Study of $A \leq 6$ helium clusters using soft-core potentials

Mario Gattobigio, A. Kievsky, and M. Viviani

Erice, 13 Octobre 2011

Institut nonlinéaire de Nice

Université Nice Sophia Antipolis

cnrs dépasser les frontières

Outline

METHOD

- Non-Symmetrized HH
  - Motivation
  - Jacobi and Hyperspherical Coordinates
  - HH properties - Raynal-Revai and Kil'dyushov coefficients
  - Hamiltonian (non)construction and diagonalization

Outline

METHOD

- Non-Symmetrized HH
  - Motivation
  - Jacobi and Hyperspherical Coordinates
  - HH properties - Raynal-Revai and Kil'dyushov coefficients
  - Hamiltonian (non)construction and diagonalization

APPLICATIONS

- Volkov Potential
  - Permutation symmetry
  - Symmetry breaking

Outline

METHOD

- Non-Symmetrized HH
  - Motivation
  - Jacobi and Hyperspherical Coordinates
  - HH properties - Raynal-Revai and Kil'dyushov coefficients
  - Hamiltonian (non)construction and diagonalization

APPLICATIONS

- Volkov Potential
  - Permutation symmetry
  - Symmetry breaking
- $A \leq 6$ helium clusters
  - Soft-core Potential description
  - Three-body force
  - Efimov physics

Method

Motivations

Motivations

- Hyperspherical Harmonics as systematic expansion basis

Motivations

- Hyperspherical Harmonics as systematic expansion basis
  - ☹ Difficulties in constructing A-particles basis functions with a given permutation symmetry
  - ☹ Difficulties to take care of permutation-symmetry-breaking terms

Motivations

- Hyperspherical Harmonics as systematic expansion basis
  - ☹ Difficulties in constructing A-particles basis functions with a given permutation symmetry
  - ☹ Difficulties to take care of permutation-symmetry-breaking terms
- Hyperspherical Harmonics without precise permutation symmetry

Motivations

- Hyperspherical Harmonics as systematic expansion basis
  - ☹ Difficulties in constructing A-particles basis functions with a given permutation symmetry
  - ☹ Difficulties to take care of permutation-symmetry-breaking terms
- Hyperspherical Harmonics without precise permutation symmetry
  - ☺ No need of symmetrization procedure
  - ☺ Simpler matrix-element calculations
  - ☺ Simpler permutation-breaking calculations
  - ☹ Bigger basis set

Motivations

- Hyperspherical Harmonics as systematic expansion basis
  - ☹ Difficulties in constructing A-particles basis functions with a given permutation symmetry
  - ☹ Difficulties to take care of permutation-symmetry-breaking terms
- Hyperspherical Harmonics without precise permutation symmetry
  - ☺ No need of symmetrization procedure
  - ☺ Simpler matrix-element calculations
  - ☺ Simpler permutation-breaking calculations
  - ☹ Bigger basis set
- Method to avoid Hamiltonian construction
  - ☺ Hamiltonian as $\sum \prod$(Sparse Matrices)
  - ☺ Iterative Diagonalization (ex. Lanczos)
  - ☺ Only action on a vector needed

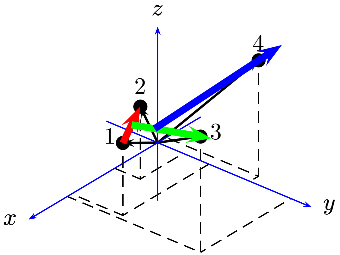
Jacobi's coordinates - $A \to N = A - 1$

Kinetic Energy

$$T = -\frac{\hbar^2}{2M}\nabla^2_{\vec{X}} - \frac{\hbar^2}{m}\sum_{i=1}^{N}\nabla^2_{\vec{x}_i}$$

Center of Mass

$$\vec{X} = \frac{1}{M}\sum_{i=1}^{A} m_i \vec{r}_i\,, \quad M = \sum_{i=1}^{A} m_i$$



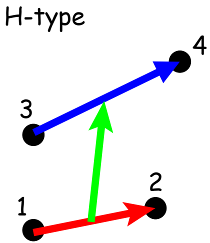
Jacobi's coordinates

$$\vec{x}_3 = \vec{r}_2 - \vec{r}_1$$

$$\vec{x}_2 = \sqrt{\frac{4}{3}}\left(\vec{r}_3 - \frac{\vec{r}_1 + \vec{r}_2}{2}\right)$$

$$\vec{x}_1 = \sqrt{\frac{3}{2}}\left(\vec{r}_4 - \frac{\vec{r}_1 + \vec{r}_2 + \vec{r}_3}{3}\right)$$

Different choices for Jacobi's coordinates



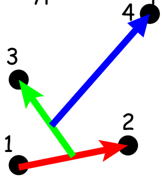
$$\vec{x}_3 = \vec{r}_2 - \vec{r}_1$$

$$\vec{x}_2 = \frac{\vec{r}_4 + \vec{r}_3}{\sqrt{2}} - \frac{\vec{r}_2 + \vec{r}_1}{\sqrt{2}}$$

$$\vec{x}_1 = \vec{r}_4 - \vec{r}_3$$

Different choices for Jacobi's coordinates

K-type 1–2 adapted



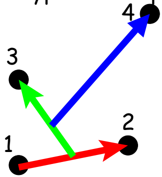
$$\vec{x}_3 = \vec{r}_2 - \vec{r}_1$$

$$\vec{x}_2 = \sqrt{\frac{4}{3}}\left(\vec{r}_3 - \frac{\vec{r}_1 + \vec{r}_2}{2}\right)$$

$$\vec{x}_1 = \sqrt{\frac{3}{2}}\left(\vec{r}_4 - \frac{\vec{r}_1 + \vec{r}_2 + \vec{r}_3}{3}\right)$$

