$\begin{aligned}
\Psi_K^{K_L, K_R}(\alpha) &= N_n^{a,b} (\sin \alpha)^{K_L} (\cos \alpha)^{K_R} P_n^{(a,b)}(\cos 2\alpha) \\
n &= \frac{K - K_L - K_R}{2} \\
a &= K_L + \nu_L/2 - 1 \\
b &= K_R + \nu_R/2 - 1 \\
N_n^{a,b} &= \sqrt{\frac{2(2n + a + b + 1)n! \Gamma(n + a + b + 1)}{\Gamma(n + a + 1)\Gamma(n + b + 1)}} \quad (7.27)
\end{aligned}$$

It is clear that $K = K_L + K_R + 2n$ and that $n \geq 0$.

7.3 The 3-body case

We begin with the Jacobi coordinates

$$\begin{aligned}
\eta_1 &= \sqrt{\frac{m_1 m_2}{M_{12} m}} (\mathbf{r}_2 - \mathbf{r}_1) \\
\eta_2 &= \sqrt{\frac{M_{12} m_3}{M_{123} m}} \left(\mathbf{r}_3 - \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{M_{12}} \right) \quad (7.28)
\end{aligned}$$

and choose the hyperspherical coordinates

$$\begin{aligned}
\eta_1 &= \rho \cos \alpha \hat{\eta}_1 \\
\eta_2 &= \rho \sin \alpha \hat{\eta}_2 \quad (7.29)
\end{aligned}$$

The complete set of six coordinates consists of ρ , θ , and the solid angles Ω_1 , Ω_2 associated with the unit vectors $\hat{\eta}_1$ and $\hat{\eta}_2$ respectively. The six dimensional volume element is given by

$$dV = \rho^5 d\rho d\Omega \equiv \rho^5 d\rho \sin^2(\alpha) \cos^2(\alpha) d\alpha d\hat{\eta}_1 d\hat{\eta}_2 \quad (7.30)$$

where $d\Omega$ is the angular volume element associated with the 6 dimensional hypersphere. The hyperangle α varies in the range $\frac{\pi}{2} \geq \alpha \geq 0$.

7.3.1 The Laplace operator in hyperspherical coordinates

The internal kinetic energy operator for a two-particle system is given by the three-dimensional Laplace operator, expressed in terms of the relative motion Jacobi coordinate η_1 and the corresponding angular coordinates Ω_1 ,

$$\Delta_1 = \Delta_{\eta_1} = \Delta_{\eta_1} - \frac{1}{\eta_1^2} \hat{\ell}_1^2 \quad (7.31)$$

where the radial part is

$$\Delta_{\eta_1} = \frac{\partial^2}{\partial \eta_1^2} + \frac{2}{\eta_1} \frac{\partial}{\partial \eta_1} \quad (7.32)$$

and $\hat{\ell}_1$ is the angular momentum operator of the relative motion.

The internal kinetic energy of a three-particle system is described by the six-dimensional Laplace operator which is a sum over the three dimensional Laplace operators that act on the coordinates η_1 and η_2 separately.

$$\Delta^{(2)} = \Delta_1 + \Delta_2 = \Delta_{\eta_1} + \Delta_{\eta_2} - \frac{1}{\eta_1^2} \hat{\ell}_1^2 - \frac{1}{\eta_2^2} \hat{\ell}_2^2 \quad (7.33)$$

Using Eqs. (7.29) we can transform the two radial coordinates η_1 and η_2 into the hyper-radial coordinate ρ and the hyper-angular coordinate α . Using (7.22) and noting that $\nu = 6$ we can write

$$\Delta^{(2)} = \frac{\partial^2}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial}{\partial \rho} - \frac{1}{\rho^2} \hat{K}^2 \quad (7.34)$$

Here we have used the notation $\hat{K}^2 = \Lambda^2$. Noting that $\nu_L = \nu_R = 3$, and that $\Lambda_R^2 = \hat{\ell}_1^2$ and $\Lambda_L^2 = \hat{\ell}_2^2$, the hyperspherical angular momentum operator \hat{K}^2 is expressed in terms of the hyper-angular coordinate α and the two angular momentum operators $\hat{\ell}_1^2$ and $\hat{\ell}_2^2$ as follows, Eq. (7.23),

$$\hat{K}^2 = -\frac{\partial^2}{\partial \alpha^2} - 4 \cot(2\alpha) \frac{\partial}{\partial \alpha} + \frac{1}{\cos^2 \alpha} \hat{\ell}_1^2 + \frac{1}{\sin^2 \alpha} \hat{\ell}_2^2 \quad (7.35)$$

7.3.2 Commuting set of operators

An important observation can be drawn now. The 3-body hyperspherical (some times also called 'grand') angular momentum operator commutes with $\hat{\ell}_1$, and $\hat{\ell}_2$. Therefore $\hat{K}^2, \hat{\ell}_1^2, \hat{\ell}_2^2, \hat{\ell}_{1,z}, \hat{\ell}_{2,z}$. These operators form a complete set of commuting hyperspherical operators, and therefore of quantum numbers, i.e. $K, \ell_1, m_1, \ell_2, m_2$. Of course these operators also commute with $\Delta^{(2)}$.

The internal angular momentum operator of the three-particle system is $\hat{\mathbf{L}} = \hat{\ell}_1 + \hat{\ell}_2$. Note that \hat{L}^2 and also \hat{L}_z commute with these operators.

7.3.3 The 3-body hyperspherical functions

Following the derivation in Sec. 7.2.3 the 3-body hyperspherical harmonics functions can be written as

$$\mathcal{Y}_{K\ell_1 m_1 \ell_2 m_2}(\Omega) = \Psi_K^{\ell_2, \ell_1}(\alpha) Y_{\ell_1 m_1}(\hat{\boldsymbol{\eta}}_1) Y_{\ell_2 m_2}(\hat{\boldsymbol{\eta}}_2) \quad (7.36)$$

As we have already seen the eigenfunctions of \hat{K}^2 , Eq. (7.35), are functions of the hyper-angular coordinate α (Eq. (??)) and depend on the value of the quantum number K as well as on the values of ℓ_2 and ℓ_1 , as follows

$$\Psi_K^{\ell_2, \ell_1}(\alpha) = N_n^{\ell_2+1/2, \ell_1+1/2} (\sin \alpha)^{\ell_2} (\cos \alpha)^{\ell_1} P_n^{(\ell_2+\frac{1}{2}, \ell_1+\frac{1}{2})}(\cos 2\alpha), \quad (7.37)$$

where $P_n^{(\ell_2+\frac{1}{2}, \ell_1+\frac{1}{2})}$ is the Jacobi polynomial, and n is a non-negative integer such that

$$n = \frac{K - \ell_1 - \ell_2}{2}. \quad (7.38)$$

The normalization constant is, Eq. (7.27), [Efros72]

$$N_n^{(\ell_2+1/2, \ell_1+1/2)} = \left[\frac{(2K+4)n!\Gamma(n+\ell_2+\ell_1+2)}{\Gamma(n+\ell_2+\frac{3}{2})\Gamma(n+\ell_1+\frac{3}{2})} \right]^{\frac{1}{2}}. \quad (7.39)$$

The eigenvalues of \hat{K}_2^2 corresponding to the eigenfunctions (7.37) are $K(K+4)$, where $K \geq \ell_1 + \ell_2 \geq 0$ and has the same parity as $\ell_1 + \ell_2$ (cf. Eq. (7.38)).

The angular part of the internal state for two particles is described by the spherical harmonic $Y_{\ell_1 m_1}(\hat{\boldsymbol{\eta}}_1)$. Adding one more particle belonging to the state $Y_{\ell_2 m_2}(\hat{\boldsymbol{\eta}}_2)$ we can form a three-particle state $\Phi_{L_2 M_2; \ell_1 \ell_2}(\hat{\boldsymbol{\eta}}_1, \hat{\boldsymbol{\eta}}_2)$, which is an eigenstate of the operators $\hat{\ell}_1^2, \hat{\ell}_2^2, \hat{L}^2$ and \hat{L}_z . This three-particle state is obtained by conventional angular momentum coupling

$$\Phi_{LM; \ell_1 \ell_2}(\hat{\boldsymbol{\eta}}_1, \hat{\boldsymbol{\eta}}_2) = \sum_{m_1 m_2} (\ell_1 m_1 \ell_2 m_2 | LM) Y_{\ell_1, m_1}(\hat{\boldsymbol{\eta}}_1) Y_{\ell_2, m_2}(\hat{\boldsymbol{\eta}}_2) \quad (7.40)$$

The hyperspherical function for three particles, which is an eigenfunction of \hat{K}^2 as well as of \hat{L}^2 , can now be written as

$$\mathcal{Y}_{[K]}(\Omega) = \Psi_K^{\ell_2, \ell_1}(\alpha) \Phi_{L_2 M_2; \ell_1 \ell_2}(\hat{\boldsymbol{\eta}}_1, \hat{\boldsymbol{\eta}}_2) \quad (7.41)$$

The symbol $[K]$ stands for the aggregate of five good quantum numbers K, L, M, ℓ_1 and ℓ_2 , which completely label the state since there are five (internal) coordinates, *i.e.*, $\hat{\boldsymbol{\eta}}_1 = (\theta_1, \phi_1)$, $\hat{\boldsymbol{\eta}}_2 = (\theta_2, \phi_2)$, and α .

7.4 The A-body case

To construct the A-body hyperspherical harmonics functions we shall use an inductive prescription. Consider k Jacobi coordinates and assume that we have already constructed states for $k-1$ coordinates.

The Jacobi coordinates $\{\boldsymbol{\eta}_k\}_{k=1 \dots N}$ consists of a radial coordinate η_k and a pair of angular coordinates $\hat{\boldsymbol{\eta}}_k \equiv (\theta_k, \phi_k)$.

In general, having defined the hyper-radial coordinate $\rho_{k-1} = \sqrt{\sum_{i=1}^{k-1} \eta_i^2}$ we define ρ_k and α_k so as to satisfy

$$\begin{aligned} \rho_{k-1} &= \rho_k \cos \alpha_k \\ \eta_k &= \rho_k \sin \alpha_k \end{aligned} \quad (7.42)$$

where

$$\rho_k^2 = \rho_{k-1}^2 + \eta_k^2 = \sum_{i=1}^k \eta_i^2 = \frac{1}{2M_k} \sum_{i,j=1}^k m_i m_j (\mathbf{r}_i - \mathbf{r}_j)^2 \quad (7.43)$$

Therefore, the hyper-radial coordinate is symmetric with respect to permutations of the underlying single particle coordinates, and is invariant to the choice of the Jacobi coordinates. The $3N$ internal coordinates for the $N+1$ -particle system consist of the hyper-radial coordinate ρ_N , the $N-1$ hyper-angular coordinates $\alpha^{(N)} \equiv \{\alpha_2, \alpha_3, \dots, \alpha_N\}$, and the $2N$ angular coordinates $\{\hat{\boldsymbol{\eta}}_1, \hat{\boldsymbol{\eta}}_2, \dots, \hat{\boldsymbol{\eta}}_N\}$.

These coordinates depend on the set of Jacobi coordinates specified in Eq. (3.8). For a different ordering of particle indices a different set of hyper-angular coordinates as well as a permuted set of angular coordinates is obtained. On the other hand, the hyper-radial coordinate is independent of the order of the particle indices, *cf.* Eq. (7.43). The volume element associated with the N Jacobi coordinates η_1, \dots, η_N is

$$dV_{3N} = \rho_N^{3N-1} d\rho_N d\Omega_{3N} \equiv \rho_N^{3N-1} d\rho_N \sin^2(\alpha_N) \cos^{3N-4}(\alpha_N) d\alpha_N d\hat{\eta}_N d\Omega_{3(N-1)} \quad (7.44)$$

where $d\Omega_{3(N-1)}$ is the volume element associated with the $3(N-1)$ dimensional hyper sphere. The hyper angle α_N varies in the range $\frac{\pi}{2} \geq \alpha_N \geq 0$.

7.4.1 The Laplace operator in hyperspherical coordinates

The $3N$ -dimensional Laplace operator, describing the internal kinetic energy of the $A = N + 1$ -particle system, is a sum over the three-dimensional Laplace operators that act on the coordinates $\eta_1, \eta_2, \dots, \eta_N$

$$\Delta^{(N)} = \sum_{i=1}^N \Delta_i = \sum_{i=1}^N \left(\Delta_{\eta_i} - \frac{1}{\eta_i^2} \hat{\ell}_i^2 \right) \quad (7.45)$$

This $N + 1$ -particle Laplace operator can be expressed by means of the recurrence relation

$$\Delta^{(N)} = \Delta^{(N-1)} + \Delta_{\eta_N} = \Delta_{\rho_{N-1}} + \Delta_{\eta_N} - \frac{1}{\rho_{N-1}^2} \hat{K}_{N-1}^2 - \frac{1}{\eta_N^2} \hat{\ell}_N^2 \quad (7.46)$$

We can apply Eq. (7.42) and transform the coordinates ρ_{N-1} and η_N into the hyper-radial coordinate ρ_N and the hyper-angular coordinate α_N . In this case the $3N$ dimensional Laplace operator, Eq. (7.45), can be written in the form

$$\Delta^{(N)} = \Delta_{\rho_N} - \frac{1}{\rho_N^2} \hat{K}_N^2 \quad (7.47)$$

where the radial part is

$$\Delta_{\rho_N} = \frac{\partial^2}{\partial \rho_N^2} + \frac{3N-1}{\rho_N} \frac{\partial}{\partial \rho_N} \quad (7.48)$$

\hat{K}_N^2 , the $N + 1$ -particle hyperspherical angular momentum operator, can be expressed in terms of \hat{K}_{N-1}^2 and $\hat{\ell}_N^2$ as follows [Efros72]

$$\hat{K}_N^2 = -\frac{\partial^2}{\partial \alpha_N^2} + \frac{3N-6-(3N-2)\cos(2\alpha_N)}{\sin(2\alpha_N)} \frac{\partial}{\partial \alpha_N} + \frac{1}{\cos^2 \alpha_N} \hat{K}_{N-1}^2 + \frac{1}{\sin^2 \alpha_N} \hat{\ell}_N^2 \quad (7.49)$$

where we define $\hat{K}_1^2 \equiv \hat{\ell}_1^2$. The internal $N + 1$ -particle angular momentum operator is $\hat{\mathbf{L}}_N = \hat{\mathbf{L}}_{N-1} + \hat{\ell}_N$. The operators \hat{K}_{N-1}^2 , $\hat{\ell}_N^2$, \hat{K}_N^2 , \hat{L}_N^2 and \hat{L}_{Nz} commute with each other, thus each hyperspherical state is labeled by the complete set of quantum numbers K_N, K_{N-1}, \dots, K_2 corresponding to the hyperspherical angular momentum, $L_N, L_{N-1}, \dots, L_2, M_{Nz}$ corresponding to the spatial angular momentum, and $\ell_N, \ell_{N-1}, \dots, \ell_2, \ell_1$ corresponding to the angular part of the Jacobi coordinates.

