Electromagnetic properties of nuclei: from few- to many-body systems

Lecture 7

Few-body methods

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Lecture series for SFB 1245
TU Darmstadt

Ab-initio methods

After having wormed up with the deuteron
we will present the modern perspective

Ab-initio methods

Most representative approaches

	Few-body: A≲12	**Many-body: 12≲A≲40 or more**
Structure Bound states	• *Faddeev Yakubowski (FY)* • **Diagonalization methods** *(on different basis)* • *Green Function Monte Carlo*	• *Coupled Cluster (CC)* • *Other Monte Carlo methods* • *IMSRG* • *Self consistent Green's function*
Reactions scattering states	• *Faddeev Yakubowski (FY)* • *HH Kohn-Variational P. (2 fragments)* • *NCSMC (only at very low energy)*	

Focus on diagonalization methods

Keep in mind we want to be able to compute the ground-state and the Schrödinger-like equation appearing in the integral transform approach to electro-weak reactions

Diagonalization methods

Given a complete set of basis states:

Solve Schroedinger equation by expanding the w.f. on a complete basis states

$$H|\psi\rangle = E|\psi\rangle \qquad |\psi\rangle = \sum_i^{\infty \to N} c_i |\psi_i\rangle$$

cannot store an infinite vector

controlled increasing N

→ basis states

$$\langle\psi_j| \times H \sum_i^N c_i |\psi_i\rangle = E \sum_i^N c_i |\psi_i\rangle$$

$$\sum_i^N \underbrace{\langle\psi_j| H |\psi_i\rangle}_{H_{ji}} c_i = E \sum_i^N c_i \underbrace{\langle\psi_j|\psi_i\rangle}_{\delta_{ji}}$$

$$\boxed{\mathbf{Hc} = E\mathbf{c}}$$

Eigenvalue problem for an Hermitian matrix

$$\mathbf{H} = \mathbf{H}^\dagger$$

Diagonalize H

Computationally challenging for growing N and mass number A → High Performance Computing

My choice of basis:
Hyper-spherical harmonic expansions

Hyper-spherical Harmonics

- The study of nuclear systems composed of A-nucleons have led to the construction of the hyper-spherical harmonics, which are harmonic polynomials in 3(A-1) dimensional space.

- The hyper-spherical coordinates and the hyper-spherical harmonics are generalization of the spherical harmonics from 3D space into the general case

- The HH were introduced in 1935 by Zernike and Brinkman

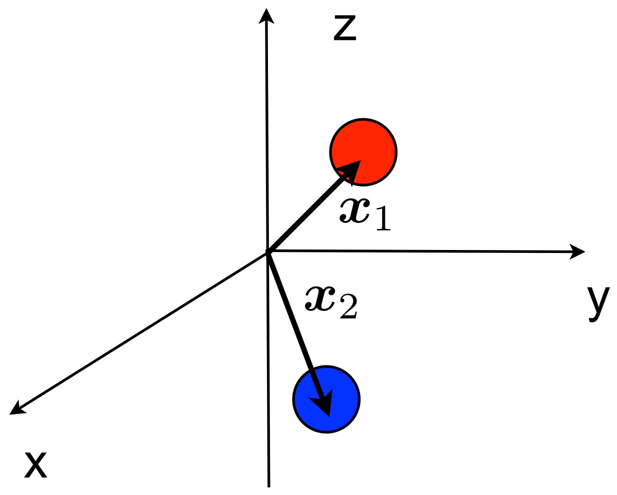
- They were reintroduced 25 years later by Delves and Smith

- ….

- Present developers, practitioners: Barnea, Efros, Gattobigio, Viviani etc…

They are built starting from relative coordinates

Two-body problem *recap*

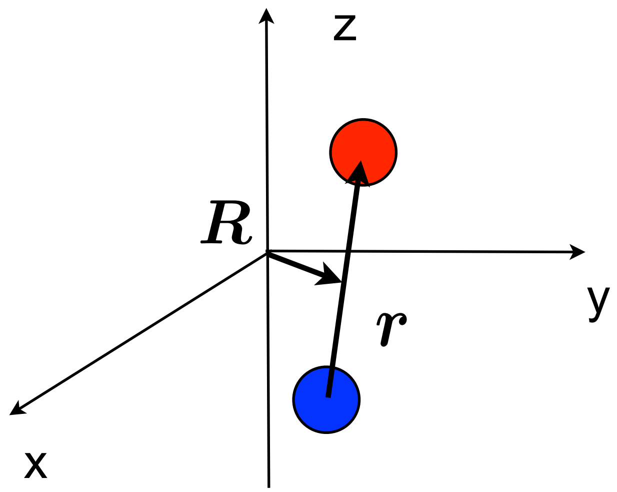


$$\psi(\boldsymbol{x}_1, \boldsymbol{x}_2) = \langle \boldsymbol{x}_1 \boldsymbol{x}_2 | \psi \rangle$$

