Hyperspherical formalism and its applications from light nuclei to light atomic clusters

N.K. Timofeyuk

University of Surrey
1966  HH method introduced into nuclear physics (Simonov and Badalian).
      First applications to $^3$H and $^3$He

1970s  First generalization to $A > 4$ nuclei (Baz, Demin, Zhukov)
      Development of mathematical background behind the HH method basing on group theory, fractional parentage expansions of HHs (Smirnov, Shitikova)
      Applications to p-shell nuclei, giant monopole resonances (Shitikova)
      Applications to deformed nuclei (Grin, Kochetov)
      First study of $^3$H and $^3$He with realistic forces known at that time (Demin, Efros)
      Methods to include binary channels, first application to $^4$He+n scattering (Baz, Zhukov)
      Potential harmonics (Efros)

1980s  Adiabatic approximation to the HH method (F. De la Ripelle)
      Integro-differential equations (F. De la Ripelle)
      First applications to Borromean nuclei
1990s  Correlated HH expansion for bound and unbound $A = 3,4$ systems, application to scattering and reactions (Rosati, Viviani, Kievsky)
Electromagnetic properties of $A=3,4$ nuclei using Integral Transforms (Efros, Orlandini, Leidemann)
Continuum response in Borromean nuclei (Danilin, Thompson, Zhukov)

1999  Correlated HHs for $A > 4$ nuclei (N. Barnea)

2000s  Effective interactions and projected Faddeev-Yakubovskii equations for $A < 6$ nuclei (N. Barnea)
Construction of HHs for arbitrary $A$ using link to the shell model states (Timofeyuk)
Construction of HHs responsible for long-range behaviour (Timofeyuk)

2010s  Effective hyperspherical interactions for non-local potentials (Barnea, Leidemann, Orlandini)
3N and 4N scattering with bound-state-like functions (Kievsky et al)
Three-body model

3-body system is described by 6 co-ordinates:

$x \ \theta_x \ \varphi_x \ \rightarrow \ \ y \ \theta_y \ \varphi_y$

Hyperspherical co-ordinates for 3-body system:
Hypperradius $\rho$,
Hyperangles: $\alpha, \theta_x, \varphi_x, \theta_y, \varphi_y$

$x = \rho \cos \alpha \quad \quad \rho^2 = x^2 + y^2$
$y = \rho \sin \alpha \quad \quad \quad \quad \quad \quad \quad \alpha = \arctan(y/x)$
Kinetic energy operator in hyperspherical co-ordinates

\[ T = -\frac{\hbar^2}{2m} \left( \frac{1}{\rho^5} \frac{\partial}{\partial \rho} \left( \rho^5 \frac{\partial}{\partial \rho} \right) - \frac{1}{\rho^2} \Delta \rho \right) \]

Eigenvalues and eigenfunctions of $\Delta \rho$ (hyperspherical harmonics)

\[ \Delta \hat{\rho} Y_{Kl_xl_y} (\hat{\rho}) = K(K + 4) Y_{Kl_xl_y} (\hat{\rho}) \]

$K$ is the hypermoment

Explicit expression for HHs

\[ Y_{Kl_xl_ym_xm_y} (\hat{\rho}) = N_{Kl_xl_y} \cos^{l_x} \alpha \sin^{l_y} \alpha \]

\[ \times P_{(K-l_x-l_y)/2}^{l_y+1/2,l_x+1/2} (\cos 2\alpha) Y_{l_xm_x} (\hat{x}) Y_{l_ym_y} (\hat{y}) \]

$P$ is Jacobi polynomial

HHs $Y$ are supplemented by spin-isospin part and then antisymmetrized.
The 3-body wave function is expanded onto hyperspherical functions basis

\[ \Psi(1,2,3) = \rho^{-5/2} \sum_{K=K_{\text{min}},Y}^{\infty} \chi_{K \gamma}(\rho) Y_{K \gamma}(\hat{\rho}) \]