Theorem 7.4.1 The hyperspherical angular momentum operator \hat{K}_N^2 is the Casimir operator of the group O_{3N} the same way that \hat{L}^2 is the Casimir operator of $O(3)$. Consequently, \hat{K}_N^2 is invariant under any rotation in the $3N$ dimensional space.

7.4.2 The hyperspherical functions

Following the foot steps we have presented in Sec. 7.2.3 and employed previously to the 3-body case in Sec. 7.3 we can easily see that HH functions corresponding to the tree displayed in Fig. 7.2 is given by

$$\begin{aligned} \mathcal{Y}_{[K_N]} &= \left[\prod_{j=1}^N Y_{\ell_j, m_j}(\hat{\eta}_j) \right] \\ &\times \left[\prod_{j=2}^N N_{n_j}^{\ell_j + \frac{1}{2}, K_{j-1} + \frac{3j-5}{2}} (\sin \alpha_j)^{\ell_j} (\cos \alpha_j)^{K_{j-1}} P_{n_j}^{(\ell_j + \frac{1}{2}, K_{j-1} + \frac{3j-5}{2})}(\cos(2\alpha_j)) \right] \end{aligned}$$

Here

$$n_j = \frac{K_j - \ell_j - K_{j-1}}{2} \quad (7.50)$$

and $[K_N]$ stands for the $3N - 1$ quantum numbers

$$[K_N] = \{K_N, K_{N-1}, \dots, K_2, \ell_N, \ell_{N-1}, \dots, \ell_1, m_N, m_{N-1}, \dots, m_1\}$$

coupling recursively angular momenta of the single Jacobi vectors we may get HH functions with well defined angular momentum

$$\begin{aligned} \mathcal{Y}_{[K_N]} &= \sum_{m_1, m_2, \dots, m_N} \prod_{j=2}^N (L_{j-1} M_{j-1} \ell_j m_j | L_j M_j) \left[\prod_{j=1}^N Y_{\ell_j, m_j}(\hat{\eta}_j) \right] \\ &\times \left[\prod_{j=2}^N N_{n_j}^{\ell_j + \frac{1}{2}, K_{j-1} + \frac{3j-5}{2}} (\sin \alpha_j)^{\ell_j} (\cos \alpha_j)^{K_{j-1}} P_{n_j}^{(\ell_j + \frac{1}{2}, K_{j-1} + \frac{3j-5}{2})}(\cos(2\alpha_j)) \right] \end{aligned}$$

Here $M_j = M_{j-1} + m_j$, $M_1 = m_1$ and $L_1 = \ell_1$.

Being normalized eigenvectors of the commuting operators $\{\hat{K}_j, \hat{L}_j^2, \hat{\ell}_j^2\}$ and $L_{N,z}$ the HH are a complete orthogonal set, therefore

$$\begin{aligned} \langle \mathcal{Y}_{[K_N]} | \mathcal{Y}_{[K'_N]} \rangle &= \delta_{[K_N], [K'_N]} \\ &= \delta_{K_N, K'_N} \delta_{L_N, L'_N} \delta_{M_N, M'_N} \delta_{\ell_N, \ell'_N} \\ &\times \delta_{K_{N-1}, K'_{N-1}} \delta_{L_{N-1}, L'_{N-1}} \delta_{\ell_{N-1}, \ell'_{N-1}} \\ &\times \dots \\ &\times \delta_{K_2, K'_2} \delta_{L_2, L'_2} \delta_{\ell_2, \ell'_2} \delta_{\ell_1, \ell'_1} \end{aligned} \quad (7.51)$$

The sequential scheme described above is one of many available routes A different route or “tree” structure corresponding to different hyperspherical coupling scheme is presented in Fig. 7.3. In this case the last two coordinates are coupled together before being coupled to the rest of the tree.

Figure 7.2: The “tree” structure that represents the scheme for constructing the eigenfunctions of the hyperspherical angular momentum operator \hat{K}_N^2 . The particles are added sequentially.

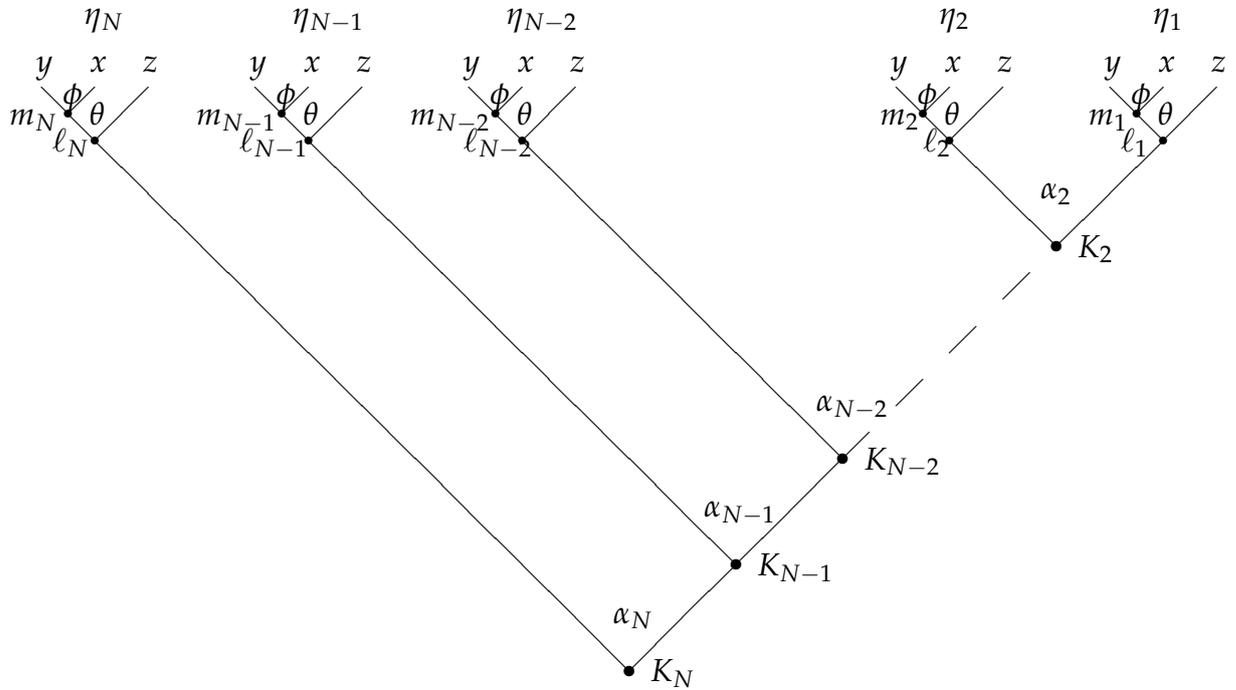
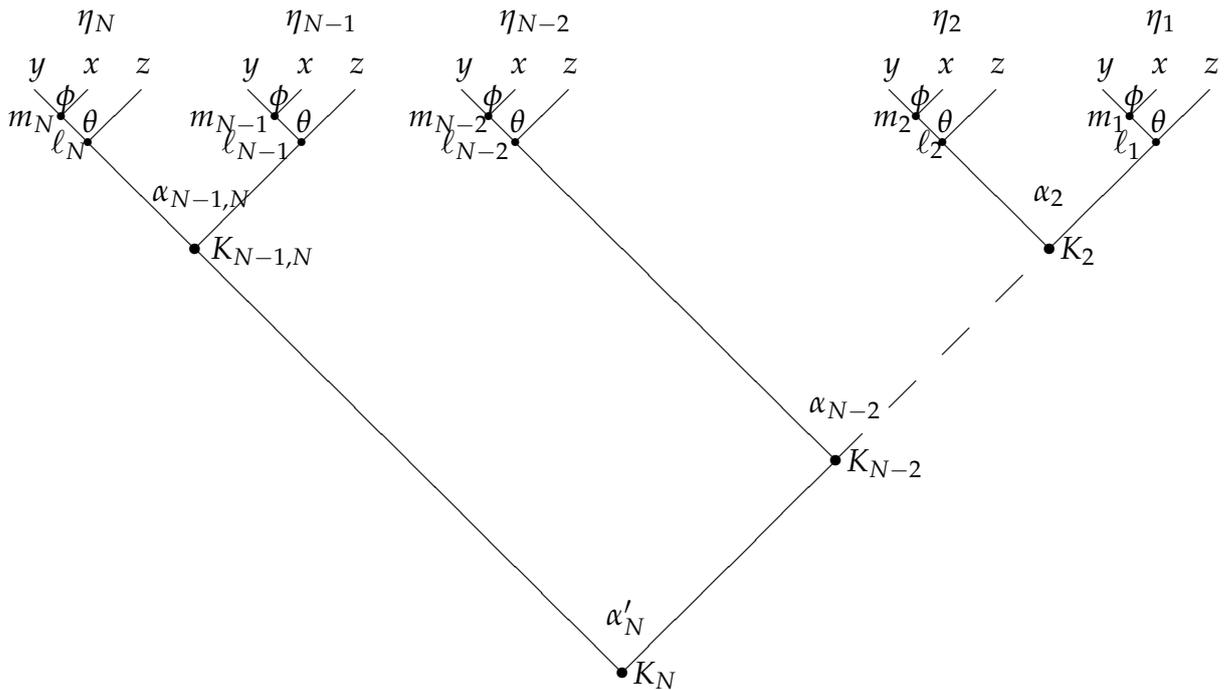


Figure 7.3: The “tree” structure that represents the scheme for constructing the eigenfunctions of the hyperspherical angular momentum operator \hat{K}_N^2 . The last two particles are coupled to one another before they are coupled to the rest of the system.



7.4.3 Relation to the HO basis

In view of Eqs. (7.47) and (7.43) it is evident that the HO Hamiltonian, written in the form

$$\sum_{j=1}^N \left(-\frac{\Delta_j}{2} + \frac{1}{2} \omega^2 \eta_j^2 \right) = \frac{1}{2} \left(-\frac{\partial^2}{\partial \rho^2} - \frac{3N-1}{\rho} \frac{\partial}{\partial \rho} + \frac{\hat{K}_N^2}{\rho^2} + \omega^2 \rho^2 \right), \quad (7.52)$$

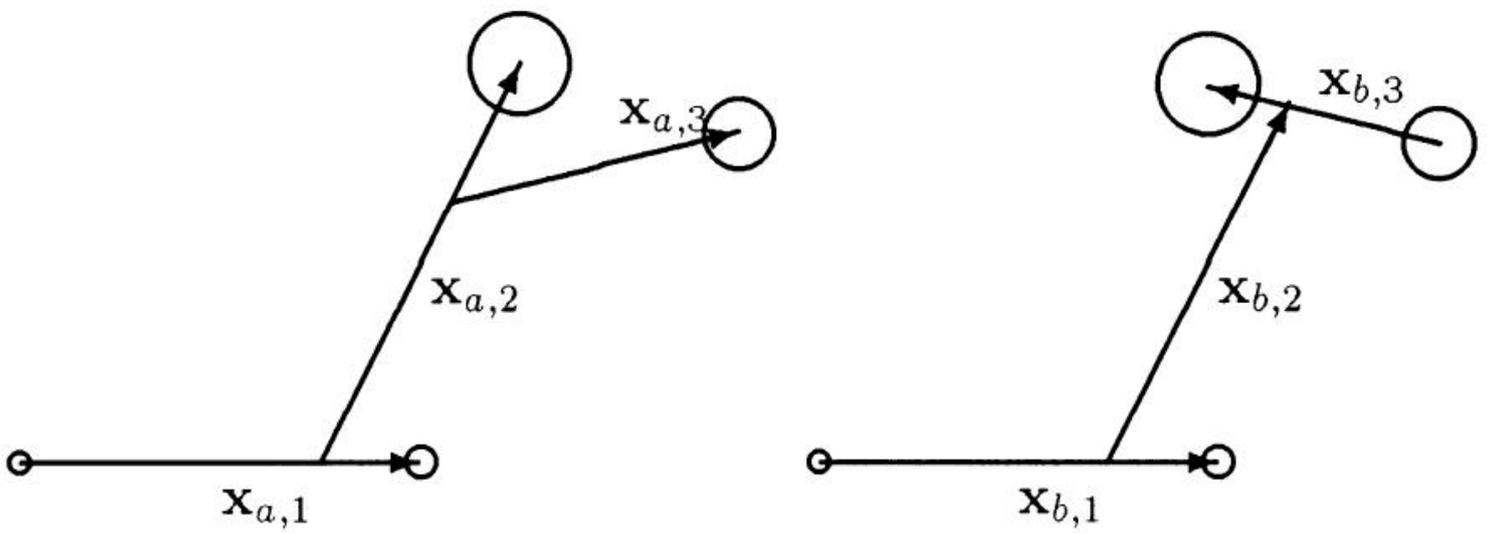
has eigenvectors of the form

$$\Psi_{HO} = R_{n_\rho}(\rho) \mathcal{Y}_{[K_N]}(\Omega) \quad (7.53)$$

with eigenvalues

$$E_n = \hbar\omega \left(\frac{3(A-1)}{2} + n \right) = \hbar\omega \left(\frac{3(A-1)}{2} + 2n_\rho + K_N \right). \quad (7.54)$$

Therefore the HH K_N -quantum number can be associated with the quanta of excitations of the HO wave function.