Different choices for Jacobi's coordinates

K-type 1–2 adapted

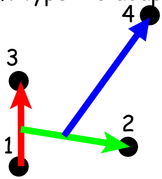


$$\vec{x}_3 = \vec{r}_2 - \vec{r}_1$$

$$\vec{x}_2 = \sqrt{\frac{4}{3}}\left(\vec{r}_3 - \frac{\vec{r}_1 + \vec{r}_2}{2}\right)$$

$$\vec{x}_1 = \sqrt{\frac{3}{2}}\left(\vec{r}_4 - \frac{\vec{r}_1 + \vec{r}_2 + \vec{r}_3}{3}\right)$$

K-type 1–3 adapted



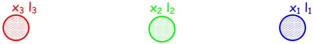
$$\vec{x}_3 = \vec{r}_3 - \vec{r}_1$$

$$\vec{x}_2 = \sqrt{\frac{4}{3}}\left(\vec{r}_2 - \frac{\vec{r}_1 + \vec{r}_3}{2}\right)$$

$$\vec{x}_1 = \sqrt{\frac{3}{2}}\left(\vec{r}_4 - \frac{\vec{r}_1 + \vec{r}_2 + \vec{r}_3}{3}\right)$$

Hyperspherical Coordinates

Hyperradius



$$\rho = \left(x_1^2 + x_2^2 + x_3^2\right)^{1/2}$$

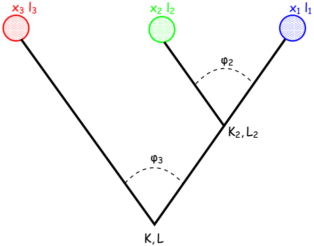
Hyperspherical Coordinates

Hyperradius

$$\rho = \left(x_1^2 + x_2^2 + x_3^2\right)^{1/2}$$

Hyperangles

$$\Omega_3 = (\hat{x}_1, \hat{x}_2, \hat{x}_3, \varphi_2, \varphi_3)$$



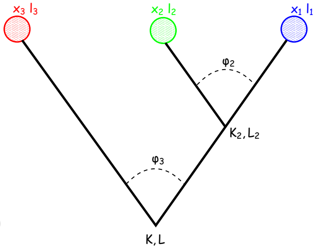
Hyperspherical Coordinates

Hyperradius

$$\rho = \left(x_1^2 + x_2^2 + x_3^2\right)^{1/2}$$

Hyperangles

$$\Omega_3 = (\hat{x}_1, \hat{x}_2, \hat{x}_3, \varphi_2, \varphi_3)$$

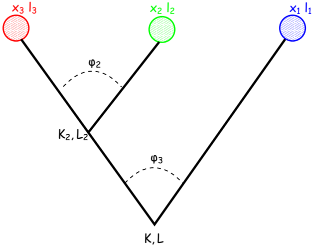


$$x_3 = \rho \cos \varphi_3$$
$$x_2 = \rho \sin \varphi_3 \cos \varphi_2$$
$$x_1 = \rho \sin \varphi_3 \sin \varphi_2$$

Hyperspherical Coordinates

Hyperradius

$$\rho = \left(x_1^2 + x_2^2 + x_3^2\right)^{1/2}$$



Hyperangles

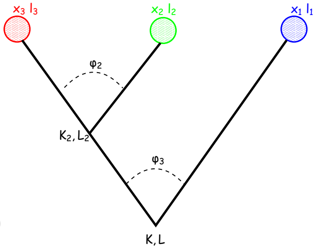
$$\Omega_3 = (\hat{x}_1, \hat{x}_2, \hat{x}_3, \varphi_2, \varphi_3)$$

$$x_3 = \rho \cos\varphi_3 \cos\varphi_2$$
$$x_2 = \rho \cos\varphi_3 \sin\varphi_2$$
$$x_1 = \rho \sin\varphi_3$$

Hyperspherical Coordinates

Hyperradius

$$\rho = \left(x_1^2 + x_2^2 + x_3^2\right)^{1/2}$$



Hyperangles

$$\Omega_3 = (\hat{x}_1, \hat{x}_2, \hat{x}_3, \varphi_2, \varphi_3)$$

$$x_3 = \rho \cos\varphi_3 \cos\varphi_2$$
$$x_2 = \rho \cos\varphi_3 \sin\varphi_2$$
$$x_1 = \rho \sin\varphi_3$$

Grand-Angular Momentum Λ_N^2

$$\Delta = \sum_{i=1}^{N} \nabla_{\mathbf{x}_i}^2 = \left(\frac{\partial^2}{\partial\rho^2} + \frac{3N-1}{\rho}\frac{\partial}{\partial\rho} + \frac{\Lambda_N^2(\Omega_N)}{\rho^2} \right)$$

Hyperspherical Harmonics

Defining Equation

$$\left(\Lambda_N^2(\Omega_N) + K(K + 3N - 2)\right)\mathcal{Y}_{[K]}(\Omega_N) = 0$$

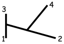
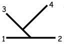
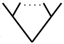
Hyperspherical Harmonics

Defining Equation

$$\left(\Lambda_N^2(\Omega_N) + K(K + 3N - 2)\right)\mathcal{Y}_{[K]}(\Omega_N) = 0$$

Memory of the coordinates

$\mathcal{Y}_{[K]}^{LM}(\Omega_N)$ depends on

- Jacobi: $\mathcal{Y}_{[K]}($  $) \neq \mathcal{Y}_{[K]}($  $)$
- Hyperspherical: $\mathcal{Y}_{[K]}($  $) \neq \mathcal{Y}_{[K]}($  $)$

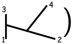
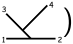
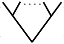
Hyperspherical Harmonics

Defining Equation

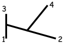
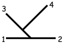
$$\left(\Lambda_N^2(\Omega_N) + K(K+3N-2)\right)\mathcal{Y}_{[K]}(\Omega_N) = 0$$

Memory of the coordinates

$\mathcal{Y}^{LM}_{[K]}(\Omega_N)$ depends on

- Jacobi: $\mathcal{Y}_{[K]}($  $) \neq \mathcal{Y}_{[K]}($  $)$
- Hyperspherical: $\mathcal{Y}_{[K]}($  $) \neq \mathcal{Y}_{[K]}($  $)$

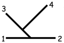
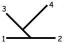
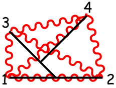
Raynal-Revai