$$H\psi = E\psi$$

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

Two-body problem *recap*



$$\psi(\boldsymbol{x}_1, \boldsymbol{x}_2) = \langle \boldsymbol{x}_1 \boldsymbol{x}_2 | \psi \rangle$$

$$H\psi = E\psi$$

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

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

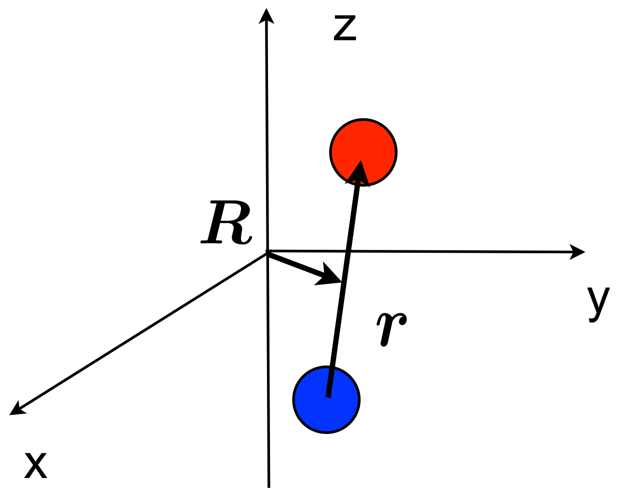
$$\boldsymbol{R} = \frac{1}{M_{12}}(m_1\boldsymbol{x}_1 + m_2\boldsymbol{x}_2) \qquad \text{with } M_{12} = m_1 + m_2$$

$$\boldsymbol{r} = (\boldsymbol{x}_2 - \boldsymbol{x}_1)$$

The internal Hamiltonian is given by

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

Two-body problem *recap*



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

Going to spherical coordinates in $\boldsymbol{r}$

Angular momentum operator

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

$$\hat{\ell}^2 Y_{\ell m}(\hat{\boldsymbol{r}}) = \ell(\ell+1)Y_{\ell m}(\hat{\boldsymbol{r}})$$

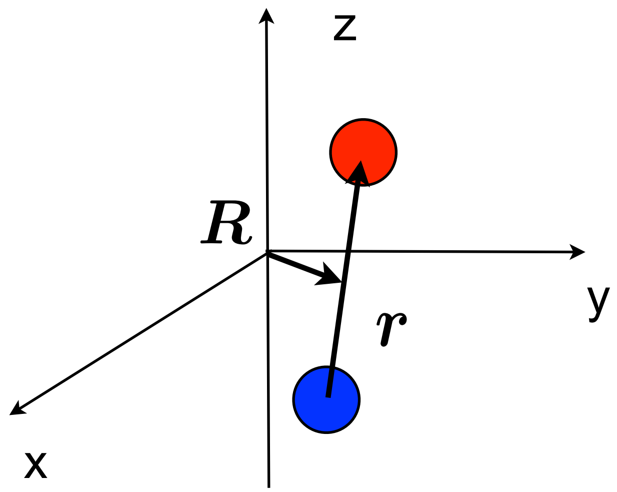
$$\hat{\ell}_z Y_{\ell m}(\hat{\boldsymbol{r}}) = m Y_{\ell m}(\hat{\boldsymbol{r}})$$

$$\hat{\mathbf{r}} = (\theta, \phi)$$

Spherical harmonics

Intrinsic wave function $\psi(\boldsymbol{r}) = Y_{\ell m}(\hat{\boldsymbol{r}})R_\ell(r)$

Two-body problem *recap*



Intrinsic wave function $\psi(\boldsymbol{r}) = Y_{\ell m}(\hat{\boldsymbol{r}}) R_\ell(r)$

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} \right) + V(r) \right] R_\ell(r) = E R_\ell(r)$$

Radial Schrödinger equation

If you know the potential, you can solve it either on a grid or expanding the radial wave function on a basis

Jacobi coordinates A=2

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

$$\boldsymbol{R} = \frac{1}{M_{12}} (m_1 \boldsymbol{x}_1 + m_2 \boldsymbol{x}_2)$$

$$\boldsymbol{r} = (\boldsymbol{x}_2 - \boldsymbol{x}_1)$$

With $M_{12} = m_1 + m_2$

It should be noted that this transformation is not orthogonal.