8. HH - The A-Body problem

8.1 Solving the Schroedinger Equation

The HH expansion in few steps

- Remove the center of mass

$$r_1, r_2, \dots, r_A \longrightarrow R_{c.m.}, \eta_1 \eta_2 \dots \eta_{A-1}$$

- Introduce hyperspherical coordinates

$$\eta_1 \eta_2 \dots \eta_{A-1} \longrightarrow \rho = \sqrt{\eta_1^2 + \eta_2^2 + \dots + \eta_{A-1}^2}, \Omega$$

- Expand the wave function using hyperspherical harmonics

$$\Psi(\rho, \Omega) = \sum_{[K], K \leq K_{\max}} R_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega)$$

- Transform the Hamilton

$$H = -\frac{1}{2} \sum_{k=1}^{A-1} \nabla_k^2 + \sum_{i<j} V_{ij} \left(+ \sum_{i<j<k} V_{ijk} + \dots \right)$$

to hyperspherical coordinates

$$H = -\frac{1}{2} \left(\frac{\partial^2}{\partial \rho^2} + \frac{3A-4}{\rho} \frac{\partial}{\partial \rho} - \frac{\hat{K}^2}{\rho^2} \right) + \sum_{i<j} V_{ij}$$

- Evaluate the matrix elements

$$V_{[K],[K']}(\rho) = \langle [K] | \sum_{i<j} V_{ij} | [K'] \rangle = \int d\Omega \mathcal{Y}_{[K]}^*(\Omega) \sum_{i<j} V_{ij}(\rho, \Omega) \mathcal{Y}_{[K']}(\Omega)$$

- Solve the Schrödinger equation

$$-\frac{1}{2} \left(\frac{\partial^2}{\partial \rho^2} + \frac{3A-4}{\rho} \frac{\partial}{\partial \rho} - \frac{K(K+3A-5)}{\rho^2} \right) R_{[K]}(\rho) + \sum_{[K']}^{K_{\max}} V_{[K],[K']}(\rho) R_{[K']}(\rho) = ER_{[K]}(\rho)$$

8.2 Convergence rate

Evaluating the convergence rate if the HH we follow T. R. Schneider, Phys. Lett. B, 40, 439 (1972).

Definition 8.2.1 Denote the exact wave function by

$$\Psi(\rho, \Omega) = \sum_{[K]} R_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega)$$

and an approximated wave function

$$\Psi_K(\rho, \Omega) = \sum_{[K]}^{K_{\max}} R_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega)$$

We also define another approximation to the wave function

$$\Psi'_K(\rho, \Omega) = \sum_{[K]}^{K_{\max}} R'_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega)$$

Ψ is the solution of $H\Psi = E\Psi$, and Ψ_K is Ψ limited to the subspace $K \leq K_{\max}$. In contrast Ψ'_K is the solution of $H_K\Psi'_K = E_K\Psi'_K$, where H_K is the Hamiltonian restricted to the subspace $[K] \leq K_{\max}$.

Also denote by

$$P_{[K]} = \int \rho^{3N-1} d\rho |R_{[K]}(\rho)|^2$$

the probability of the system being in HH state $[K]$.

Theorem 8.2.1 If the quantity $\|\hat{K}^p|\Psi\rangle\|$ is bound then the expansion coefficients are also bounded

$$P_{[K]} \leq \frac{\|\hat{K}^p|\Psi\rangle\|^2}{K^{2p}}$$

and

$$\sum_{[K]=K} P_{[K]} \leq \frac{\|\hat{K}^p|\Psi\rangle\|^2}{K^{2p}}$$

Here the sum is restricted to the HH states with principle quantum number K .

This can be easily seen as

$$\begin{aligned} \|\hat{K}^p|\Psi\rangle\|^2 &= \langle\Psi|\hat{K}^{2p}|\Psi\rangle \\ &= \sum_{[K]} \int \rho^{3N-1} d\rho |R_{[K]}(\rho)|^2 \{K(K+3A-5)\}^p \end{aligned}$$

$$= \sum_{[K]} P_{[K]} \{K(K + 3A - 5)\}^p \quad (8.1)$$

It can be shown on general grounds, applicable to any basis expansion, that

$$\| |\Psi\rangle - |\Psi'_K\rangle \| \leq C \| |\Psi\rangle - |\Psi_K\rangle \| \quad (8.2)$$

and

$$\| E_K - E \| \leq D \| |\Psi\rangle - |\Psi_K\rangle \|^2 \quad (8.3)$$

It follows that

$$\| E_K - E \| \leq D \sum_{[K] > K_{\max}} P_{[K]} \leq D \| \hat{K}^p |\Psi\rangle \|^2 \sum_{K > K_{\max}} \frac{1}{K^{2p}} \quad (8.4)$$

Theorem 8.2.2 If $\hat{K}^{2p}V$ is square integrable, then the quantity $\| \hat{K}^{2p+2} |\Psi\rangle \|$ is bounded.

Proof. The bound state wave function of the A -body system is a square integrable function. From the theory of square integrable functions it follows that if f, g are square integrable then also are fg and $f + g$.

If the potential V is square integrable, then $V|\Psi\rangle$ is also square integrable. As $|\Psi\rangle$ is an eigenstates of H

$$E|\Psi\rangle - V|\Psi\rangle = -\frac{1}{2}\Delta_\rho|\Psi\rangle + \frac{1}{2}\frac{\hat{K}^2}{\rho^2}|\Psi\rangle \quad (8.5)$$

As $H|\Psi\rangle$ is square integrable and so are the terms on the lhs, the rhs must also be square integrable. The wave function $|\Psi\rangle$ is continuous and differentiable, it is regular at the origin and therefore $\Delta_\rho|\Psi\rangle$ must be bound. Consequently also $\frac{\hat{K}^2}{\rho^2}|\Psi\rangle$ must be bound. As $\langle \rho | \Psi \rangle \rightarrow \exp(-\kappa\rho)$ for large ρ the square integrability of $\frac{\hat{K}^2}{\rho^2}|\Psi\rangle$ implies that also $\hat{K}^2|\Psi\rangle$ is square integrable.

Assume now that $\hat{K}^{2k}V$ is square integrable for $k < p$, and that $\| \hat{K}^{2k+2} |\Psi\rangle \|$ is bounded. If $\hat{K}^{2p}V$ is square integrable so also

$$-\hat{K}^{2p}V|\Psi\rangle = -\hat{K}^{2p}E|\Psi\rangle - \frac{1}{2}\Delta_\rho\hat{K}^{2p}|\Psi\rangle + \frac{1}{2}\frac{\hat{K}^{2p+2}}{\rho^2}|\Psi\rangle \quad (8.6)$$

Consequently $\| \hat{K}^{2p+2} / \rho^2 |\Psi\rangle \|$ is bounded and following the same argument as above so also is $\| \hat{K}^{2p+2} |\Psi\rangle \|$. ■

We can consider now few examples of short range potentials. Each is less singular than r^{-2} and falls off faster than r^{-3} .

- Yukawa potential -

$$V(r) = V_0 \exp(-r/a)/r$$

Here all the difficulties are introduced by the $1/r$ singularity. This potential is square integrable but \hat{K}^2V is not square integrable. It is expected that the binding energy will converge at least as fast as K^{-3} .

- Square well potential - The potential is square integrable, but the discontinuity at makes $\hat{K}^2 V$ not square integrable. Therefore it is expected that the binding energy will converge at least as fast as K^{-3} .
- Gaussian -

$$V(r) = V_0 \exp(-r^2/a^2)$$

The Gaussian is finite every-where, and it is infinitely differentiable, while it and all of its derivatives are square integrable. Hence $\hat{K}^{2p} V$ is bounded for all values of p . The convergence rate will be faster than any inverse power of p , exponentially fast.

8.3 Evaluation of Matrix Elements

8.3.1 The 2-body integral

The evaluation of the 2-body potential matrix elements is simple when the *last* Jacobi coordinate in the tree is proportional to the interparticle distance. Let us denote by $\{\eta_1^{(ij)}, \eta_2^{(ij)}, \dots, \eta_N^{(ij)}\}$ a coordinate system in which

$$\eta_N^{(ij)} = \sqrt{\frac{1}{2}}(r_i - r_j) \quad (8.7)$$

Using the 'K' tree coupling scheme

$$r_{ij} = \sqrt{2}\rho \sin \alpha_N \quad (8.8)$$

This coordinate system defined a specific set of hyperspherical coordinates Ω_{ij} and a corresponding HH basis $|[K_N]_{ij}\rangle$. In general we shall denote these coordinates and states by ij but will omit this subscript in this subsection.

The 2-body matrix elements reads

$$\begin{aligned} V_{[K_N],[K'_N]}^{(ij)}(\rho) &= \langle [K_N] | V_{ij}(r_{ij}) | [K'_N] \rangle \\ &= \int d\Omega \mathcal{Y}_{[K_N]}^*(\Omega) V_{ij}(\sqrt{2}\rho \sin \alpha_N) \mathcal{Y}_{[K'_N]}(\Omega) \\ &= \delta_{[K_{N-1}], [K'_{N-1}]} \delta_{\ell_N, \ell'_N} \delta_{L_N, L'_N} V_{K_N, K'_N; K_{N-1}, \ell_N}^{(ij)}(\rho) \end{aligned} \quad (8.9)$$

$$\begin{aligned} V_{K_N, K'_N; K_{N-1}, \ell_N}^{(ij)}(\rho) &= \int d\alpha_N \sin^2 \alpha_N \cos^{3N-4} \alpha_N \\ &\quad \times [N_n^{a,b}(\sin \alpha_N)^{\ell_N} (\cos \alpha_N)^{K_{N-1}} P_n^{(a,b)}(\cos(2\alpha_N))] \\ &\quad \times V_{ij}(\sqrt{2}\rho \sin \alpha_N) \\ &\quad \times [N_{n'}^{a,b}(\sin \alpha_N)^{\ell_N} (\cos \alpha_N)^{K_{N-1}} P_{n'}^{(a,b)}(\cos(2\alpha_N))] \\ &= N_n^{a,b} N_{n'}^{a,b} \int d\alpha_N \sin^{2a+1} \alpha_N \cos^{2b+1} \alpha_N \\ &\quad \times P_n^{(a,b)}(\cos(2\alpha_N)) V_{ij}(\sqrt{2}\rho \sin \alpha_N) P_{n'}^{(a,b)}(\cos(2\alpha_N)) \end{aligned} \quad (8.10)$$

where

$$\begin{aligned}
 a &= \ell_N + \frac{1}{2} \\
 b &= K_{N-1} + \frac{3N-5}{2} \\
 n &= \frac{K_N - K_{N-1} - \ell_N}{2} \\
 n' &= \frac{K'_N - K_{N-1} - \ell_N}{2}
 \end{aligned} \tag{8.11}$$

These expressions become a bit more complicated for non central potentials.

8.3.2 The general case

In general we need to transform the coordinate system so that the desired pair is in the last Jacobi coordinate.

$$\langle [K_N] | V_{ij} | [K'_N] \rangle = \sum_{[K_N]_{ij}, [K'_N]_{ij}} \langle [K_N] | [K_N]_{ij} \rangle V_{[K_N]_{ij}, [K'_N]_{ij}}^{(ij)}(\rho) \langle [K'_N]_{ij} | [K'_N] \rangle \tag{8.12}$$

The overlap matrix elements

$$\langle [K_N] | [K_N]_{ij} \rangle = \int d\Omega \mathcal{Y}_{[K_N]}^*(\Omega) \mathcal{Y}_{[K_N]_{ij}}(\Omega_{ij}) \tag{8.13}$$

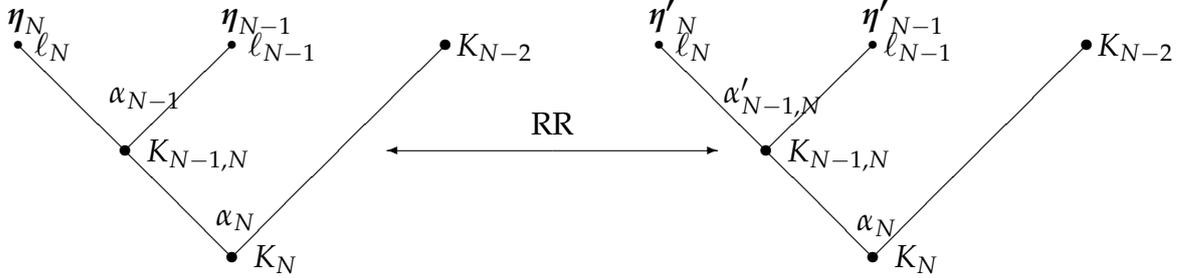
should be evaluated. In view of the transformation properties of the HH function it is clear that K_N, L_N define an invariant subspace under the rotation. A few methods to calculate the transformation matrix elements will be presented in the following sections.