$\mathcal{Y}_{[K]}($  $) = \sum_{K'} A^{(23)}_{[K],[K']}\mathcal{Y}_{[K']}($  $)$

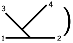
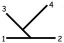
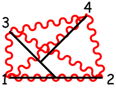
Kil'dyushov T-coefficients

$\mathcal{Y}_{[K]}($  $) = \sum_{K'} \mathcal{T}_{[K],[K']}\mathcal{Y}_{[K']}($  $)$

Potential Energy

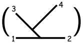
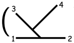
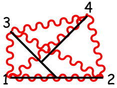
$V_{[K],[K']} = \langle \mathcal{Y}_{[K]}($  $)| \sum_{i<j}^{A} V(r_{ij}) |\mathcal{Y}_{[K']}($  $)\rangle =$ 

Potential Energy

$V_{[K],[K']} = \langle \mathcal{Y}_{[K]}($  $)| \sum_{i<j}^{A} V(r_{ij}) |\mathcal{Y}_{[K']}($  $)\rangle =$ 

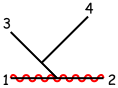
- ☹ Huge dimension of the basis
- ☹ Huge Dense Matrix!!!

Potential Energy

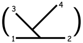
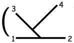
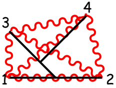
$V_{[K],[K']} = \langle \mathcal{Y}_{[K]}($  $)| \sum_{i<j}^{A} V(r_{ij}) | \mathcal{Y}_{[K']}($  $)\rangle =$ 

- ☹ Huge dimension of the basis
- ☹ Huge Dense Matrix!!!

BUT !!!

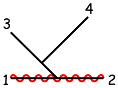
$V(r_{12}) =$ 

Potential Energy

$V_{[K],[K']} = \langle \mathcal{Y}_{[K]}($  $)| \sum_{i<j}^{A} V(r_{ij}) |\mathcal{Y}_{[K']}($  $)\rangle =$ 

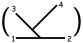
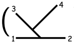
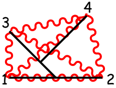
- ☹ Huge dimension of the basis
- ☹ Huge Dense Matrix!!!

BUT !!!

$V(r_{12}) =$ 

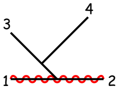
- ☺ Huge but Sparse Matrix!!!

Potential Energy

$V_{[K],[K']} = \langle \mathcal{Y}_{[K]}($  $)| \sum_{i<j}^{A} V(r_{ij}) |\mathcal{Y}_{[K']}($  $)\rangle =$ 

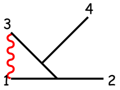
- ☹ Huge dimension of the basis
- ☹ Huge Dense Matrix!!!

BUT !!!

$V(r_{12}) =$ 

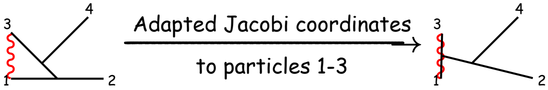
- ☺ Huge but Sparse Matrix!!!
- ☺ Sparse is Good!!!

“Adapted” Jacobi coordinates

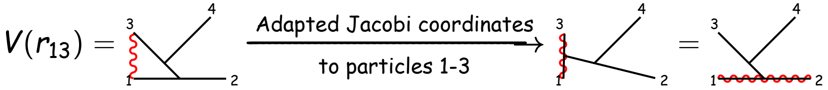
$V(r_{13}) =$ 

"Adapted" Jacobi coordinates

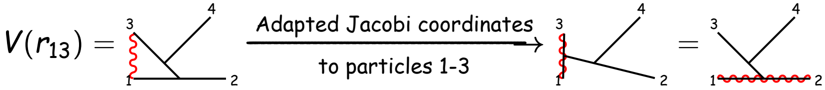
$V(r_{13}) =$



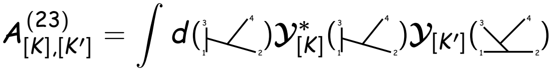
"Adapted" Jacobi coordinates



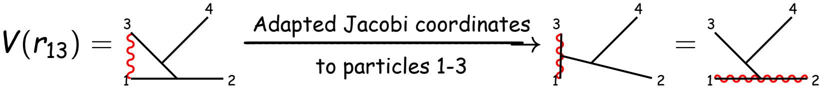
“Adapted” Jacobi coordinates



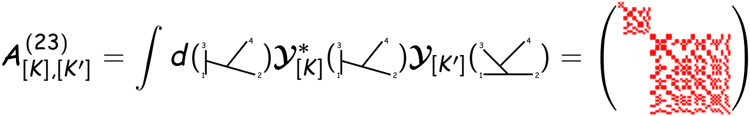
Rotation (Transposition) Matrix



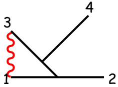
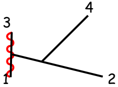
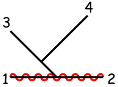
"Adapted" Jacobi coordinates



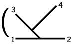
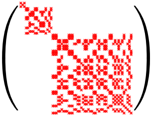
Rotation (Transposition) Matrix



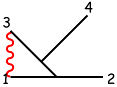
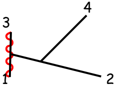
“Adapted” Jacobi coordinates

$V(r_{13}) =$  $\xrightarrow[\text{to particles 1-3}]{\text{Adapted Jacobi coordinates}}$  $=$ 

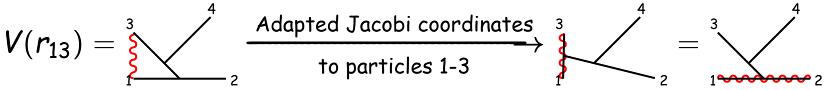
Rotation (Transposition) Matrix

$A^{(23)}_{[K],[K']} = \int d($  $)\mathcal{Y}^{*}_{[K]}($  $)\mathcal{Y}_{[K']}($  $) =$ 