The orthogonal transformation is

m arbitrary mass, typically taken to be the nucleon mass

$$\boldsymbol{\eta}_0 = \sqrt{\frac{1}{M_{12}}} (m_1 \boldsymbol{r}_1 + m_2 \boldsymbol{r}_2)$$ ← CoM

$$\boldsymbol{\eta}_1 = \sqrt{\frac{m_1 m_2}{M_{12} m}} (\boldsymbol{r}_2 - \boldsymbol{r}_1)$$ ← Relative

A two-body problem is reduced to a one-body problem, once the CoM is removed

Jacobi coordinates A=3

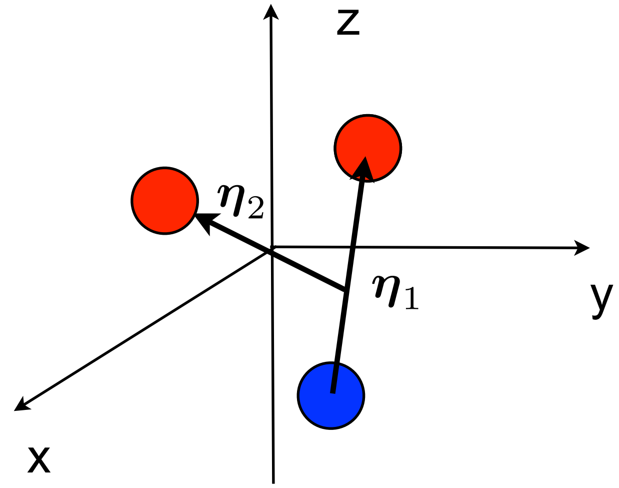
A three-body problem is reduced to a two-body problem, once the CoM is removed

$$\boldsymbol{\eta}_0 = \sqrt{\frac{1}{M_{123}}}(m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2 + m_3\boldsymbol{r}_3)$$ ← CoM

Relative:

$$\boldsymbol{\eta}_1 = \sqrt{\frac{m_1 m_2}{M_{12} m}}(\boldsymbol{r}_2 - \boldsymbol{r}_1)$$

$$\boldsymbol{\eta}_2 = \sqrt{\frac{M_{12} m_3}{M_{123} m}}\left(\boldsymbol{r}_3 - \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{M_{12}}\right)$$



Jacobi coordinates general A

An A-body problem is reduced to an (A-1)-body problem, once the CoM is removed

Mass-weighted Jacobi coordinates

$$\boldsymbol{\eta}_0 = \sqrt{\frac{1}{M_{1\ldots k}}}(m_1\mathbf{r}_1 + m_2\mathbf{r}_2 + \cdots + m_A\mathbf{r}_A)$$

← CoM

$$\boldsymbol{\eta}_{k-1} = \sqrt{\frac{M_{1\ldots k-1}m_k}{M_{1\ldots k}\ m}}\left(\mathbf{r}_k - \frac{1}{M_{1\ldots k-1}}(m_1\mathbf{r}_1 + m_2\mathbf{r}_2 + \cdots + m_{k-1}\mathbf{r}_{k-1})\right)$$

Relative (A-1) coordinates

NB: one can write this as an orthogonal transformation and then compute the expressions of the gradients

Jacobi coordinates general A

Normalized equal mass (A-1) Jacobi coordinates

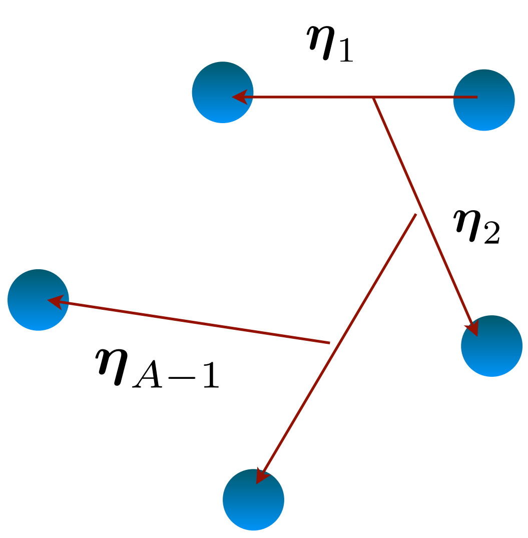
$$\boldsymbol{\eta}_1 = \sqrt{\frac{1}{2}}\Big(\boldsymbol{r}_2 - \boldsymbol{r}_1\Big)$$

$$\boldsymbol{\eta}_2 = \sqrt{\frac{2}{3}}\Big(\boldsymbol{r}_3 - \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_3)\Big)$$

$$\cdots$$

$$\boldsymbol{\eta}_{A-2} = \sqrt{\frac{A-2}{A-1}}\Big(\boldsymbol{r}_{A-2} - \frac{1}{A-2}(\boldsymbol{r}_1 + \boldsymbol{r}_2 + \cdots + \boldsymbol{r}_{A-3})\Big)$$

$$\boldsymbol{\eta}_{A-1} = \sqrt{\frac{A-1}{A}}\Big(\boldsymbol{r}_{A-1} - \frac{1}{A-1}(\boldsymbol{r}_1 + \boldsymbol{r}_2 + \cdots + \boldsymbol{r}_{A-1})\Big)$$