8.4 The Raynal-Revai and the T-coefficients

The hyperspherical functions, as constructed in the previous section, depend on the choice of the Jacobi coordinates, Eq. (3.8), as well as on the “tree” diagram chosen for coupling the various single-Jacobi coordinate functions. I first consider the transformation of the hyperspherical harmonics which results from transforming between different sets of *two* Jacobi coordinates connected to the same node in the “tree” diagram. This transformation is effected by means of the Raynal-Revai coefficients presented in Subsection 8.4.1. In Subsection 8.4.2 I discuss the transformation between the two sets of hyperspherical functions corresponding to two different coupling schemes, i.e. two different “tree” diagrams, that is effected by means of the T-coefficients. It can be easily verified that the transformation of the HH induced by *any* transformation of the Jacobi coordinates can be expressed in terms of these two sets of coefficients.

At the end of this section we shall present a simple numerical algorithm due to V. Efros that allows for a simple calculation of the HH transformation coefficients.

Figure 8.1: A schematic representation of the Raynal-Revai coefficients, RR , between two sets of Jacobi coordinates coupled to the same node. Only the relevant part of the “tree” is plotted.



8.4.1 The Raynal-Revai coefficients

To enable the transformation between sets of hyperspherical functions obtained for the same physical system using different choices of Jacobi coordinates we use the Raynal-Revai coefficients. More specifically these coefficients are needed in order to apply transformations between different sets of *two* Jacobi coordinates connected to the same node in the “tree” diagram, as can be seen in Fig. 8.1.

As was pointed out at the bottom of Section 7.4.1 the $N + 1$ -particle hyperspherical angular momentum operator \hat{K}_N^2 is independent of the set of the angular coordinates Ω_N and of the structure of the “tree” or of the choice of the Jacobi coordinates. Let us consider the two Jacobi coordinates η_{N-1} and η_N . The hyperspherical functions constructed from these two Jacobi coordinates are uniquely specified by the quantum numbers ℓ_{N-1} , ℓ_N , $K_{N-1,N}$, $L_{N-1,N}$ and $M_{N-1,N}$. These hyperspherical functions can be expressed in terms of the hyperspherical functions depending on two different Jacobi coordinates η'_{N-1} and η'_N , that are related to the first two by means of a rotation by an angle γ ,

$$\begin{pmatrix} \eta'_{N-1} \\ \eta'_N \end{pmatrix} = \begin{pmatrix} \cos \gamma & -\sin \gamma \\ \sin \gamma & \cos \gamma \end{pmatrix} \begin{pmatrix} \eta_{N-1} \\ \eta_N \end{pmatrix} \quad (8.14)$$

using the Raynal-Revai coefficients as follows:

$$\begin{aligned} & |(\ell_{N-1}; \ell_N) K_{N-1,N} L_{N-1,N} M_{N-1,N} \rangle \\ = & \sum_{\ell'_{N-1} \ell'_N} \langle \ell_{N-1} \ell_N | \gamma | \ell'_{N-1} \ell'_N \rangle_{K_{N-1,N} L_{N-1,N}} |(\ell'_{N-1}; \ell'_N) K_{N-1,N} L_{N-1,N} M_{N-1,N} \rangle, \end{aligned} \quad (8.15)$$

here ℓ'_{N-1}, ℓ'_N are the values of the single-coordinate angular momentum operators corresponding to the rotated coordinates η'_{N-1} and η'_N . The sum in Eq. (8.15) is restricted by the relation $|\ell'_{N-1} - \ell'_N| \leq L_{N-1,N} \leq \ell'_{N-1} + \ell'_N \leq K_{N-1,N}$ such that $\ell'_{N-1} + \ell'_N$ has the same parity as $K_{N-1,N}$. Note that the quantum numbers $K_{N-1,N}$ and $L_{N-1,N}$ (as well as $M_{N-1,N}$) are common to both sets of hyperspherical functions, as was explained above.

The Raynal-Revai coefficients defined by Eq. (8.15) can be expressed in terms of the harmonic-oscillator Talmi-Moshinsky brackets [Raynal73]. Using this relation,

an analytic expression for the transformation brackets for hyperspherical functions was obtained by Raynal and Revai for three particles [Raynal70], [Raynal73]. A generalization to four particles was studied in Ref. [Jibuti77].

The Raynal-Revai coefficients can be calculated through the action of the infinitesimal generator of the Raynal-Revai rotation,

$$\hat{X}_{N-1,N} = i(\boldsymbol{\eta}_{N-1} \cdot \boldsymbol{\nabla}_N - \boldsymbol{\eta}_N \cdot \boldsymbol{\nabla}_{N-1}) , \quad (8.16)$$

on the hyperspherical harmonics. Analytic expressions for the matrix elements of the operator $\hat{X}_{N-1,N}$ in the hyperspherical basis were obtained by Raynal [Raynal73]. This operator can change the values of ℓ_{N-1} and ℓ_N by ± 1 and does not change the other quantum numbers $K = K_{N-1,N}$, $L = L_{N-1,N}$ and $M_{N-1,N}$. The expressions obtained by Raynal are (Eqs. (23) and (24) in Ref. [Raynal73])

$$\begin{aligned} & \langle \ell'_{N-1} \ell'_N | \hat{X}_{N-1,N} | \ell_{N-1} \ell_N \rangle_{K,L} = [n(n + \ell_{N-1} + \ell_N + 2)(L + \ell_{N-1} + \ell_N + 2)]^{\frac{1}{2}} \\ & \times \left[\frac{(L + \ell_{N-1} + \ell_N + 3)(\ell_{N-1} + \ell_N - L + 1)(\ell_{N-1} + \ell_N - L + 2)}{(2\ell_{N-1} + 1)(2\ell_N + 1)(2\ell'_{N-1} + 1)(2\ell'_N + 1)} \right]^{\frac{1}{2}} \end{aligned} \quad (8.17)$$

where $\ell'_{N-1} = \ell_{N-1} + 1$ and $\ell'_N = \ell_N + 1$, and

$$\begin{aligned} & \langle \ell'_{N-1} \ell'_N | \hat{X}_{N-1,N} | \ell_{N-1} \ell_N \rangle_{K,L} = \left[(n + \ell_N + \frac{1}{2})(n + \ell_{N-1} + \frac{3}{2}) \right]^{\frac{1}{2}} \\ & \times \left[\frac{(L + \ell_N - \ell_{N-1} - 1)(L + \ell_N - \ell_{N-1})(L + \ell_{N-1} - \ell_N + 1)(L + \ell_{N-1} - \ell_N + 2)}{(2\ell_{N-1} + 1)(2\ell_N + 1)(2\ell'_{N-1} + 1)(2\ell'_N + 1)} \right]^{\frac{1}{2}} \end{aligned} \quad (8.18)$$

where $\ell'_{N-1} = \ell_{N-1} + 1$ and $\ell'_N = \ell_N - 1$. The variable n is given by

$$n = \frac{K - \ell_{N-1} - \ell_N}{2} . \quad (8.19)$$

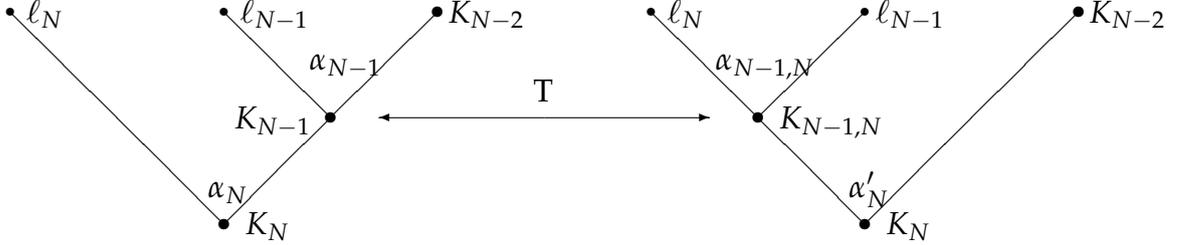
The other two non-zero matrix elements i.e., $\ell'_{N-1} = \ell_{N-1} - 1$, $\ell'_N = \ell_N - 1$ and $\ell'_{N-1} = \ell_{N-1} - 1$, $\ell'_N = \ell_N + 1$ have the same expressions as in Eqs. (8.17) and (8.18), respectively, but with opposite signs.

8.4.2 The hyperspherical recoupling coefficients - the T-coefficients

The hyperspherical recoupling coefficients are the recoupling coefficients that enable the expression of a hyperspherical function obtained by coupling of three subsystems in a particular order in terms of the set of hyperspherical functions describing the same composite system, obtained using a different coupling order.

For example consider the transformation from the “tree” diagram given in Fig. 7.2 to the “tree” diagram given in Fig. 7.3. This transformation is effected by means of the hyperspherical recoupling coefficients (of type F) introduced in Ref. [Kildyushov72]. The transformation is presented in Fig. 8.3 which is the figure of case F in Ref. [Kildyushov72]); Only the relevant parts of the two “trees” are

Figure 8.2: A schematic representation of the T-coefficient between the “tree” of Fig. 7.2 and the “tree” of Fig. 7.3. Only the relevant parts of the two “trees” are plotted. The two-headed arrow points to the two different intermediate quantum numbers.



plotted. This hyperspherical recoupling coefficients are known as the T-coefficients, where "T" stands for “tree” recoupling coefficients.

More specifically, the T-coefficients presented many years ago by Kil'dyushov [Kildyushov73] are the hyperspherical analogs of the celebrated angular momentum $6j$ symbols, and indeed they could as justly be called $6K$ symbols. Let us denote by $K_i, i = 1, 2, 3$ an harmonic polynomial over a coordinate space of dimension ν_i . We can couple three polynomials to create an harmonic polynomial of order K over $\nu_1 + \nu_2 + \nu_3$ dimensional space in, essentially, two different ways. We can couple K_1 and K_2 to obtain K_{12} and then couple K_{12} with K_3 , or couple K_1 and K_3 to obtain K_{13} and then couple K_{13} with K_2 . The T-coefficients, like the $6j$ coefficients, are the matrix elements of the transformation between these two sets of functions,

$$|((K_1; K_2)K_{12}; K_3)K \rangle = \sum_{K_{13}} T_{K_{12}K_{13}}^{K; K_1 K_2 K_3} |((K_1; K_3)K_{13}; K_2)K \rangle \quad (8.20)$$

We introduce the following definitions

$$\begin{aligned} \alpha_i &\equiv K_i + \frac{3}{2}\nu_i - 1 \\ n_{12} &\equiv \frac{K_{12} - K_1 - K_2}{2} \quad ; \quad n_{13} \equiv \frac{K_{13} - K_1 - K_3}{2} \\ n &\equiv \frac{K - K_1 - K_2 - K_3}{2} \end{aligned} \quad (8.21)$$

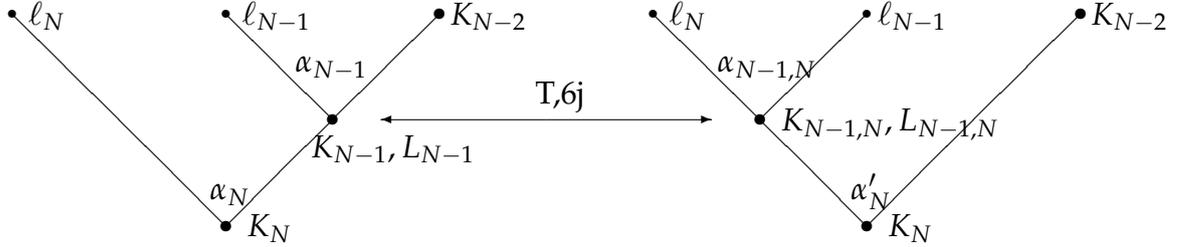
and follow Raynal derivation in Ref. [Raynal73b] to obtain

$$\begin{aligned} T_{K_{12}K_{13}}^{K; K_1 K_2 K_3} &= (-)^{n-n_{12}-n_{13}} B_n(n_{12}, \alpha_1, \alpha_2, \alpha_3) B_n(n_{13}, \alpha_1, \alpha_3, \alpha_2) \\ &{}_4F_3(n_{12} - n, n_{13} - n, -n - n_{12} - \alpha_1 - \alpha_2 - 1, -n - n_{13} - \alpha_1 - \alpha_3 - 1; \\ &-2n - \alpha_1 - \alpha_2 - \alpha_3 - 1, -n - \alpha_1, -n; 1) \end{aligned} \quad (8.22)$$

where

$$\begin{aligned} B_n(n_{12}, \alpha_1, \alpha_2, \alpha_3) &= \left[\frac{n!}{n_{12}!(n-n_{12})!} \frac{(2n_{12} + \alpha_1 + \alpha_2 + 1)\Gamma(n_{12} + \alpha_1 + \alpha_2 + 1)}{\Gamma(n + n_{12} + \alpha_1 + \alpha_2 + 2)\Gamma(n - n_{12} + \alpha_3 + 1)} \right]^{\frac{1}{2}} \\ &\left[\frac{\Gamma(2n + \alpha_1 + \alpha_2 + \alpha_3 + 2)\Gamma(n_{12} + \alpha_2 + 1)\Gamma(n + \alpha_1 + 1)}{\Gamma(n_{12} + \alpha_1 + 1)\Gamma(n + n_{12} + \alpha_1 + \alpha_2 + \alpha_3 + 2)} \right]^{\frac{1}{2}} \end{aligned} \quad (8.23)$$

Figure 8.3: A schematic representation of the transformation between the “tree” of Fig. 7.2 and the “tree” of Fig. 7.3. Only the relevant parts of the two “trees” are plotted. The two-headed arrow points to the two different intermediate quantum numbers.



and $B_n(n_{13}, \alpha_1, \alpha_3, \alpha_2)$ has the same expression as (8.23) with the appropriate substitutions. The function ${}_4F_3$ is the generalized hypergeometric function defined by the relation

$${}_4F_3(a_1, a_2, a_3, a_4; b_1, b_2, b_3; x) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k (a_3)_k (a_4)_k}{(b_1)_k (b_2)_k (b_3)_k} \frac{x^k}{k!} = \sum_{k=0}^{\infty} c_k x^k \quad (8.24)$$

where

$$c_k = \frac{(a_1 + k - 1)(a_2 + k - 1)(a_3 + k - 1)(a_4 + k - 1)}{(b_1 + k - 1)(b_2 + k - 1)(b_3 + k - 1)k} c_{k-1} \quad (8.25)$$

and $c_0 = 1$.