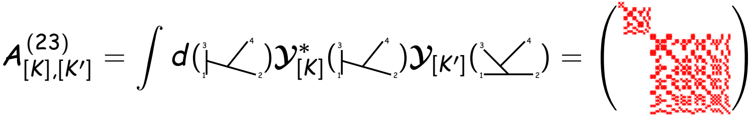
V_{13} as Product of Sparse Matrices

 $= A^{(23)} \cdot$  $\cdot A^{(23)}$

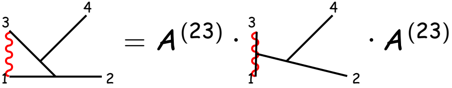
“Adapted” Jacobi coordinates



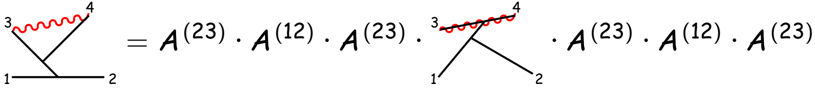
Rotation (Transposition) Matrix



V_{13} as Product of Sparse Matrices



Always possible! Use Jacobi-adjacent transpositions



Three-body force

Hyper-central three-body force

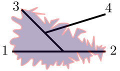
$$V^{(3)} = \sum_{i<j<k} W(\rho_{ijk}) \quad \text{with} \quad \rho_{ijk}^2 = \frac{2}{3}(r_{ij}^2 + r_{jk}^2 + r_{ik}^2)$$

Three-body force

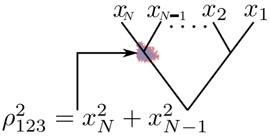
Hyper-central three-body force

$$V^{(3)} = \sum_{i<j<k} W(\rho_{ijk}) \quad \text{with} \quad \rho_{ijk}^2 = \frac{2}{3}(r_{ij}^2 + r_{jk}^2 + r_{ik}^2)$$

$\widetilde{W}(\rho_{123}) =$



$=$

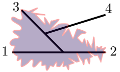


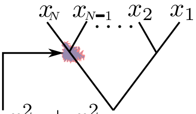
$=$ Sparse Matrix

Three-body force

Hyper-central three-body force

$$V^{(3)} = \sum_{i<j<k} W(\rho_{ijk}) \quad \text{with} \quad \rho_{ijk}^2 = \frac{2}{3}(r_{ij}^2 + r_{jk}^2 + r_{ik}^2)$$

$\widetilde{W}(\rho_{123}) =$ 

$=$ 

$= $ Sparse Matrix

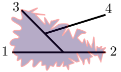
$$\rho_{123}^2 = x_N^2 + x_{N-1}^2$$

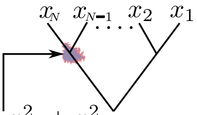
$$W(\rho_{123}) = \mathcal{T} \cdot \widetilde{W}(\rho_{123}) \cdot \mathcal{T}^\dagger$$

Three-body force

Hyper-central three-body force

$$V^{(3)} = \sum_{i<j<k} W(\rho_{ijk}) \quad \text{with} \quad \rho_{ijk}^2 = \frac{2}{3}(r_{ij}^2 + r_{jk}^2 + r_{ik}^2)$$

$\widetilde{W}(\rho_{123}) =$ 

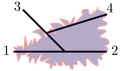
$=$ 

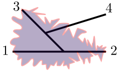
$= $ Sparse Matrix

$$\rho_{123}^2 = x_N^2 + x_{N-1}^2$$

$$W(\rho_{123}) = \mathcal{T} \cdot \widetilde{W}(\rho_{123}) \cdot \mathcal{T}^\dagger$$

Adapted Jacobi coordinates



$= A^{(12)} \cdot$ 

$\cdot A^{(12)}$

$$W(\rho_{124}) = A^{(12)} \cdot \mathcal{T} \cdot \widetilde{W}(\rho_{123}) \cdot \mathcal{T}^\dagger \cdot A^{(12)}$$

How to use Hyperspherical Harmonics

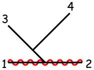
How to use Hyperspherical Harmonics

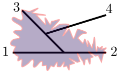
- Use the full set – Life is simpler!
  - Avoid the symmetrization step
  - Matrix elements easier to calculate
  - Simpler to introduce permutation-breaking terms

How to use Hyperspherical Harmonics

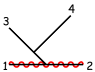
- Use the full set – Life is simpler!
  - Avoid the symmetrization step
  - Matrix elements easier to calculate
  - Simpler to introduce permutation-breaking terms
- $A^{(i\,i+1)}$ and $\mathcal{T}$ potential-independents
  - Calculated once for all - Library

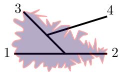
How to use Hyperspherical Harmonics

- Use the full set – Life is simpler!
  - Avoid the symmetrization step
  - Matrix elements easier to calculate
  - Simpler to introduce permutation-breaking terms
- $A^{(i\,i+1)}$ and $\mathcal{T}$ potential-independents
  - Calculated once for all - Library
- Only calculate $V(r_{12}) =$ 

and $\widetilde{W}(\rho_{123}) =$ 

How to use Hyperspherical Harmonics

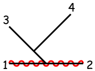
- Use the full set – Life is simpler!
  - Avoid the symmetrization step
  - Matrix elements easier to calculate
  - Simpler to introduce permutation-breaking terms
- $A^{(i\,i+1)}$ and $\mathcal{T}$ potential-independents
  - Calculated once for all - Library
- Only calculate $V(r_{12}) =$ 

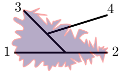
and $\widetilde{W}(\rho_{123}) =$ 

- Do not construct the Hamiltonian!!

$$H = \sum \left(\prod \text{Sparse Matrices} \right)$$

How to use Hyperspherical Harmonics

- Use the full set – Life is simpler!
  - Avoid the symmetrization step
  - Matrix elements easier to calculate
  - Simpler to introduce permutation-breaking terms
- $A^{(i\,i+1)}$ and $\mathcal{T}$ potential-independents
  - Calculated once for all - Library
- Only calculate $V(r_{12}) =$ 

and $\widetilde{W}(\rho_{123}) =$ 

- Do not construct the Hamiltonian!!