One may start these definitions with an arbitrary permutation of particles

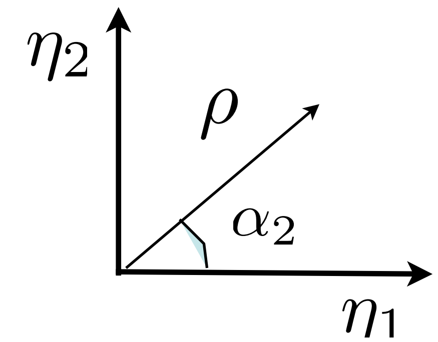
Once you have the Jacobi coordinates, you can perform another transformation to hyperspherical harmonics coordinates

Hyper-spherical coordinates

Recursive definition of hyper-spherical coordinates

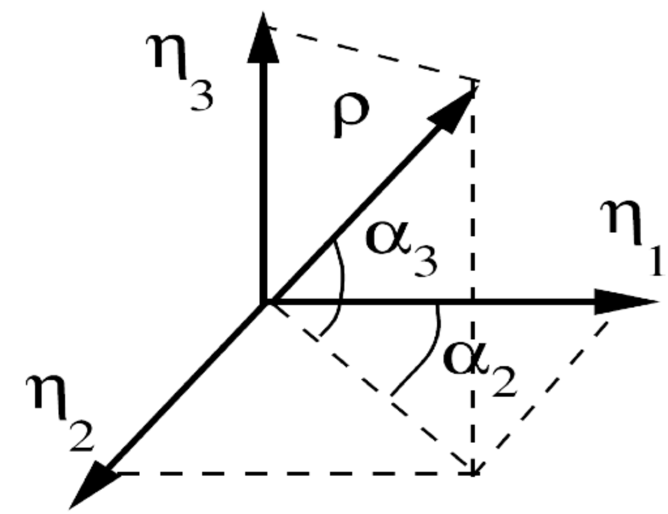
A=3

$$\begin{cases} \boldsymbol{\eta}_1 = \{\eta_1, \theta_1, \phi_1\} \\ \boldsymbol{\eta}_2 = \{\eta_2, \theta_2, \phi_2\} \end{cases} \qquad \begin{cases} \rho = \sqrt{\eta_1^2 + \eta_2^2} \\ \sin\alpha_2 = \frac{\eta_2}{\rho} \end{cases}$$



A=4

$$\begin{cases} \boldsymbol{\eta}_1 = \{\eta_1, \theta_1, \phi_1\} \\ \boldsymbol{\eta}_2 = \{\eta_2, \theta_2, \phi_2\} \\ \boldsymbol{\eta}_3 = \{\eta_3, \theta_3, \phi_3\} \end{cases} \qquad \begin{cases} \rho = \sqrt{\eta_1^2 + \eta_2^2 + \eta_3^2} \\ \sin\alpha_2 = \frac{\eta_2}{\rho} \\ \sin\alpha_3 = \frac{\eta_3}{\rho} \end{cases}$$



In general $\qquad \boldsymbol{\eta}_1, \dots \boldsymbol{\eta}_A \longrightarrow \rho, \Omega$

Hyper-radius

Hyper-angles

$$\rho = \sqrt{\sum_{i=1}^{A-1} \eta_i^2}$$

$$\Omega = (\hat{\eta}_1, \dots, \hat{\eta}_{A-1}, \alpha_2, \dots, \alpha_{A-1})$$

How many angular coordinates in total? $\qquad$ 2(A-1)+A-2 = 3A-4

How many HH coordinates in total? $\qquad$ 3A-3

Hyper-spherical coordinates

Exercise: prove this property of the hyper-radius

$$\rho^2 = \sum_{i=1}^{A} r_i^2 = \sum_{i=1}^{A-1} \eta_i^2$$

Nuclear matter radius is related simply to the hyper-radius

Once we have a new set of coordinates, we need to rewrite our Hamiltonian in these coordinates

1) Kinetic energy

Laplace operator in hyper-spherical coordinates

A=2 Recap

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 $\boldsymbol{\eta}_1$ and the corresponding angle coordinates Ω

$$\Delta_{(1)} = \Delta_{\boldsymbol{\eta}_1} = \Delta_{\eta_1} - \frac{1}{\eta_1^2}\hat{\ell}_1^2$$

N.B.: $\Delta = \nabla^2$

Where the radial part is

$$\Delta_{\eta_1} = \frac{\partial^2}{\partial \eta_1^2} + \frac{2}{\eta_1}\frac{\partial}{\partial \eta_1}$$

And $\hat{\ell}_1^2$ is the angular momentum operator of the relative motion

Laplace operator in hyper-spherical coordinates

A=3

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 $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$ separately.

$$\Delta_{(2)} = \Delta_{\boldsymbol{\eta}_1} + \Delta_{\boldsymbol{\eta}_2} = \Delta_{\eta_1} + \Delta_{\eta_2} - \frac{1}{\eta_1^2}\hat{\ell}_1^2 - \frac{1}{\eta_2^2}\hat{\ell}_2^2$$