It should be noted that expression (8.22) is symmetric with respect to permutation of the indices 2 and 3. In addition, since some of the variables in the function ${}_4F_3$ are negative integers (see Eq. (8.22)) the sum in Eq. (8.24) reduces to a polynomial of the order of the lowest absolute value of these negative integers.

When working with a coupled angular momentum basis the T coefficients needs to be accompanied with the 6j coefficients to recoupled the angular momentum quantum numbers.

$$\begin{aligned} & |((K_1 L_1; K_2 L_2) K_{12} L_{12}; K_3 L_3) KL\rangle = \\ & = \sum_{K_{23} L_{23}} \sqrt{(2L_{12} + 1)(2L_{23} + 1)(-1)^{L_1 + L_2 + L_3 + L}} \begin{Bmatrix} L_1 & L_2 & L_{12} \\ L_3 & L & L_{23} \end{Bmatrix} T_{K_{12} K_{23}}^{K; K_2 K_1 K_3} \\ & \quad \times |(K_1 L_1; (K_2 L_2; K_3 L_3) K_{23} L_{23}) KL\rangle \end{aligned} \quad (8.26)$$

8.4.3 The Efros trick

Consider the orthogonal transformation $O(a \rightarrow b) \in O_N$ of the Jacobi coordinates from one coordinate set a to a different set b

$$\eta_k^b = \sum_{k'=1}^N O_{kk'}(a \rightarrow b) \eta_{k'}^a \quad (8.27)$$

Each set of Jacobi vectors defines a set hyperspherical angles $\Omega_{a/b}$, and a corresponding set of HH states $|[K]_{a/b}\rangle$. By this notation we mean that $\langle \Omega || [K]_{a/b} \rangle =$

$\mathcal{Y}_{[K]}(\Omega_{a/b})$. As $[\hat{K}_N, O_N] = [\hat{L}_N, O_N] = 0$ the quantum numbers K_N, L_N define an invariant subspace under the rotations $O \in O_N$, in particular for each vector $|[K_N]_a\rangle$ in this subspace we can write

$$|[K_N]_b\rangle = O(a \rightarrow b)|[K_N]_a\rangle = \sum_{[K'_N]_a; K'_N=K_N, L'_N=L_N} \langle [K'_N]_a | [K_N]_b \rangle |[K'_N]_a\rangle \quad (8.28)$$

This is an algebraic equation in a N_{KL} , and the $N_{KL} \times N_{KL}$ overlap matrix is given by

$$\langle [K_N]_a | [K'_N]_b \rangle = \int d\Omega_a \mathcal{Y}_{[K_N]}^*(\Omega_a) \mathcal{Y}_{[K'_N]}(\Omega_b) \quad (8.29)$$

Equation (8.28) holds for any point on the hypersphere

$$\mathcal{Y}_{[K_N]}(\Omega_b) = \sum_{[K'_N]_a; K'_N=K_N, L'_N=L_N} \langle [K'_N]_a | [K_N]_b \rangle \mathcal{Y}_{[K'_N]}(\Omega_a) \quad (8.30)$$

choosing a set of N_{KL} arbitrary points we get a set of $N_{KL} \times N_{KL}$ which we can solve for the transformation coefficients.

$$\langle [K'_N]_a | [K_N]_b \rangle = \sum_{p=1}^{N_{KL}} U^{-1}(a)_{[K'_N]_p} U(b)_p [K'_N] \quad (8.31)$$

where

$$\begin{aligned} U(a)_p [K'_N] &= \mathcal{Y}_{[K_N]}(\Omega_a^p) \\ U(b)_p [K'_N] &= \mathcal{Y}_{[K_N]}(\Omega_b^p) \end{aligned} \quad (8.32)$$

The condition for this procedure to succeed is $\det(U(a)) > 0$.

8.5 Symmetrization of the Hyperspherical Harmonics

The (anti)symmetrization of the HH basis is a difficult problem. Over the years many strategies were suggested to address this issue. In the following we shall briefly discuss different approaches to the problem.

- A. Apply the anti-symmetrization to the HH basis (including internal degrees of freedom)

$$\mathcal{A} = \frac{1}{\sqrt{A!}} \sum_{p \in S_A} \text{sign}(p) \hat{p}$$

The cost is $A!$ operations. The resulting basis states are (i) non orthogonal and (ii) over complete.

- B. Generate HH states from HO Slater determinant.

$$\det(HO) = e^{-\frac{1}{2}\rho^2} \rho^K \hat{A} \left(\mathcal{Y}(\Omega) \mathcal{X}(s_i, t_i) \right)$$

This works very well for the lowest K in a closed shell, for larger K or open shells the factorization of the CM and the separation between hyperspherical and hyperradial excitations becomes more involved. This is probably the only viable way to extend the HH expansion to large systems.

C. Using the Casimir eigenvalues and the relation

$$\hat{C}_2(n) = \hat{C}_2(n-1) + \sum_{i=1}^{n-1} (i, n) \quad (8.33)$$

a recursive symmetrization procedure can be formulated. Assume that $\{|\Phi_A(1\dots n-1)\rangle\}$ is a set of antisymmetric basis states and $\{|\phi_a(n)\rangle\}$ are “single particle” states, such that $|\Phi_A\phi_a\rangle$ form an invariant subspace. Utilizing the operator relation

$$(i, n) = (i, n-1)(n, n-1)(i, n-1) \quad (8.34)$$

We see that

$$\begin{aligned} \langle \Phi_A\phi_a | \hat{C}_2(n) | \Phi_B\phi_b \rangle &= \langle \Phi_A\phi_a | \hat{C}_2(n-1) + \sum_{i=1}^{n-1} (i, n) | \Phi_B\phi_b \rangle \\ &= -\delta_{AB}\delta_{ab} \frac{(n-1)(n-2)}{2} + \langle \Phi_A\phi_a | \sum_{i=1}^{n-1} (i, n-1)(n, n-1)(i, n-1) | \Phi_B\phi_b \rangle \\ &= -\delta_{AB}\delta_{ab} \frac{(n-1)(n-2)}{2} + (n-1) \langle \Phi_A\phi_a | (n, n-1) | \Phi_B\phi_b \rangle \end{aligned} \quad (8.35)$$

Thus at the cost of evaluating the matrix elements of the operator $(n, n-1)$ and diagonalizing the matrix \hat{C}_2 we can construct antisymmetric states. This procedure can be generalized to any S_n irrep.

D. Use the group of kinematic rotations O_{A-1} , $\eta_i \longrightarrow \eta'_i = g\eta_i$, the HH symmetrization can be carried out in two steps

$$HH \longrightarrow O_{(A-1)}$$

and

$$O_{(A-1)} \longrightarrow S_A$$

In short we use the following group-subgroup chain

$$\begin{array}{ccccccc} O_{3(A-1)} & \subset & O_3 & \otimes & O_{(A-1)} & \subset & O_3 \otimes S_A \\ & & K & & LM & \Lambda_{A-1} & LM & Y_A \end{array} \quad (8.36)$$

For both steps the method is based on the eigenvalues of the Casimir operator. This method is much more efficient but also much more complicated than any of the others.

E. The Hamiltonian commutes with S_A therefore we can “ignore the whole issue”, built the Hamiltonian matrix diagonalize it and select the physical states at the end. This procedure might be very expensive for larger system but it is extremely simple. A variant of this procedure is to introduce a generalized Hamiltonian

$$\tilde{H} = H + \lambda \hat{C}_2 \quad (8.37)$$

For λ large and positive the Casimir operator pushes the antisymmetric states to the bottom of the spectrum, negative values push the symmetric states.

K	HH $\rightarrow S_A$	HH $\rightarrow O_{(A-1)}$	$O_{(A-1)} \rightarrow S_A$	Ratio
2	198	56	108	1.21
4	11308	728	1528	5.01
6	516647	8771	16511	20.44
8	10^7	84700	127544	47.12

Table 8.1: The 6-body system – A comparison between direct symmetrization and symmetrization through the kinematical group O_{A-1} .

8.6 Convergence Accelaration

Convergence - Statement of the problem

- For potentials with Coulomb type singularities the HH expansion of Ψ converge as K_{max}^{-2} and energy as K_{max}^{-4}
- For Gaussian potentials Ψ converge as $e^{-cK_{max}}$.
- Actually. The problem is not the only slow convergence rate but rather the fast growth in the number of HH states.

Different Strategies were used to address this major problem.

8.6.1 Correlations

Correlations in the wave-function where used by few groups (CHH, PHH, CFHHM ...)

$$\Psi(\rho, \Omega) = \prod_{ij} F(r_{ij}) \sum_{K \leq K_{max}} R_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega)$$

The introduction of the correlation function came as a solution to the hard core problem in the nuclear force and in order to reproduce the cusp in the wave function for Coulomb problems.

8.6.2 Basis reduction

Adressing the problem of the fast growth in the number of basis states Fabre de-la Rippe suggested to use only a small subset of the HH basis, solving a Faddeev like equation. For the bosonic case the resulting equations take the form

$$\Psi = \sum \Psi_{ij} \quad (8.38)$$

where

$$\Psi_{ij} = \sum_{[K]} R_{[K]}^{(2)}(\rho) \mathcal{Y}_{[K]}(\Omega_{ij}) \quad (8.39)$$

and

$$\left[-\frac{1}{2}\Delta - E \right] \Psi_{ij} = -V_{ij}\Psi \quad (8.40)$$

The wave function is then approximated by taking all quantum number to be zero but K_N , this is call the potential basis (PB) approximation. For central potentials this method was quite succesful. Its can also be generalized to Fermionic systems and was applied for $A \geq 10$ systems. For larger system this method is equivalent

to the configuration interaction method (CI) which doesn't fulfill the linked cluster theorem and therefore cannot be a very good approximation to the many body wave function.

A simpler basis reduction method was suggested by other groups restricting the partial angular momenta to small values, or generalizing the PB approximation. For example in a bose-system this generalized expansion may take the following form

$$\Psi(\rho, \Omega) = \sum_{ij} \sum_{[K]} R_{[K]}^{(2)}(\rho) \mathcal{Y}_{[K]}(\Omega_{ij}) + \sum_{ij,kl} \sum_{[K]} R_{[K]}^{(2,2)}(\rho) \mathcal{Y}_{[K]}(\Omega_{ij,kl}) + \dots$$

8.6.3 Effective interaction

The basic principle beyond the effective interaction approach is that one can accelerate the convergence rate by modifying the Hamiltonian while increasing the size of our basis expansion, i.e.

$$V^{(2)} \longrightarrow V_{eff}^{(2)}$$

$$V^{(3)} \longrightarrow V_{eff}^{(3)}$$

There are different ways to achieve this goal. The Bloch-Horowitz transformation for one or the Lee-Suzuki. In the Lee Suzuki approach one can construct an energy independent effective interaction. This method was introduced to the few-body community through the NCSM method by Navratil and Barrett.