$$H = \sum \left(\prod \text{Sparse Matrices} \right)$$

Only action on a vector (Iterative Diagonalization)

$$\vec{v}_{out} = H \cdot \vec{v}_{in}$$

Applications

Volkov's Potential

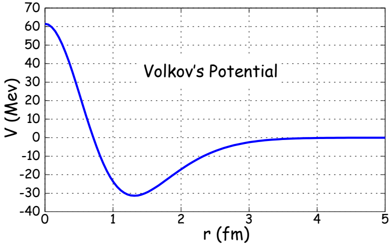
- Mass parameter

$$\hbar^2/m = 41.47 \text{ Mev fm}^2$$

- Potential

$$V(r) = E_1\, e^{-r^2/R_1^2} + E_2\, e^{-r^2/R_2^2}$$

- $E_1 = 144.86$ Mev, $R_1 = 0.82$ fm, $E_2 = -83.34$ Mev, $R_2 = 1.6$ fm



Volkov's Potential

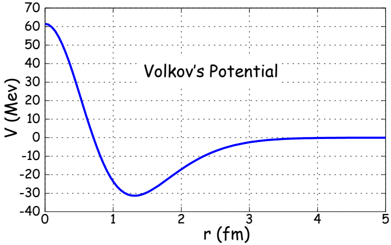
- Mass parameter

$$\hbar^2/m = 41.47 \text{ Mev fm}^2$$

- Potential

$$V(r) = E_1 \, e^{-r^2/R_1^2} + E_2 \, e^{-r^2/R_2^2}$$

- $E_1 = 144.86$ Mev, $R_1 = 0.82$ fm, $E_2 = -83.34$ Mev, $R_2 = 1.6$ fm



- S-wave potential – only acts when $l_{ij} = 0$

Spectrum & Symmetries

Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

Spectrum & Symmetries

Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

Spectrum & Symmetries

Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

- For $A = 6$ with Volkov potential ($L^\pi = 0^+$, $K = 22$)

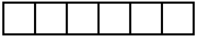
Spectrum & Symmetries

Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

- For $A = 6$ with Volkov potential ($L^{\pi} = 0^{+}$, $K = 22$)

-122.78 MeV [6] =  (1 level)

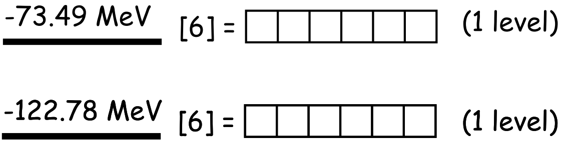
Spectrum & Symmetries

Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

- For $A = 6$ with Volkov potential ($L^\pi = 0^+$, $K = 22$)



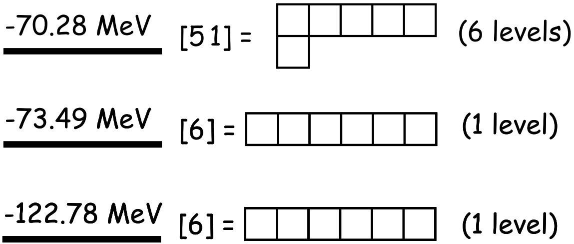
Spectrum & Symmetries

Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

- For $A = 6$ with Volkov potential ($L^\pi = 0^+$, $K = 22$)



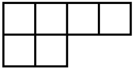
Spectrum & Symmetries

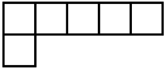
Permutation of the A particles is a symmetry

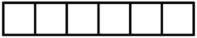
$$[H, S_A] = 0$$

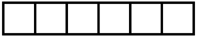
The Eigenvalues are organized according to irreps of S_A

- For $A = 6$ with Volkov potential ($L^\pi = 0^+$, $K = 22$)

-66.49 MeV [4 2] =  (9 levels)

-70.28 MeV [5 1] =  (6 levels)

-73.49 MeV [6] =  (1 level)

-122.78 MeV [6] =  (1 level)

Spectrum & Symmetries

Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

Spectrum & Symmetries

Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

... or irreps of subgroups ...

Spectrum & Symmetries

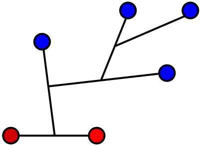
Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

... or irreps of subgroups ...

Coulomb Interaction



Spectrum & Symmetries

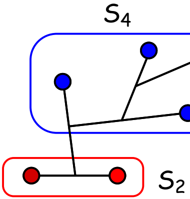
Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

... or irreps of subgroups ...

Coulomb Interaction



Spectrum & Symmetries

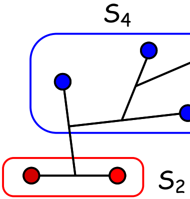
Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

... or irreps of subgroups ...

Coulomb Interaction



Symmetry breaking

$$S_6 \rightarrow S_2 \otimes S_4$$

Spectrum & Symmetries

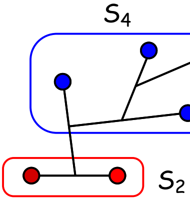
Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

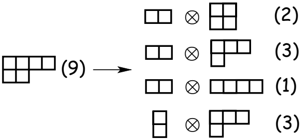
... or irreps of subgroups ...

Coulomb Interaction



Symmetry breaking

$$S_6 \to S_2 \otimes S_4$$



Spectrum & Symmetries

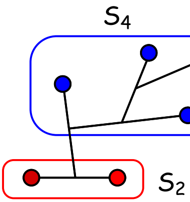
Permutation of the A particles is a symmetry

$$[H, S_A] = 0$$

The Eigenvalues are organized according to irreps of S_A

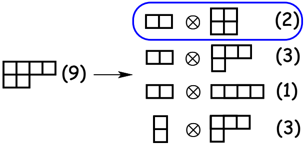
... or irreps of subgroups ...