Now transforming to HH coordinates using the definition of hyper-radius and

$$\eta_1 = \rho\cos\alpha_2$$
$$\eta_2 = \rho\sin\alpha_2$$

one gets

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

with

$$\hat{K}^2 = -\frac{\partial^2}{\partial\alpha_2^2} - 4\cot(2\alpha_2)\frac{\partial}{\partial\alpha_2} + \frac{1}{\cos^2\alpha_2}\hat{\ell}_1^2 + \frac{1}{\sin^2\alpha_2}\hat{\ell}_2^2$$

Grand-angular momentum operator

Important observations

$\hat{K}^2, \hat{\ell}_1^2, \hat{\ell}_{1,z}, \hat{\ell}_2^2, \hat{\ell}_{2,z}$ These operators form a complete set of commuting hyper-spherical operators, and therefore we can introduce a set of quantum numbers

$K, \ell_1, m_1, \ell_2, m_2$ These operators commute also with $\Delta_{(2)}$ and $\hat{L}^2, \hat{L}_z$

obtained from the internal angular momentum of the three-particle system

$$\hat{\mathbf{L}} = \hat{\boldsymbol{\ell}}_1 + \hat{\boldsymbol{\ell}}_2$$

Since it is a recursive definition, it should be labelled by the number of particles

$\rho_{A-1}, \hat{K}^2_{A-1}$

Laplace operator in hyper-spherical coordinates

General A

The Laplace operator in 3(A-1) dimensions, that describes the internal kinetic energy of an A-body system, is

$$\Delta_{(A-1)} = \sum_{i=1}^{A-1} \Delta_{\boldsymbol{\eta}_i} = \sum_{i=1}^{A-1} \left(\Delta_{\eta_i} - \frac{1}{\eta_i^2} \hat{\ell}_i^{\,2} \right)$$

Now transforming to A-body HH coordinates it becomes

$$\Delta_{(A-1)} = \Delta^{A-1}_{\rho_{A-1}} - \frac{1}{\rho_{A-1}^2} \hat{K}^{\,2}_{A-1}$$

Radial part

Angular part

with $\Delta^{A-1}_{\rho_{A-1}} = \frac{\partial^2}{\partial \rho_{A-1}^2} + \frac{3(A-1)-1}{\rho_{A-1}} \frac{\partial}{\partial \rho_{A-1}}$ and

$$\hat{K}^{\,2}_{A-1} = -\frac{\partial^2}{\partial \alpha_{A-1}^2} + \frac{3A-9-(3A-5)\cos(2\alpha_{A-1})}{\sin(2\alpha_{A-1})} \frac{\partial}{\partial \alpha_{A-1}} + \frac{\hat{\ell}^{\,2}_{A-1}}{\sin^2 \alpha_{A-1}} + \frac{\hat{K}^{\,2}_{A-2}}{\cos^2 \alpha_{A-1}}$$

Grand-angular momentum operator

Important observations

$$\hat{K}^2_{A-2}, \hat{\ell}^2_{A-1}, \hat{K}^2_{A-1}, \hat{L}^2_{A-1}, \hat{L}_{A-1_z}$$

These operators form a complete set of commuting hyper-spherical operators.
The recursion can be used so that at the end we can introduce a set of quantum numbers corresponding to operators that commute

$$[K_{A-1}] = K_{A-1}, K_{A-2}, \ldots, K_2, \ell_{A-1}, \ell_{A-2}, \ldots, \ell_2, \ell_1, m_{A-1}, m_{A-2}, \ldots, m_2, m_1$$

Cumulative quantum number

$\hat{K}^2_{A-1}$ commutes with the kinetic energy

Once we have a new set of coordinates, we need to rewrite our Hamiltonian in these coordinates

2) Potential

The simplest potential you can use is an hyper-radial potential $V(\rho)$

In general, NN potentials are more complicated…

Hyper-spherical Harmonics

HH

Are eigenfunctions of the grand-angular momentum operator

Hyper-spherical Harmonics

A=2 spherical harmonics $Y_{\ell_1,m_1}(\hat{\eta}_1)$

A=3 Start of hpyer-spherical harmonics

$$\mathcal{Y}_{[K_2]}(\Omega_{(2)},\alpha_2) = \psi_{K_2;\ell_2\ell_1}(\alpha_2)\,\Phi_{L_2M_2;\ell_1\ell_2}\left(\Omega_{(2)}\right)$$

coupled spherical harmonics

$$\Phi_{L_2M_2;\ell_1\ell_2}\left(\Omega_{(2)}\right) = \sum_{m_1,m_2} \langle \ell_1\ell_2L_2|m_1m_2M_2\rangle\, Y_{\ell_1m_1}(\hat{\eta}_1)\, Y_{\ell_2m_2}(\hat{\eta}_2)$$