In the Effective Interaction Hyperspherical Harmonics (EIHH) The effective 2-body potential $V_{eff}^{(2)}$ is derived from a "2-body" Hamiltonian

$$H_2(\rho) = \frac{1}{2m} \frac{\hat{K}^2}{\rho^2} + V(\vec{r} = \sqrt{2}\rho \sin \alpha_N \cdot \hat{\eta}_N), \quad (8.41)$$

The effective Hamiltonian is constructed through the Lee-Suzuki similarity transformation

$$H_{2\,eff}(\rho) = U^\dagger(\rho) H_2(\rho) U(\rho) \quad ; \quad U = \frac{1 + \omega}{\sqrt{P(1 + \omega^\dagger \omega)P}} \quad (8.42)$$

The operator $\omega = Q\omega P$ is given by

$$\langle q|i \rangle = \sum_{\alpha} \langle q|\omega|p \rangle \langle p|i \rangle \quad ; \quad H_2|i \rangle = E_i|i \rangle \quad (8.43)$$

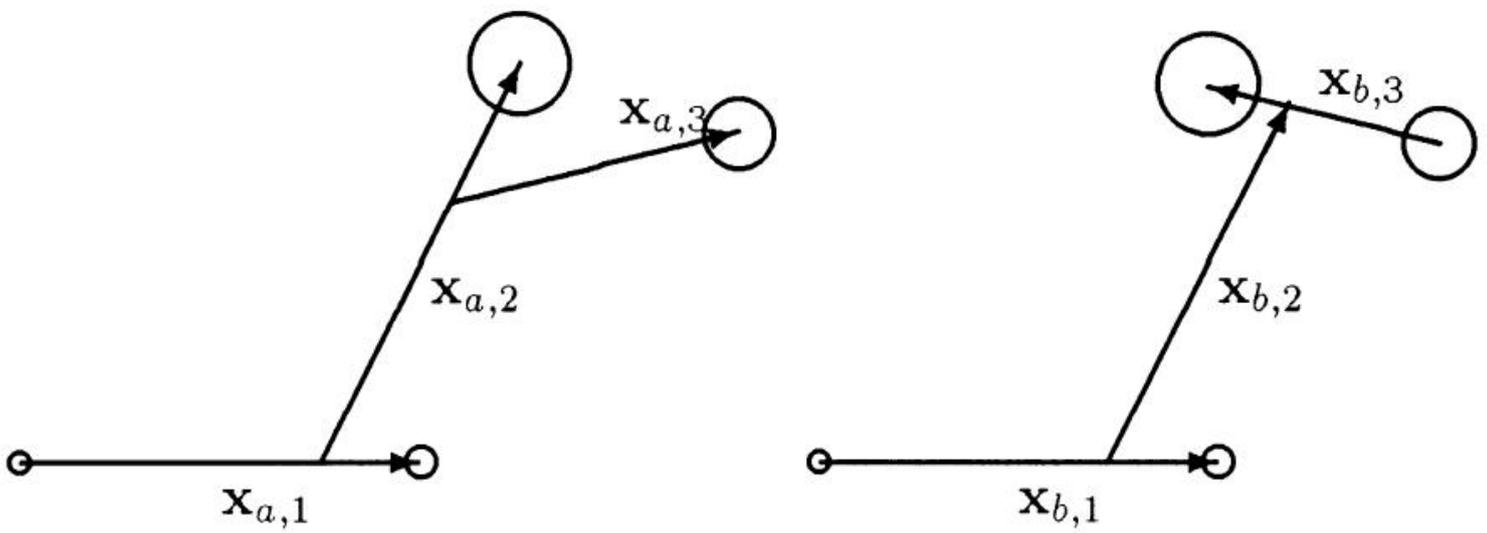
Finally the **effective interaction** is given by

$$V_{2\,eff}(\rho) = H_{2\,eff}(\rho) - \frac{1}{2m} \frac{\hat{K}^2}{\rho^2} \quad (8.44)$$

■ **Example 8.1** 4-body ground-state - Bare vs Effective ■

K_{max}	AV18		AV18+UIX	
	E_b	$\langle r^2 \rangle^{\frac{1}{2}}$	E_b	$\langle r^2 \rangle^{\frac{1}{2}}$
6	25.312	1.506	26.23	1.456
8	25.000	1.509	27.63	1.428
10	24.443	1.520	27.861	1.428
12	24.492	1.518	28.261	1.427
14	24.350	1.518	28.324	1.428
16	24.315	1.518	28.397	1.430
18	24.273	1.518	28.396	1.431
20	24.268	1.518	28.418	1.432
FY [Nogga]	24.25		28.50	
FY [Lazauskas]	24.22	1.516		
HH [Viviani]	24.21	1.512	28.46	1.428
GFMC [Wiringa]			28.34	1.44

Table 8.2: The 4-body ground-state – Convergence of the EIHH method for ${}^4\text{He}$ binding energy E_b [MeV] and root mean square matter radius $\langle r^2 \rangle^{\frac{1}{2}}$ [fm] with AV18 and AV18+UIX potentials.



9. Monte Carlo methods

9.1 References

Here we follow the following sources:

- [HLK17] Morten Hjorth-Jensen, Maria Paola Lombardo, and Ubirajara van Kolck. *An Advanced Course in Computational Nuclear Physics*. Springer Cham, 2017. DOI: <https://doi.org/10.1007/978-3-319-53336-0>.
- [KFS96] Ioan Kosztin, Byron Faber, and Klaus Schulten. "Introduction to the diffusion Monte Carlo method". In: *American Journal of Physics* 64.5 (1996), pages 633–644. DOI: 10.1119/1.18168. eprint: <https://doi.org/10.1119/1.18168>. URL: <https://doi.org/10.1119/1.18168>.

9.2 Evaluating expectation values

Suppose we have solved the Schroedinger equation

$$H\Psi_0(X) = E_0\Psi_0(X) \quad (9.1)$$

where X stand for all the coordiantes and the internal degree of freedom and we want to evaluate the observable

$$\langle O \rangle \equiv \langle \Psi_0 | O | \Psi_0 \rangle = \frac{\int dXdX' \langle \Psi_0 | X \rangle \langle X | O | X' \rangle \langle X' | \Psi_0 \rangle}{\int dX |\langle X | \Psi_0 \rangle|^2} . \quad (9.2)$$

Here the integration stands for both integration over the coordinates and summation over internal degrees of freedom.

In order to evaluate such integrals numerically we can try to create a grid of points in each direction, the number of sampling for reaching a given accuracy would scale as $(L/\Delta)^D$, with L the typicall size of the system, Δ the required

spatial step, and D the dimension. It follows that the number of integration points grows exponentially with the dimension of the system. Based on the central limit theorem, the Monte Carlo techniques allows for an integration techniques that has a way better scaling than that.

We start by rewriting the expectation value as

$$\langle O \rangle = \frac{1}{\int dX |\langle X | \Psi_0 \rangle|^2} \int dX |\langle X | \Psi_0 \rangle|^2 \frac{\langle X | O \Psi_0 \rangle}{\langle X | \Psi_0 \rangle}. \quad (9.3)$$

For the moment we assume that this integral is well behaved. We note that in our understanding of quantum mechanics, the term

$$P(X) = \frac{|\langle X | \Psi_0 \rangle|^2}{\int dX |\langle X | \Psi_0 \rangle|^2}, \quad (9.4)$$

is just the probability density function (PDF) of finding the system in the state $|X\rangle$. Thus,

$$\langle O \rangle = \int dX P(X) \frac{\langle X | O \Psi_0 \rangle}{\langle X | \Psi_0 \rangle}. \quad (9.5)$$

is the average of the function $O(X) \equiv \langle X | O \Psi_0 \rangle / \langle X | \Psi_0 \rangle$, which we call *the local operator*, weighted with the probability $P(X)$. The integral in Eq. (9.5) has a clear physical interpretation. In an experimental measurement of $\langle O \rangle$ we would observe a sampling of $P(X)$. Sampling N points X_k according to the distribution $P(X)$ the integral Eq. (9.5) can be approximated by

$$\langle O \rangle \approx \frac{1}{N} \sum_{k=1}^N O(X_k). \quad (9.6)$$

The random aspect of the sampling process is the reason this family of algorithms, used not only in physics, is generally known as Monte Carlo techniques.

9.3 The central limit theorem

To evaluate the accuracy of this sampling process we use the Central Limit Theorem. Given a distribution $P(X)$ over a suitable event space X , and an arbitrary function $F(X)$, we can define the sum

$$S_N(F) = \frac{1}{N} \sum_{k=1}^N F(X_k), \quad (9.7)$$

where the events $X_k \sim P(X)$ are assumed to be independent random variables. The notation $X_k \sim P(X)$ implies that $P(X)$ is the distribution of X . Being a sum of random values $S_N(F)$ is a stochastic variable, which in turn has its own distribution $P(S_N)$. According to the Central Limit Theorem for large N the PDF $P(S_N)$ will converge into normal distribution,

$$\lim_{N \rightarrow \infty} P(S_N) = \frac{1}{\sqrt{2\pi\sigma_N^2(F)}} \exp\left(-\frac{1}{2} \frac{(S_N - \langle F \rangle)^2}{\sigma_N^2(F)}\right). \quad (9.8)$$

Here

$$\sigma_N^2(F) = \frac{1}{N} \left(\langle F^2 \rangle - \langle F \rangle^2 \right) = \frac{1}{N} \sigma_F^2, \quad (9.9)$$

is the variance of the normal distribution, while

$$\sigma_F^2 = \langle F^2 \rangle - \langle F \rangle^2 \quad (9.10)$$

is the variance of F , and

$$\langle F^n \rangle = \int dX P(X) F^n(x), \quad (9.11)$$

is the n 'th moment of F . The case $n = 1$ corresponds to $\langle F \rangle$, the mean value of F , which we estimate using the sum $S_N(F)$. The variance of F is evaluated using the unbiased estimate $\sigma_F^2 \approx \frac{N}{N-1} (S_N(F^2) - S_N^2(F))$.

The importance of the Central Limit Theorem stems from its implications to the accuracy of our estimate. In view of Eq. (9.8) $S_N(F) \rightarrow \langle F \rangle \pm \sigma_N(F)$ as $N \rightarrow \infty$. And since $\sigma_N(F) \propto 1/\sqrt{N}$, it follows that we need $\mathcal{O}(N^2)$ sampling points to reach a given accuracy in our integral. As a consequence, we understand that in general Monte Carlo techniques are more efficient than “grid” integration methods already for the 3-dimensional case.

9.4 The Metropolis–Hastings algorithm

The crux of the matter is the random sampling of the distribution $P(X)$ in a computer simulation. The (quasi) random series produced by the computer form a uniform distribution. In order to create a 1-dimensional distribution $P_{1D}(X)$ we need to invert the cumulative distribution function of $P_{1D}(X)$. This procedure can work out in 1-dimension but not in general. In the following we present the Metropolis–Hastings algorithm which allow us to sample from an arbitray (multi dimensional) distribution.

To elucidate the basic idea of the Metropolis–Hastings algorithm we can think of a sample of N points X_0 which we choose in our Hilbert space according to some PDF $P_0(X_0)$. In order make this a sample distributed according to our desired PDF $P(X)$ we need to find a *transition matrix* $\tilde{T}(X \leftarrow X_0)$ such that the sample X obtained via the action $\tilde{T}(X \leftarrow X_0)$ has the desired properties. Of course if we knew how to construct such a transition matrix there would be no problem. The solution suggested by the Metropolis–Hastings algorithm is to construct \tilde{T} as a sequence of well defined transformations $T_k(X_{k+1} \leftarrow X_k)$ that in the limit will yield the desired result.

Taking a more formal look at the process, we consider at first a configuration X_0 sampled from the PDF $P_0(X_0)$, and the transition matrix $T_0(X_1 \leftarrow X_0)$. The probability density of finding the system in configuration X_1 is then

$$P_1(X_1) = \int dX_0 T_0(X_1 \leftarrow X_0) P_0(X_0). \quad (9.12)$$

Or in the short hand notation

$$P_1(X_1) = \hat{T}_0 P_0(X_0), \quad (9.13)$$

with \hat{T}_0 the integral operator associated with $T_0(X_1 \leftarrow X_0)$. Following this example it is clear that the PDF obtained after k steps is given by

$$P_k(X_k) = \hat{T}_{k-1}P_{k-1}(X_{k-1}) = \hat{T}_{k-1} \dots \hat{T}_1 \hat{T}_0 P_0(X_0). \quad (9.14)$$

The sequence of stochastic variables $\{X_0, X_1, \dots, X_k\}$ generated by this procedure is called a *Markov chain*. It is also customary to refer to a point X_0 moving through a series of transitions $\{X_0, X_1, \dots, X_k\}$ as a walker, as the Markov chain produce an arbitrary walk in X .

Now let us make a bold move taking the same transition operators for all steps. In this case

$$P_k(X_k) = \hat{T}P_{k-1}(X_{k-1}) = \hat{T} \dots \hat{T} \hat{T}P_0(X_0) = \hat{T}^k P_0(X_0). \quad (9.15)$$

One might wonder now if this sequence is convergent, i.e. if a limiting probability density $P_\infty(X)$ exists. In the following we will avoid this question and simply assume that for the family of transition operators we consider the sequence converge. That is

$$\lim_{k \rightarrow \infty} \hat{T}P_{k-1}(X_{k-1}) = \lim_{k \rightarrow \infty} P_k(X_k), \quad (9.16)$$

or

$$\hat{T}P_\infty(X) = P_\infty(X). \quad (9.17)$$

We may conclude now that $P_\infty(X)$ is an eigenvector of \hat{T} with eigenvalue 1. This latter result follow from our demand that $\hat{T}P_\infty(X)$ is a normalized PDF.

As it turns out, the properties of such stationary Markov chain can be utilized to sample an arbitrary PDF $P(X)$. Given a target distribution $P_\infty(X)$ it is not too difficult to construct a transition operators \hat{T} such that Eq. (9.17) holds. Moreover, starting with an arbitrary initial PDF a repeated application of \hat{T} will eventually generate the distribution $P_\infty(X)$.

The trick is to write \hat{T} as a product of a simple transition matrix $S(X' \leftarrow X)$, that creates a step in the X space, and an unknown factor $A(X' \leftarrow X)$ that we call the “acceptance probability”

$$\hat{T} = \hat{A}\hat{S}. \quad (9.18)$$

For example, assuming that X is a vector in a D -dimensional coordinate space we can take $S(X' \leftarrow X)$ to be a uniform distribution within a box of size Δ ,

$$S(X' \leftarrow X) = \begin{cases} \frac{1}{\Delta^D} & \text{if } |X'_i - X_i| \leq \frac{\Delta}{2} \text{ for all } i = 1, \dots, D \\ 0 & \text{otherwise} \end{cases} \quad (9.19)$$

For a stationary distribution we expect that anywhere the probability density will not change due to the application of the transition operator. Transitions away from X must be balanced by transitions into X :

$$\int dX' T(X' \leftarrow X) P(X) = \int dX' T(X \leftarrow X') P(X'). \quad (9.20)$$

The equilibrium condition can be replaced with the more stringent *detailed balance* condition:

$$T(X' \leftarrow X) P(X) = T(X \leftarrow X') P(X') \quad (9.21)$$

which we can use as a condition on the acceptance probability,

$$\frac{A(X' \leftarrow X)}{A(X \leftarrow X')} = \frac{P(X') S(X \leftarrow X')}{P(X) S(X' \leftarrow X)}. \quad (9.22)$$

We can rewrite this condition as

$$A(X' \leftarrow X) = \min \left(\frac{P(X') S(X \leftarrow X')}{P(X) S(X' \leftarrow X)}, 1 \right). \quad (9.23)$$

This expression is called the *acceptance ratio*. It holds the probability by which we decide whether to accept the new configuration X' or to remain in the old one X .