Coulomb Interaction



Symmetry breaking

$$S_6 \rightarrow S_2 \otimes S_4$$

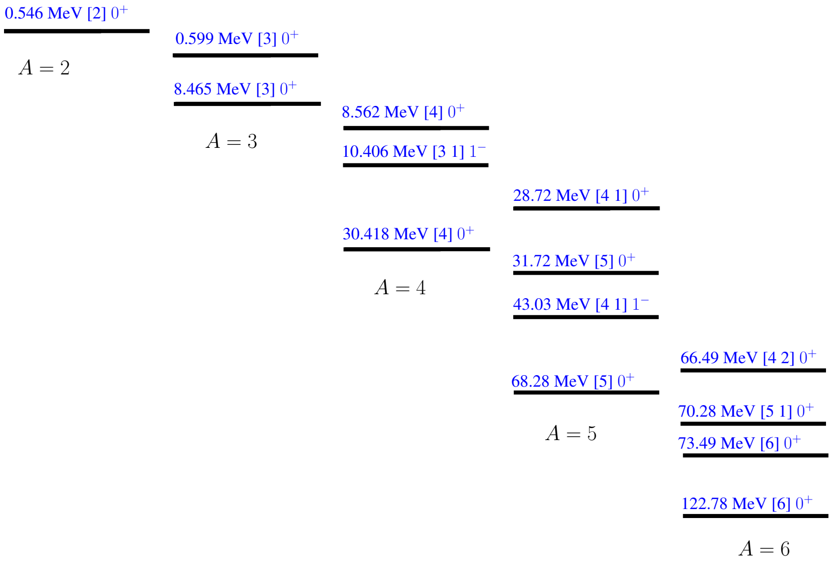


All-wave Volkov for $A = 6, L^{\pi} = 0^{+}$

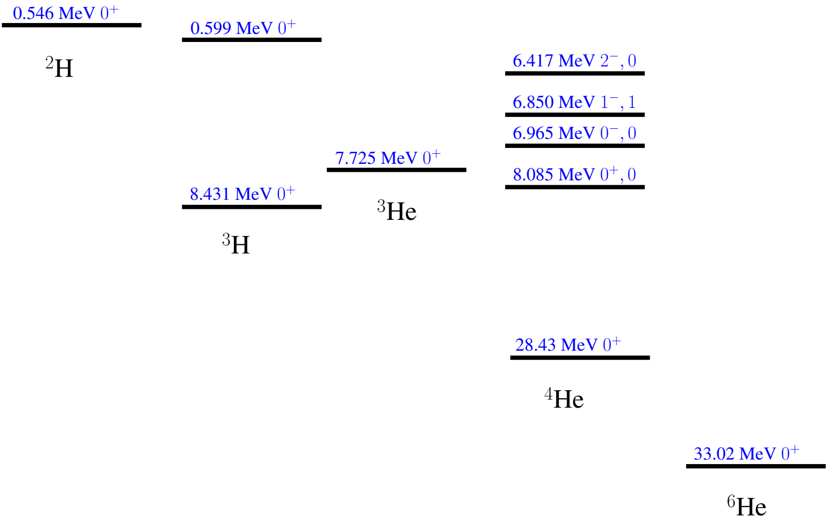
K_{max}	N_{HH}	E_0 (MeV) [6]	E_1 (MeV) [6]	E_2 (MeV) [5 1]	E_3 (MeV) [4 2]
2	15	117.205	64.701	62.513	61.142
4	120	118.861	69.450	64.277	62.015
6	680	120.345	70.544	66.268	63.377
8	3045	121.738	71.443	67.280	64.437
10	11427	122.317	71.923	68.371	65.354
12	37310	122.597	72.477	69.029	65.886
14	108810	122.711	72.822	69.531	66.201
16	288990	122.752	73.101	69.842	66.360
18	709410	122.768	73.284	70.051	66.437
20	1628328	122.774	73.407	70.189	66.474
22	3527160	122.776	73.485	70.283	66.491
SVM*					66.25

* K. Varga and Y. Suzuki, Phys. Rev. *C* **52**, 2885 (1995)

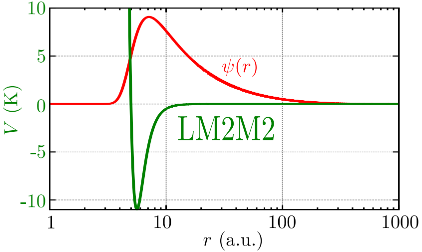
All-wave Volkov - Summary



S-wave Volkov - "Physics"



Helium Potential



- Helium-Helium interaction

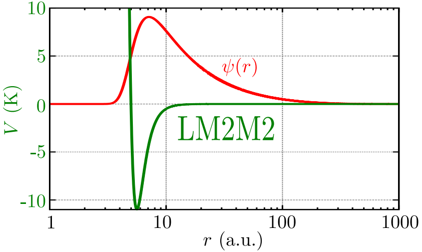
$\ell_{vdW} \approx 10a.u.$

$r_0 \approx 14$ a.u.

$a_0 \approx 190$ a.u.

$E_2 \approx -1.30$ mK

Helium Potential



- Helium-Helium interaction

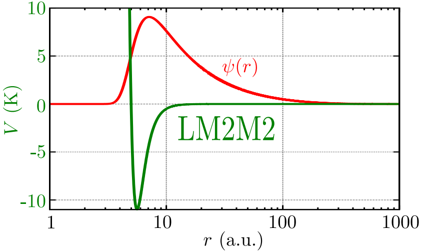
$$\ell_{vdW} \approx 10 a.u.$$
$$r_0 \approx 14 \text{ a.u.}$$
$$a_0 \approx 190 \text{ a.u.}$$
$$E_2 \approx -1.30 \text{ mK}$$

- Efimov physics

$$r_0/a_0 \approx (\hbar^2/2ma_0^2 - E_2)/E_2$$

$$E_3^{(0)} \simeq -126 \text{ mK} \quad \text{and} \quad E_3^{(1)} \simeq -2.3 \text{ mK}$$

Helium Potential



- Helium-Helium interaction

$$\ell_{vdW} \approx 10 a.u.$$
$$r_0 \approx 14 \text{ a.u.}$$
$$a_0 \approx 190 \text{ a.u.}$$
$$E_2 \approx -1.30 \text{ mK}$$