Hyper-angular function and polynomial

$$\psi_{K_2;\ell_2\ell_1}(\alpha_2) = \mathcal{N}_2(K_2;\ell_2\ell_1)(\sin\alpha_2)^{\ell_2}(\cos\alpha_2)^{\ell_1}\, P_{n_2}^{\left(\ell_2+\frac{1}{2},\ell_1+\frac{1}{2}\right)}(\cos 2\alpha_2)$$

$$\mathcal{N}_2(K_2;\ell_2\ell_1) = \left[\frac{(2K_2+4)\,n_2!\,\Gamma(n_2+\ell_2+\ell_1+2)}{\Gamma\left(n_2+\ell_2+\frac{3}{2}\right)\Gamma\left(n_2+\ell_1+\frac{3}{2}\right)}\right]^{\frac{1}{2}}$$

Jacobi polynomial

Hyper-spherical Harmonics

General A

$$\mathcal{Y}_{[K_{A-1}]}\left(\Omega_{(A-1)},\alpha_{(A-1)}\right) = \boxed{\psi_{K_{A-1};\ell_{A-1}K_{A-2}}\left(\alpha_{(A-1)}\right)}\boxed{\Phi_{L_{A-1}M_{A-1};[K_{A-2}]\ell_{A-1}}\left(\Omega_{(A-1)},\alpha_{(A-2)}\right)}$$

coupled spherical and hyper-spherical harmonics

$$\Phi_{L_{A-1}M_{A-1};[K_{A-2}]\ell_{A-1}}\left(\Omega_{(A-1)},\alpha_{(A-2)}\right) =$$
$$\sum_{M_{A-2},m_{A-1}} \langle L_{A-2}\ell_{A-1}L_{A-1}|M_{A-2}m_{A-1}M_{A-1}\rangle \mathcal{Y}_{[K_{A-2}]}(\Omega_{(A-2)},\alpha_{(A-2)})Y_{\ell_{A-1}m_{A-1}}(\hat{\eta}_{A-1})$$

Hyper-angular function and polynomial

$$\psi_{K_{A-1};\ell_{A-1}K_{A-2}}\left(\alpha_{A-1}\right) =$$
$$\mathcal{N}_{A-1}!\,(K_{A-1};\ell_{A-1}K_{A-2})(\sin\alpha_{A-1})^{\ell_{A-1}}(\cos\alpha_{A-1})^{K_{A-2}}P_{n_{A-1}}^{\left(\ell_{A-1}+\frac{1}{2},K_{A-2}+\frac{3A-8}{2}\right)}(\cos 2\alpha_{A-1})$$

Jacobi polynomial

with

$$K_{A-1} = 2n_{A-1} + K_{A-2} + \ell_{A-1}$$

Hyper-spherical Harmonics

To make the long story short:

- The Laplacian can be written as

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

depends on particle number

- The HH are eigenstates of $\hat{K}^2$

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

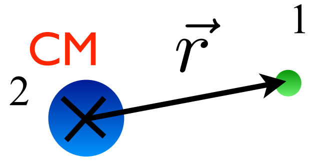
- The HH are eigenstates of the kinetic energy operator

- The HH form a complete set of orthonormal states

$$\langle \mathcal{Y}_{[K]}(\Omega') | \mathcal{Y}_{[K']}(\Omega) \rangle = \delta_{[K],[K']}$$

Understanding with an analogy

Hydrogen atom



- Solve the problem in the CM frame

$$[T + V(r)]\,\psi(\vec{r}) = E\psi(\vec{r})$$

- Use spherical coordinates

$$\vec{r} = (r, \underbrace{\theta, \phi}_{\Omega})$$

$$\psi(\vec{r}) \sim Y_{\ell m}(\Omega) u_\ell(r)$$

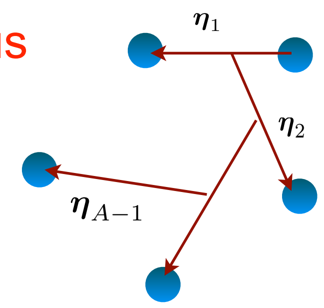
$$T = -\frac{\hbar^2}{2m}\left[\Delta_r - \frac{\hat{\ell}^2}{r^2}\right]$$

$$\hat{\ell}^2\; Y_{\ell m}(\Omega) = \ell(\ell+1) Y_{\ell m}(\Omega)$$

- Solve the radial equation

$$\left\{-\frac{\hbar^2}{2m}\left[\Delta_r - \frac{\hat{\ell}^2}{r^2}\right] - E + V(r)\right\} R_\ell(r) = 0$$

A-body Nucleus



- Solve the problem in the CM frame

$$[T + V]\Psi(\boldsymbol{\eta}_1, \ldots \boldsymbol{\eta}_A) = E\Psi(\boldsymbol{\eta}_1, \ldots \boldsymbol{\eta}_A)$$