We note that for a symmetric transition \hat{S} the acceptance ratio Eq. (9.23) can be further simplified

$$A(X' \leftarrow X) = \min \left(\frac{P(X')}{P(X)}, 1 \right). \quad (9.24)$$

The Metropolis–Hastings will converge to the right distribution if (1) every allowed state can be reached from any other by a finite number of steps, and (2) the cycle condition is fulfilled.

Definition 9.4.1 — Kolmogorov Cycle Condition. We say that the cycle condition is satisfied if given a cycle of states $X_0, X_1, \dots, X_n = X_0$ with $T(X_{i+1} \leftarrow X_i) > 0$ for $i = 0, \dots, n-1$, we have

$$\prod_{i=0}^{n-1} T(X_{i+1} \leftarrow X_i) = \prod_{i=0}^{n-1} T(X_i \leftarrow X_{i+1}). \quad (9.25)$$

9.4.1 The algorithm

At this point we can formulate the application of the Metropolis–Hastings algorithm for a few-body problem. For simplicity we ignore internal degrees of freedom, denote $\mathbf{R} = (\mathbf{R}_1, \dots, \mathbf{R}_A)$, and assume that the potential and the trial wave-function depend only on \mathbf{R} , $V = V(\mathbf{R})$, and $\Psi_T = \Psi_T(\mathbf{R})$.

1. Start from an arbitrary configuration of the system \mathbf{R} .
2. Utilizing the S operator generate a new position \mathbf{R}' . If $i = 1, \dots, A$ denotes the particle index and $a = x, y, z$ denotes the spatial direction then

$$S(\mathbf{R}' \leftarrow \mathbf{R}) = \begin{cases} \frac{1}{\Delta} & \text{if } |R'_{i,a} - R_{i,a}| \leq \frac{\Delta}{2} \\ 0 & \text{otherwise} \end{cases} \quad (9.26)$$

Implemented in a computer code we just write

$$R'_{i,a} = R_{i,a} + (\text{rand}() - 0.5)\Delta. \quad (9.27)$$

Here $\text{rand}()$ is a function that generates a random number with a uniform distribution in the range $[0, 1)$.

3. Evaluate the acceptance ratio

$$A(\mathbf{R}' \leftarrow \mathbf{R}) = \min \left(\frac{|\Psi_T(\mathbf{R}')|^2}{|\Psi_T(\mathbf{R})|^2}, 1 \right) \quad (9.28)$$

4. Now we select a new random number $\eta = \text{rand}()$. If $\eta \leq A$ we accept the new configuration, i.e. setting $\mathbf{R} = \mathbf{R}'$. Otherwise we reject it keeping the old configuration \mathbf{R} .
5. Having decided on the configuration we sum over the local energy

$$\begin{aligned}\Sigma_E &\leftarrow \Sigma_E + \frac{H\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} \\ \Sigma_{E^2} &\leftarrow \Sigma_{E^2} + \left(\frac{H\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})}\right)^2\end{aligned}\quad (9.29)$$

6. The process described in points 2-5 is now to be repeated. We first have to make some warm-up steps until the distribution stabilizes.
7. After the warm-up steps we repeat points 2-5, this time we actually start to accumulate the sums Σ_E, Σ_{E^2} . If we have made N_{steps} actual steps then our estimate for the energy is given by $\langle E \rangle \pm \Delta E$, where

$$\begin{aligned}\langle E \rangle &= \frac{1}{N_{\text{steps}}} \Sigma_E \\ \Delta E &= \sqrt{\frac{1}{N_{\text{steps}} - 1} \left(\frac{\Sigma_{E^2}}{N_{\text{steps}}} - \langle E \rangle^2 \right)}.\end{aligned}\quad (9.30)$$

The same procedure may be used for evaluating any integral,

$$\int dX F(X) = \int dX P(X) \frac{F(X)}{P(X)}.\quad (9.31)$$

9.4.2 Autocorrelations

Earlier we have discussed the Central Limit Theorem. The main assumption underlying this analysis was that the series X_1, \dots, X_N is a set of independent random variables. By construction, this requirement is not fulfilled for a Markov chain. On the other hand we expect that in a Markov chain the correlation between steps will diminish with the distance between them.

Consider the integral

$$I = \int dX P(X) F(X) \approx \frac{1}{N} \sum_{i=1}^N F(X_i),\quad (9.32)$$

with the points X_i chosen randomly as we discussed above. Repeating this evaluation of I with different sets of points we can discuss the average value of the integral $\langle I \rangle$ and its variance $(\Delta I)^2$,

$$\begin{aligned}\langle I \rangle &= \frac{1}{N} \sum_{i=1}^N \langle F(X_i) \rangle = \langle F \rangle \\ (\Delta I)^2 &= \frac{1}{N^2} \sum_{i,j=1}^N \langle F(X_i) F(X_j) \rangle - \langle F \rangle^2.\end{aligned}\quad (9.33)$$

For a stationary Markov chain the expectation value $\langle F(X_i)F(X_j) \rangle$ depends only on the distance $\lambda = i - j$, i.e. the number of steps between event i and event j . To measure the correlation between steps we define the *autocorrelation coefficient*

$$C_\lambda(F) = \frac{\langle F(X_i)F(X_{i+\lambda}) \rangle - \langle F \rangle^2}{\langle F^2 \rangle - \langle F \rangle^2}. \quad (9.34)$$

The coefficient is normalized so that $C_0(F) = 1$. Now

$$\langle F(X_i)F(X_{i+\lambda}) \rangle = C_\lambda(F)\sigma_F^2 + \langle F \rangle^2, \quad (9.35)$$

and thus

$$\begin{aligned} (\Delta I)^2 &= \frac{1}{N^2} \sum_{i,j=1}^N \langle F(X_i)F(X_j) \rangle - \langle F \rangle^2 \\ &= \frac{1}{N} \sigma_F^2 \sum_{\lambda=1}^N C_\lambda(F) + \langle F \rangle^2 - \langle F \rangle^2 = \frac{1}{N} \sigma_F^2 \sum_{\lambda=1}^N C_\lambda(F). \end{aligned} \quad (9.36)$$

The autocorrelations reduce the efficiency of our sampling process. Usually the autocorrelation coefficient $C_\lambda(F)$ has exponential decay $C_\lambda(F) \sim \exp(-\lambda/\bar{\lambda})$. The sum in Eq. (9.36) can thus be approximated as

$$\sum_{\lambda=1}^N C_\lambda(F) \sim \int_0^\infty d\lambda \exp(-\lambda/\bar{\lambda}) = \bar{\lambda}, \quad (9.37)$$

and therefore

$$\Delta I \approx \sqrt{\frac{1}{N-1} \sigma_F^2 \bar{\lambda}}. \quad (9.38)$$

This result has a simple interpretation: when we make N steps in our markov chain, we generate only $N/\bar{\lambda}$ independent samples of the variables X .

To minimize the autocorrelation the step width Δ is chosen so that the acceptance fraction is about 30%-40%.

Once $\bar{\lambda}$ has been evaluated we can arrange the calculation to get a more realistic error estimate. The idea is to divide the points into blocks of size $N_b \geq \bar{\lambda}$, and then use the block average quantities

$$F_b = \frac{1}{N_b} \sum_{i \in b} F(X_i) \quad (9.39)$$

to estimate the standard deviation of I .

9.5 Variational Monte Carlo

Given a trial wave function Ψ_T we can use the Metropolis–Hastings algorithm to estimate the ground state energy (E_0)

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0. \quad (9.40)$$

In general, the wave-function will depend on a set of variational parameters $\alpha = \{\alpha_1, \alpha_2, \dots\}$. In that case we can improve our estimate of E_0 and of the wave-function by demanding

$$\frac{\delta E_T(\alpha)}{\delta \alpha_k} = 0 \quad (9.41)$$

for all the variational parameters. The solution of multi-dimensional minimization problem is not that simple but there are various techniques to achieve this goal. Discussing these techniques is beyond the scope of these lectures.

9.6 Diffusion Monte Carlo

Variational Monte Carlo can take only as far as we can guess the real form of the wave-function. To go further we introduce imaginary time propagation.

Recalling the real time Schroedinger equation

$$-i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle, \quad (9.42)$$

we introduce the *imaginary time* $\tau = it/\hbar$, having units of inverse energy, and write

$$- \frac{\partial}{\partial \tau} |\Psi(\tau)\rangle = H |\Psi(\tau)\rangle. \quad (9.43)$$

The formal solution of this equation is

$$|\Psi(\tau)\rangle = e^{-H\tau} |\Psi(0)\rangle. \quad (9.44)$$

The crux of the method lays with the observation that the imaginary time propagation of any trial wave function Ψ_T is proportional to the ground state Ψ_0 given that τ is long enough. To see that we write

$$|\Psi_T\rangle = \sum_n c_n |\Phi_n\rangle \quad (9.45)$$

with Φ_n the eigenfunctions of H , $H|\Phi_n\rangle = E_n|\Phi_n\rangle$. Now

$$\begin{aligned} e^{-H\tau} |\Psi_T\rangle &= \sum_n c_n e^{-E_n\tau} |\Phi_n\rangle \\ &= e^{-E_0\tau} \left(c_0 |\Phi_0\rangle + \sum_{n>1} c_n e^{-(E_n-E_0)\tau} |\Phi_n\rangle \right), \end{aligned} \quad (9.46)$$

and if the ground state is not degenerated, then $(E_n - E_0) > 0$, and

$$|\Psi(\tau)\rangle = e^{-H\tau} |\Psi_T\rangle \xrightarrow{\tau \rightarrow \infty} c_0 e^{-E_0\tau} |\Phi_0\rangle. \quad (9.47)$$

The imaginary time propagator selects, or projects, the trial function on the ground state.

In practice we introduce an energy $E_R \approx E_0$ as an estimate of the ground state energy. Now, since

$$e^{-(H-E_R)\tau} |\Psi_T\rangle \approx e^{-(E_0-E_R)\tau} c_0 |\Phi_0\rangle, \quad (9.48)$$

we may conclude that

- For $E_0 > E_R$ the amplitude $|\Psi(\tau)\rangle$ declines.
- For $E_0 < E_R$ the amplitude $|\Psi(\tau)\rangle$ grows.
- For $E_0 = E_R$ the amplitude $|\Psi(\tau)\rangle$ is stable.

9.6.1 Path integral formalism

In the following we will limit our discussion to (a) bosonic systems where the ground state wave function is positive definite, and (b) local interactions. In this case the propagator is easily expressed in coordinate space.

Formally

$$\Psi(\mathbf{R}, \tau) = \int d\mathbf{R}' \langle \mathbf{R} | e^{-(H-E_R)\tau} | \mathbf{R}' \rangle \Psi_T(\mathbf{R}') \quad (9.49)$$

with

$$G(\mathbf{R}, \mathbf{R}'; \tau) = \langle \mathbf{R} | e^{-(H-E_R)\tau} | \mathbf{R}' \rangle, \quad (9.50)$$

the imaginary time propagator. To evaluate the propagator we break the time evolution into small time steps. For example, splitting τ into two intervals we can write

$$\begin{aligned} \langle \mathbf{R} | e^{-(H-E_R)\tau} | \mathbf{R}' \rangle &= \langle \mathbf{R} | e^{-(H-E_R)\frac{\tau}{2}} e^{-(H-E_R)\frac{\tau}{2}} | \mathbf{R}' \rangle \\ &= \int d\mathbf{R}'' \langle \mathbf{R} | e^{-(H-E_R)\frac{\tau}{2}} | \mathbf{R}'' \rangle \langle \mathbf{R}'' | e^{-(H-E_R)\frac{\tau}{2}} | \mathbf{R}' \rangle \end{aligned} \quad (9.51)$$

In general we can split τ into M steps,

$$\begin{aligned} \langle \mathbf{R} | e^{-(H-E_R)\tau} | \mathbf{R}' \rangle &= \int d\mathbf{R}^1 \dots d\mathbf{R}^{M-1} \langle \mathbf{R} | e^{-(H-E_R)\frac{\tau}{M}} | \mathbf{R}^{M-1} \rangle \\ &\times \langle \mathbf{R}^{M-1} | e^{-(H-E_R)\frac{\tau}{M}} | \mathbf{R}^{M-2} \rangle \dots \langle \mathbf{R}^1 | e^{-(H-E_R)\frac{\tau}{M}} | \mathbf{R}' \rangle. \end{aligned} \quad (9.52)$$

For a short time propagation we can evaluate the propagator using the Trotter-Suzuki formula

$$e^{-(H-E_R)\Delta\tau} = e^{-(V-E_R)\frac{\Delta\tau}{2}} e^{-(T-E_R)\Delta\tau} e^{-(V-E_R)\frac{\Delta\tau}{2}} = \mathcal{O}(\Delta\tau^3), \quad (9.53)$$

which separates the propagator into a product of kinetic energy and interaction terms. The interaction is diagonal in coordinate space, therefore

$$e^{-(V-E_R)\frac{\Delta\tau}{2}} | \mathbf{R} \rangle = | \mathbf{R} \rangle e^{-(V(\mathbf{R})-E_R)\frac{\Delta\tau}{2}}. \quad (9.54)$$