The hyperradial functions \( \chi_{K \gamma}(\rho) \) satisfy the system of coupled differential equations:

\[
\left( \frac{d^2}{d \rho^2} - \frac{L_K(L_K + 1)}{\rho^2} \right) \chi_{K \gamma}(\rho) = \frac{2m}{\hbar^2} \left( E + V_{K \gamma,K \gamma} \right) \chi_{K \gamma}(\rho) + \frac{2m}{\hbar^2} \sum_{K' \gamma' \neq K \gamma} V_{K \gamma,K' \gamma'}(\rho) \chi_{K' \gamma'}(\rho)
\]

where \( L_K = K + 3/2 \) and \( m \) is the nucleon mass.

The hyperradial potentials

\[ V_{K \gamma,K' \gamma'}(\rho) = \langle Y_{K \gamma}(\hat{\rho}) | \sum_{i<j} V_{ij}(\rho - \rho_j) | Y_{K' \gamma'}(\hat{\rho}) \rangle \]

are calculated using Raynal-Revai transformation coefficients.
## Properties of $^3\text{H}$


<table>
<thead>
<tr>
<th>Potential</th>
<th>$B$</th>
<th>$\langle T \rangle$</th>
<th>$r_p$</th>
<th>$r_n$</th>
<th>$P_{S'}$</th>
<th>$P_P$</th>
<th>$P_D$</th>
<th>$P_{T=3/2}$</th>
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<tr>
<td>AV8$'$</td>
<td>7.767</td>
<td>47.605</td>
<td>1.642</td>
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<td>1.273</td>
<td>0.067</td>
<td>8.579</td>
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<td>45.678</td>
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<td>1.828</td>
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<td>1.293</td>
<td>0.066</td>
<td>8.510</td>
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<td>NJ2</td>
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<td>1.647</td>
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<td>0.064</td>
<td>8.329</td>
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<td>1.568</td>
<td>1.715</td>
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<td>0.026</td>
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<td>7.998</td>
<td>37.630</td>
<td>1.618</td>
<td>1.771</td>
<td>1.310</td>
<td>0.047</td>
<td>7.018</td>
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<td>1.655</td>
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<td>N3LO-Jülich</td>
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<td>4.316</td>
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<td>1.574</td>
<td>1.713</td>
<td>1.330</td>
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<td>4.062</td>
<td>0.0016</td>
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<td>AV18/UIX</td>
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<td>51.275</td>
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<td>–</td>
<td>1.60</td>
<td>–</td>
<td>–</td>
<td>–</td>
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<td>–</td>
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</table>
n-d scattering at 3 MeV with AV18 + N2LOL

Application to Borromean nuclei

Bound states:

\[ ^6\text{He} = ^4\text{He} + n + n \]
\[ ^{11}\text{Li} = ^9\text{Li} + n + n \]
\[ ^{14}\text{Be} = ^{12}\text{Be} + n + n \]
\[ ^{17}\text{B} = ^{15}\text{B} + n + n \]
\[ ^{17}\text{Ne} = ^{15}\text{O} + p + p \]
\[ ^{22}\text{C} = ^{20}\text{C} + n + n \]

3-body resonances

\[ ^6\text{Be} = ^4\text{He} + p + p \]
\[ ^5\text{H} = ^3\text{H} + n + n \]
\[ ^{10}\text{He} = ^8\text{He} + n + n \]
\[ ^{12}\text{O} = ^{10}\text{C} + p + p \]
\[ ^{16}\text{Ne} = ^{14}\text{O} + p + p \]
\[ ^{19}\text{Mg} = ^{17}\text{Ne} + p + p \]
\[ ^{45}\text{Fe} = ^{43}\text{Cr} + p + p \]
\[ ^{54}\text{Zn} = ^{52}\text{Ni} + p + p \]

Transitions from bound states to continuum.
$^{22}\text{C} = ^{20}\text{C} + n + n$