- Use hyperspherical coordinates

$$\boldsymbol{\eta}_1, \ldots \boldsymbol{\eta}_A \longrightarrow \rho, \Omega$$

$$\Psi(\boldsymbol{\eta}_1, \ldots \boldsymbol{\eta}_A) \sim \mathcal{Y}_{[K]}(\Omega) R_{[K]}(\rho)$$

$$T = -\frac{\hbar^2}{2m}\left[\Delta_\rho - \frac{\hat{K}^2}{\rho^2}\right]$$

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

- Solve the hyperradial equation

$$\left\{-\frac{\hbar^2}{2m}\left[\Delta_\rho - \frac{\hat{K}^2}{\rho^2}\right]\delta_{[K],[K']} - E\;\delta_{[K],[K']} + \langle \mathcal{Y}_{[K]}|V(\rho,\Omega)|\mathcal{Y}_{[K']}\rangle\right\} R_{[K]}(\rho) = 0$$

Antisymmetrization

- If we want to work with fermions, we may want to antisymmetrize HH

- Antisymmetrization can be achieved by diagonalizing the antisymmetrizer operator

- Or one can use other algorithms based on their symmetry properties

N. Barnea and A. Novoselsky, Ann. Phys (N.Y.) **256**, 192 (1997).
N. Barnea and A. Novoselsky, Phys. Rev. A 57, **48** (1998).

HH expansion

$$|\psi\rangle = \sum_{[K]}^{K_{max}} \sum_{\nu}^{\nu_{max}} c_{[K]\nu}\, \mathcal{Y}_{[K]}(\Omega)\; e^{-\rho/2b} L_\nu(\rho)$$

$K_{max} * \nu_{max}$ = # states

Exact method

When you converge your expansion,
every kind of correlation induced by the Hamiltonian
is taken into account