To evaluate the kinetic energy term we note that a free particle obeys a diffusion like equation

$$-\frac{\partial}{\partial\tau} \Psi = -\frac{\hbar^2}{2m} \nabla^2 \Psi. \quad (9.55)$$

The solution of this equation for A particles is well known

$$\Psi(\mathbf{R}, \tau) = \frac{1}{(2\pi\frac{\hbar^2}{m}\Delta\tau)^{3A/2}} \int d\mathbf{R}' \exp\left(-\frac{(\mathbf{R}-\mathbf{R}')^2}{2\frac{\hbar^2}{m}\Delta\tau}\right) \Psi(\mathbf{R}', 0). \quad (9.56)$$

The short time propagator, to order $\Delta\tau^2$, is then

$$\begin{aligned} G(\mathbf{R}, \mathbf{R}'; \Delta\tau) &= \langle \mathbf{R} | e^{-(H-E_R)\Delta\tau} | \mathbf{R}' \rangle \\ &= e^{-(V(\mathbf{R})-E_R)\frac{\Delta\tau}{2}} e^{-\frac{m}{2\hbar^2\Delta\tau}(\mathbf{R}-\mathbf{R}')^2} e^{-(V(\mathbf{R}')-E_R)\frac{\Delta\tau}{2}} \\ &= e^{-\left(\frac{1}{2}[V(\mathbf{R})+V(\mathbf{R}')]-E_R\right)\Delta\tau} e^{-\frac{m}{2\hbar^2\Delta\tau}(\mathbf{R}-\mathbf{R}')^2} \end{aligned} \quad (9.57)$$

Now we can write

$$\Psi(\mathbf{R}, \tau) = \lim_{M \rightarrow \infty} \int \prod_{j=1}^{M-1} d\mathbf{R}^j \prod_{n=1}^M G(\mathbf{R}^n, \mathbf{R}^{n-1}; \frac{\tau}{M}) \Psi_T(\mathbf{R}^0), \quad (9.58)$$

with $\mathbf{R}^M = \mathbf{R}$. In order to evaluate this multi dimensional integral we have to use the Monte Carlo method. To this end we write the propagator as a product of a transition matrix T and a weight function W ,

$$G(\mathbf{R}, \mathbf{R}'; \Delta\tau) = W(\mathbf{R}, \mathbf{R}'; \Delta\tau) T(\mathbf{R}, \mathbf{R}'; \Delta\tau) \quad (9.59)$$

with

$$\begin{aligned} W(\mathbf{R}, \mathbf{R}'; \Delta\tau) &= e^{-\left(\frac{1}{2}[V(\mathbf{R})+V(\mathbf{R}')]-E_R\right)\Delta\tau}, \\ T(\mathbf{R}, \mathbf{R}'; \Delta\tau) &= \frac{1}{(2\pi\frac{\hbar^2}{m}\Delta\tau)^{3A/2}} e^{-\frac{m}{2\hbar^2\Delta\tau}(\mathbf{R}-\mathbf{R}')^2}. \end{aligned} \quad (9.60)$$

T is clearly a transition matrix since

$$\begin{aligned} 1 &= \int d\mathbf{R} T(\mathbf{R}, \mathbf{R}'; \Delta\tau) \\ T(\mathbf{R}, \mathbf{R}'; \Delta\tau) &= \int d\mathbf{R}'' T(\mathbf{R}, \mathbf{R}''; \Delta\tau) T(\mathbf{R}'', \mathbf{R}'; \Delta\tau). \end{aligned} \quad (9.61)$$

Now we can write

$$\Psi(\mathbf{R}^M, \tau) = \int \prod_{j=0}^{M-1} d\mathbf{R}^j \prod_{n=1}^M W(\mathbf{R}^M, \dots, \mathbf{R}^0) P(\mathbf{R}^M, \dots, \mathbf{R}^0) \quad (9.62)$$

with P the probability function

$$P(\mathbf{R}^M, \dots, \mathbf{R}^0) = \prod_{n=1}^M T(\mathbf{R}^n, \mathbf{R}^{n-1}; \frac{\tau}{M}) \Psi_T(\mathbf{R}^0) \quad (9.63)$$

and W the weight function

$$W(\mathbf{R}^M, \dots, \mathbf{R}^0) = \prod_{n=1}^M W(\mathbf{R}^n, \mathbf{R}^{n-1}; \frac{\tau}{M}). \quad (9.64)$$

In this form we can estimate the integrals in Eq. (9.62) using Monte Carlo techniques, sampling the path $\mathbf{R}^M, \dots, \mathbf{R}^0$ from the distribution P . In view of Eq. (9.62), P can be written as a product of conditional distributions

$$P(\mathbf{R}^M, \dots, \mathbf{R}^0) = P(\mathbf{R}^M | \mathbf{R}^{M-1}) \dots P(\mathbf{R}^1 | \mathbf{R}^0) P(\mathbf{R}^0). \quad (9.65)$$

The interpretation of P as a distribution hangs on the assumption we made at the begining of this section, namely that the wave-function is positive and hence, we can interpret $\Psi_T(\mathbf{R}^0) > 0$ as a PDF that defines the distribution of the points $P(\mathbf{R}^0)$ (Don't worry about normalization, we'll take care of it later). The conditional distributions

$$P(\mathbf{R}^n | \mathbf{R}^{n-1}) = T(\mathbf{R}^n, \mathbf{R}^{n-1}; \Delta\tau), \quad (9.66)$$

are normal distributions around the point \mathbf{R}^{n-1} with standard deviation

$$\sigma = \sqrt{\frac{\hbar^2}{m} \Delta\tau}. \quad (9.67)$$

Now we are in position to sample a path $\mathbf{R}^M, \dots, \mathbf{R}^0$. We start picking a point \mathbf{R}^0 using the trial wave-function $\Psi_T(\mathbf{R}^0)$ as our distribution. If Ψ_T is simple enough we can do it directly, otherwise we can use the Metropolis–Hastings method. To make a step in our path, lets say from $\mathbf{R}^{n-1} \rightarrow \mathbf{R}^n$, we sample $3A$ independent random variables $\eta_{i,a}$ from a normal distribution of mean zero and standard deviation one, $\eta_{i,a} \in N(0, 1)$, now

$$R_{i,a}^n = R_{i,a}^{n-1} + \sigma \eta_{i,a}. \quad (9.68)$$

Now in principle we can integrate (9.62) either by summing the points or better using the Metropolis–Hastings algorithm. The so-called Diffusion Monte Carlo (DMC), provides a different strategy which we describe next.

9.6.2 Diffusion Monte Carlo

DMC interprets the integrand in Eq. (9.62)

$$\begin{aligned} & \underbrace{W(\mathbf{R}^M, \mathbf{R}^{M-1})}_{\text{weight } M} \underbrace{T(\mathbf{R}^M, \mathbf{R}^{M-1})}_{\text{step } M} \dots \underbrace{W(\mathbf{R}^2, \mathbf{R}^1)}_{\text{weight } 2} \underbrace{T(\mathbf{R}^2, \mathbf{R}^1)}_{\text{step } 2} \\ & \times \underbrace{W(\mathbf{R}^1, \mathbf{R}^0)}_{\text{weight } 1} \underbrace{T(\mathbf{R}^1, \mathbf{R}^0)}_{\text{step } 1} \underbrace{\Psi_T(\mathbf{R}^0)}_{\text{init } 0} \end{aligned} \quad (9.69)$$

as a product of probabilities and weights to be modeled as a sequence of stochastic processes carried out not on a single integration path but rather on an ensemble of integration paths which we call walkers. In the DMC algorithm the walkers population evolves according to the following recipe:

Initial state

We start randomly choosing N_0 points $\mathbf{R}^0(k)$ distributed according to trial wave-function $\Psi_T(\mathbf{R}^0)$. Here k is the index of the walker.

Diffusion

In the diffusion step, the positions of all the walkers are changed according to the prescription discussed above in Eq. (9.68).

Birth-Death process

Instead of accumulating the weights factors for each walker, it is more efficient to change the ensemble distribution according to the weight factors $W(\mathbf{R}^n, \mathbf{R}^{n-1})$. This way, the unnormalized wave function is given by the density of the walkers. The calculation of Ψ is simulated as diffusion-reaction process of our walkers.

To get the average number of walkers correct, we calculate for each walker the number of copies

$$m_n(k) = \min \left[\text{int} \left[W(\mathbf{R}^n, \mathbf{R}^{n-1}) + \zeta \right], 3 \right] \quad ; \quad \zeta \in U(0,1). \quad (9.70)$$

Here $\text{int}[x]$ denotes the integer part of x , and $U(0,1)$ uniform distribution in the range $[0,1]$. Now, the fate of the walker is decided according to m_n :

- In case $m_n = 0$ the walker is deleted - "death".
- In case $m_n = 1$ the walker is unaffected.
- In case $m_n = 2, 3$ the walker continues to the next step but 1 or 2 new copies of the walker are added to the ensemble - "birth".

The limitation $m_n \leq 3$ is added to avoid numerical instabilities. The error resulting from this limitation are expected to be small as in the limit of $\Delta\tau \rightarrow 0$ $W \rightarrow 1$.

Population and energy

To control the number of walkers we can introduce a modified weight

$$\tilde{W} = \frac{N_0}{N_c} e^{-\left(\frac{V(\mathbf{R})+V(\mathbf{R}')}{2} - E_R\right)\Delta\tau}, \quad (9.71)$$

where N_0 is the number of walkers we aim for, and N_c is the number of walkers in the current step. \tilde{W} introduce a bias linear in $\Delta\tau$.

The weight can also be used to estimate the energy. The population grows or decline according to the expectation value of W ,

$$\langle W \rangle \approx 1 - (\langle V \rangle - E_R)\Delta\tau. \quad (9.72)$$

Therefore, recalling that we get a stable population for $E_R = E_0$ we can conclude that

$$E_R = \langle V \rangle. \quad (9.73)$$

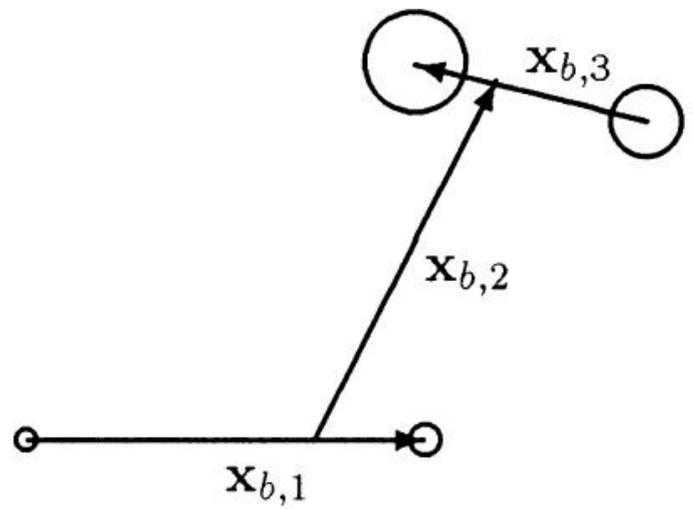
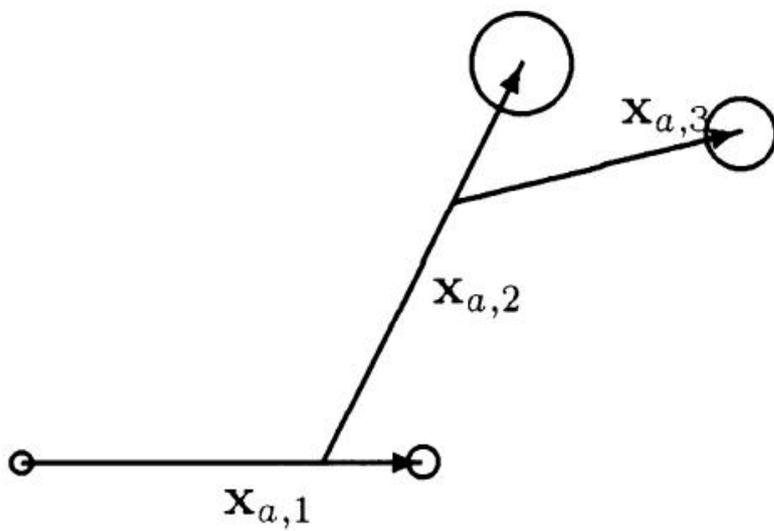
which we average over the ensemble of walkers. This estimator to the ground state energy is called the *growth energy* estimator.

Another way to evaluate the energy is to use a trial function Ψ_T and evaluate the matrix element,

$$\langle E \rangle = \frac{\langle \Psi_T | H | \Phi_0 \rangle}{\langle \Psi_T | \Phi_0 \rangle} \approx \frac{\langle \Psi_T | H | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle} \quad (9.74)$$

which, due to the hermiticity of H we can write as

$$\begin{aligned} \langle E \rangle &= \frac{\langle \Psi(\tau) | H | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle} = \frac{\int d\mathbf{R} \Psi(\mathbf{R}, \tau) H \Psi_T(\mathbf{R})}{\int d\mathbf{R} \Psi(\mathbf{R}, \tau) \Psi_T(\mathbf{R})} \\ &\approx \frac{\sum_k H \Psi_T(\mathbf{R}^n(k))}{\sum_k \Psi_T(\mathbf{R}^n(k))}. \end{aligned} \quad (9.75)$$



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