- Efimov physics

$$r_0/a_0 \approx (\hbar^2/2ma_0^2 - E_2)/E_2$$
$$E_3^{(0)} \simeq -126 \text{ mK} \quad \text{and} \quad E_3^{(1)} \simeq -2.3 \text{ mK}$$

- Strong short-range repulsion
  - Difficult to treat with orthogonal basis
  - Difficult to have converged excited states

Soft Two-Body Gaussian Potential

- Effective low-energy gaussian soft potential

$$V(r) = V_0 \; e^{-r^2/R^2}$$

  - Regularized contact interaction

Soft Two-Body Gaussian Potential

- Effective low-energy gaussian soft potential

$$V(r) = V_0 \; e^{-r^2/R^2}$$

  - Regularized contact interaction
  - Fix V_0 to reproduce one low-energy LM2M2 datum
  - Use the cut-off R to reproduce a second datum

$$V_0 = -1.227 \text{ K}$$
$$R = 10.03 \text{ a.u.}$$

$\Rightarrow$

	Soft-Gaussian	LM2M2
a_0 (a.u.)	189.95	189.05
r_0 (a.u.)	13.85	13.84
E_2 (mK)	-1.296	-1.302

Soft Two-Body Gaussian Potential

- Effective low-energy gaussian soft potential

$$V(r) = V_0 \; e^{-r^2/R^2}$$

  - Regularized contact interaction
  - Fix V_0 to reproduce one low-energy LM2M2 datum
  - Use the cut-off R to reproduce a second datum

$V_0 = -1.227$ K

$R = 10.03$ a.u.

$\Rightarrow$

	Soft-Gaussian	LM2M2
a_0 (a.u.)	189.95	189.05
r_0 (a.u.)	13.85	13.84
E_2 (mK)	-1.296	-1.302

- Problem in the three-body sector

	Soft-Gaussian	LM2M2
$E_3^{(0)}$ (mK)	-150.4	-126.4
$E_3^{(1)}$ (mK)	-2.467	-2.265

Soft Hyper-Central Three-Body Potential

- Effective low-energy three-body-soft potential

$$W(\rho_{ijk}) = W_0 \; e^{-2\rho_{ijk}^2/\rho_0^2}$$

  - Regularized three-body-contact interaction

Soft Hyper-Central Three-Body Potential

- Effective low-energy three-body-soft potential

$$W(\rho_{ijk}) = W_0 \; e^{-2\rho_{ijk}^2/\rho_0^2}$$

  - Regularized three-body-contact interaction

potential	$E_{3b}^{(0)}$ (mK)	$E_{3b}^{(1)}$ (mK)
LM2M2	−126.4	−2.265
gaussian	−150.4	−2.467
(W_0 [K], ρ_0 [a.u.])		
(306.9, 4)	−126.4	−2.283
(18.314, 6)	−126.4	−2.287
(4.0114, 8)	−126.4	−2.289
(1.4742, 10)	−126.4	−2.292
(0.721, 12)	−126.4	−2.295
(0.422, 14)	−126.4	−2.299
(0.279, 16)	−126.4	−2.302

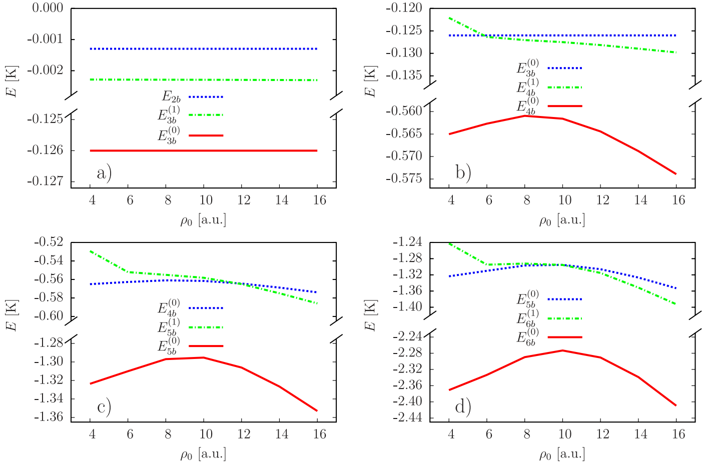
Helium Clusters with Soft Potential

- Soft Potential sum of two- and three-body terms

K	$E_{4b}^{(0)}$[mK]	$E_{4b}^{(1)}$[mK]	$E_{5b}^{(0)}$[mK]	$E_{5b}^{(1)}$[mK]	$E_{6b}^{(0)}$[mK]	$E_{6b}^{(1)}$[mK]
0	538.93	4.557	1288.1	365.1	2293.8	1109.9
2	538.93	4.557	1288.1	365.1	2293.8	1109.9
4	561.69	40.29	1319.6	460.4	2331.8	1237.3
6	566.68	67.47	1324.4	497.6	2336.6	1273.0
8	568.21	84.22	1326.1	527.0	2338.4	1307.7
10	568.58	96.04	1326.5	542.7	2338.7	1323.1
12	568.73	105.30	1326.6	554.0	2338.8	1334.4
14	568.77	111.17	1326.6	561.0	2338.9	1340.9
16	568.78	115.58	1326.6	565.9	2338.9	1345.3
18	568.79	118.78	1326.6	569.3	2338.9	1348.2
20	568.79	121.20	1326.6	571.8	2338.9	1350.2
22	568.79	122.98	1326.6	573.6	2338.9	1351.6
24	568.79	124.38	1326.6	574.9		
26	568.79	125.47				
28	568.79	126.33				
30	568.79	127.02				
32	568.79	127.57				
34	568.79	128.02				
36	568.79	128.40				
38	568.79	128.70				
40	568.79	128.96				
Lewerenz, JCP **106**, 4596 (1997)	558.4		1302.2		2319.4	
Blume&Greene, JCP **112**, 8053 (2000)	559.7	132.6	1309.3	597.1	2329.4	1346.7