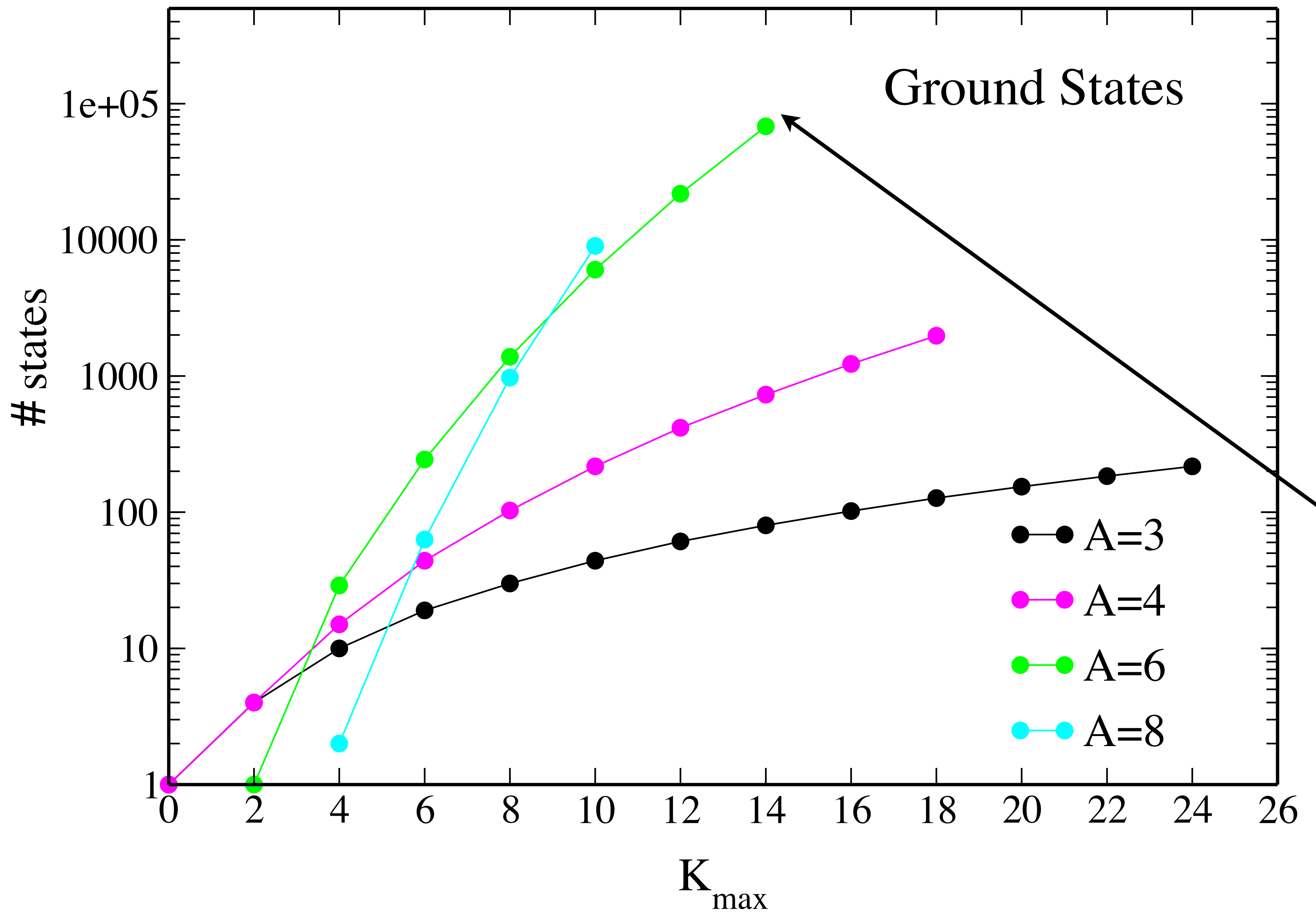
Bad computational scaling

Matrices become big very fast…

HH expansion

$$|\psi\rangle = \sum_{[K]}^{K_{max}} \sum_{\nu}^{\nu_{max}} c_{[K]\nu} \mathcal{Y}_{[K]}(\Omega)\, e^{-\rho/2b} L_\nu(\rho)$$

$K_{max} * \nu_{max}$ = # states

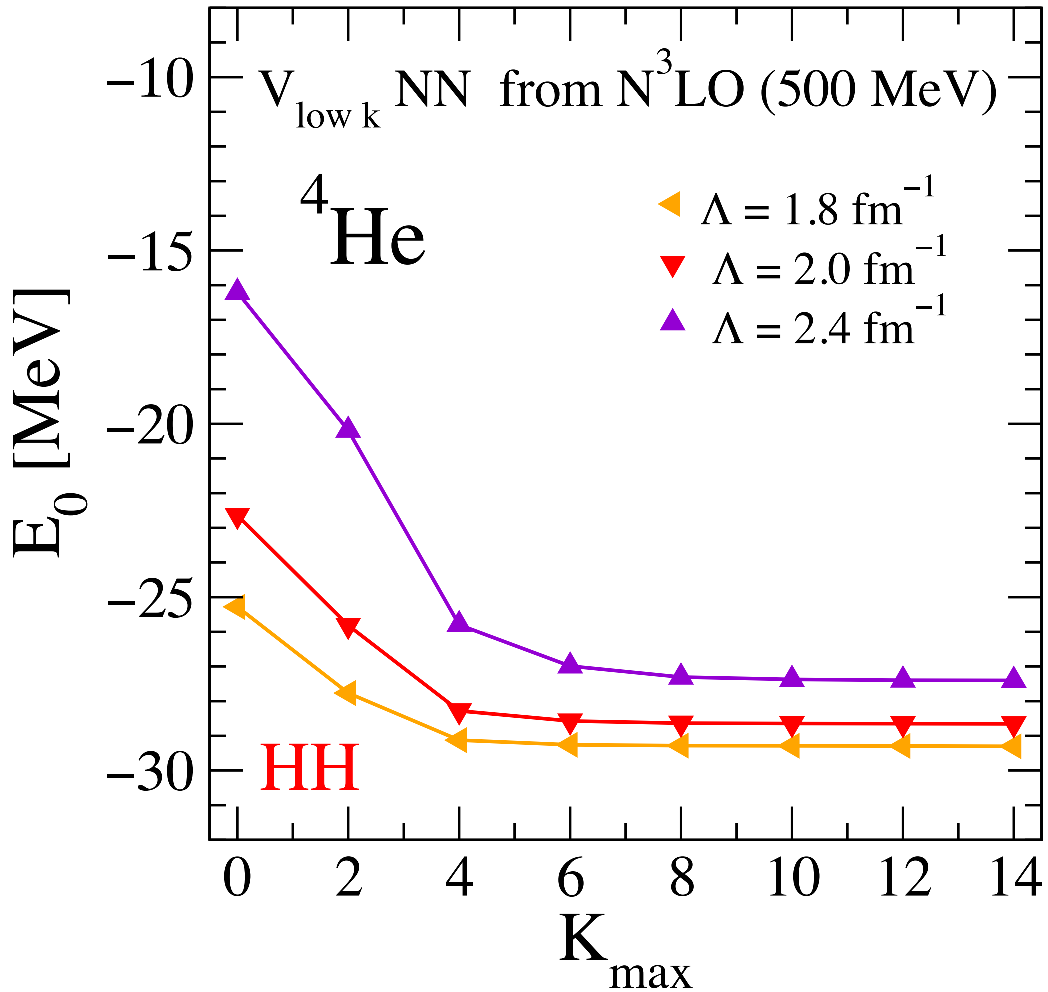


Total number of states:

10^6 dense matrix

Benchmark on ^{4}He

S.Bacca et al., Eur. Phys. J. A 42, 553 (2009)



Method	$\Lambda = 2.0\ fm^{-1}$	$E_0(^4He)$ [MeV]
Faddeev-Yakubovsky (FY)		-28.65(5)
Hyperspherical harmonics (HH)		-28.65(2)
CCSD level coupled-cluster theory (CC)		-28.44
Lambda-CCSD(T) (CC with triples corrections)		-28.63

E^{exp}=-28.296 MeV