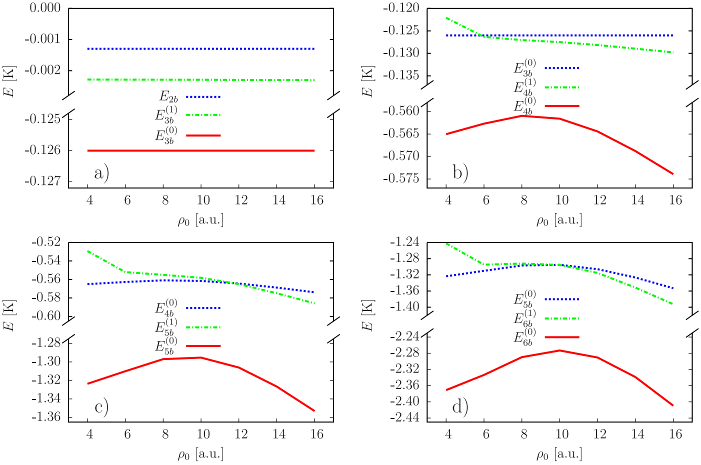
Helium Clusters with Soft Potential

- Ground and Excited states for ^4He_A with $A \leq 6$



Helium Clusters with Soft Potential

- Ground and Excited states for ^4He_A with $A \leq 6$



- The range ρ_0 is not independent . . .

$$\rho_0^2/2 \geq R^2 \quad \Rightarrow \quad \rho_0 \gtrsim 14 \text{ a.u.}$$

Helium Clusters with Soft Potential

- Two + Three Soft potential for $A \le 6$ Helium clusters
- $r_0/a_0 \approx 7\%$

Helium Clusters with Soft Potential

- Two + Three Soft potential for $A \leq 6$ Helium clusters
- $r_0/a_0 \approx 7\%$
- For (each?) Efimov state
  - Two Four-Body states
  - Two Five-Body states
  - Two Six-Body states
- Second $4 < A < 6$ excited state above the threshold and not bosonic!

Helium Clusters with Soft Potential

- Two + Three Soft potential for $A \leq 6$ Helium clusters
- $r_0/a_0 \approx 7\%$
- For (each?) Efimov state
  - Two Four-Body states
  - Two Five-Body states
  - Two Six-Body states
- Second $4 < A < 6$ excited state above the threshold and not bosonic!
- Universal ratios

ρ_0 [a.u.]	$E^{(0)}_{4b}/E^{(0)}_{3b}$	$E^{(1)}_{4b}/E^{(0)}_{3b}$	$E^{(0)}_{5b}/E^{(0)}_{3b}$	$E^{(1)}_{5b}/E^{(0)}_{4b}$	$E^{(0)}_{6b}/E^{(0)}_{3b}$	$E^{(1)}_{6b}/E^{(0)}_{5b}$
12	4.47	1.01	10.33	1.001	18.12	1.005
14	4.50	1.02	10.50	1.011	18.50	1.018
16	4.54	1.03	10.70	1.021	19.06	1.029

Conclusions

Method

Conclusions

Method

- Hyperspherical Harmonics is a good basis set

Conclusions

Method

- Hypersppherical Harmonics is a good basis set
    - ☛ How to use it?
    - ✔ Do not symmetryze the basis set!

Conclusions

Method

- Hypersperical Harmonics is a good basis set
  - ☛ How to use it?
  - ✔ Do not symmetryze the basis set!
  - ☛ What about the Huge-Basis Dimension?
  - ✔ Do not contruct the Hamiltonian!

Conclusions

Method

- Hyperspherical Harmonics is a good basis set
  - ☛ How to use it?
  - ✔ Do not symmetryze the basis set!
  - ☛ What about the Huge-Basis Dimension?
  - ✔ Do not contruct the Hamiltonian!

MG, A. Kievsky, M. Viviani, and P. Barletta, PRA **79**, 032513 (2009)
MG, A. Kievsky, and M. Viviani, PRC **83**, 024001 (2011)

Conclusions

Method

- Hyperspherical Harmonics is a good basis set
  - ☛ How to use it?
  - ✔ Do not symmetryze the basis set!
  - ☛ What about the Huge-Basis Dimension?
  - ✔ Do not contruct the Hamiltonian!

MG, A. Kievsky, M. Viviani, and P. Barletta, PRA **79**, 032513 (2009)

MG, A. Kievsky, and M. Viviani, PRC **83**, 024001 (2011)

Application

Conclusions

Method

- Hyperspherical Harmonics is a good basis set
  - ☛ How to use it?
  - ✔ Do not symmetryze the basis set!
  - ☛ What about the Huge-Basis Dimension?
  - ✔ Do not contruct the Hamiltonian!

MG, A. Kievsky, M. Viviani, and P. Barletta, PRA **79**, 032513 (2009)
MG, A. Kievsky, and M. Viviani, PRC **83**, 024001 (2011)

Application

- Helium Cluster up to A=6 - Excited states too!

Conclusions

Method

- Hyperspherical Harmonics is a good basis set
  - ☛ How to use it?
  - ✔ Do not symmetryze the basis set!
  - ☛ What about the Huge-Basis Dimension?
  - ✔ Do not contruct the Hamiltonian!

MG, A. Kievsky, M. Viviani, and P. Barletta, PRA **79**, 032513 (2009)
MG, A. Kievsky, and M. Viviani, PRC **83**, 024001 (2011)

Application

- Helium Cluster up to A=6 - Excited states too!
  - ☛ How to deal with hard-core potentials?
  - ✔ Use soft two- and three-body forces!

Conclusions

Method

- Hyperspherical Harmonics is a good basis set
  - ☛ How to use it?
  - ✔ Do not symmetryze the basis set!
  - ☛ What about the Huge-Basis Dimension?
  - ✔ Do not contruct the Hamiltonian!

MG, A. Kievsky, M. Viviani, and P. Barletta, PRA **79**, 032513 (2009)
MG, A. Kievsky, and M. Viviani, PRC **83**, 024001 (2011)

Application

- Helium Cluster up to A=6 - Excited states too!
  - ☛ How to deal with hard-core potentials?
  - ✔ Use soft two- and three-body forces!
  - ✔ Universality in $A > 3$ bound states

MG, A. Kievsky, and M. Viviani, arXiv:1106.3853, accepted PRA