FIG. 6. (Color online) Calculated $^{22}\text{C}$ dipole strength function distributions for separation energies $S_{2n} = 50$, 100, 200, and 400 keV (upper to lower curves). The insert compares dipole strength distributions for $S_{2n} = 10$ keV (upper line) and 50 keV (lower line).
\[ \alpha + \alpha + \alpha \rightarrow ^{12}\text{C} \]

*N. B. Nguyen, F. M. Nunes, I. J. Thompson, and E. F. Brown, PRL 109, 141101 (2012)*

HHR:

- HHs expansion
- R-matrix
- R-matrix propagation
- screening technique
Non-Borromean $^{12}\text{Be}$ in the $^{10}\text{Be}+n+n$ model

Deformation and excitation of the $^{10}\text{Be}$ core as in

$n+^{10}\text{Be}$ interaction in all partial waves,
$^{11}\text{Be}(1/2^+)$ and $^{11}\text{Be}(1/2^-)$ energies are reproduced

Antisymmetrization is taken into account using Pauli projections technique.
GPT potential for NN interaction, hyperspherical expansion to $K_{\text{max}} = 34$

$^{12}\text{Be}$ probability density
Overlap integral \( \langle {}^{11}\text{Be} | {}^{12}\text{Be} \rangle \)


At large \( r \) \( I(r) \sim \exp(-kr)/r \)

- Abnormally slow convergence to true asymptotic
- Enlarged rms radius due to nn correlations

<table>
<thead>
<tr>
<th>SF</th>
<th>( \langle r^2 \rangle^{\frac{1}{2}} )</th>
<th>( \langle r^2 \rangle_{\text{standard}}^{\frac{1}{2}} )</th>
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<td>( \frac{1}{2}^+ )</td>
<td>0.325</td>
<td>4.413</td>
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<tr>
<td>( \frac{1}{2}^- )</td>
<td>0.110</td>
<td>3.588</td>
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<td>( \frac{5}{2}^+ )</td>
<td>0.322</td>
<td>3.738</td>
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<tr>
<td>( E^{(12}\text{Be)} )</td>
<td>= 3.641 MeV</td>
<td></td>
</tr>
<tr>
<td>( E_{\exp}^{(12}\text{Be)} )</td>
<td>= 3.673 ( \pm ) 0.015 MeV</td>
<td></td>
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</table>
Co-ordinates in the A-body system:

- Individual: \( \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A \)

- Jacobi: \( \xi_i = \sqrt{\frac{i}{i+1}} \left( \frac{1}{i} \sum_{j=1}^{i} r_j - r_{i+1} \right) \)

- Hyperspherical: hyperradius \( \rho \), hyperangles \( \theta_1, \theta_2, \ldots, \theta_{3A-4} \)

\[
\begin{align*}
\xi_1 &= \rho \sin \theta_{3A-4} \cdots \sin \theta_2 \sin \theta_1, \\
\xi_2 &= \rho \sin \theta_{3A-4} \cdots \sin \theta_2 \cos \theta_1, \\
&\quad \vdots \\
\xi_{3A-4} &= \rho \sin \theta_{3A-4} \cos \theta_{3A-5}, \\
\xi_{3A-3} &= \rho \cos \theta_{3A-4}.
\end{align*}
\]

\[
\rho^2 = \sum_{i=1}^{A-1} \xi_i^2 = \sum_{i=1}^{A} r_i^2 - R_A^2 = \frac{1}{A} \sum_{i<j}^{A} (r_i - r_j)^2
\]
Hyperspherical Harmonics Method for $A > 3$

- In hyperspherical coordinates, the operator of kinetic energy is separated into hyperradial and hyperangular parts.

\[
T = -\frac{\hbar^2}{2m}\left(\frac{1}{\rho^{n-1}} \frac{\partial}{\partial \rho} \left( \rho^{n-1} \frac{\partial}{\partial \rho} \right) - \frac{1}{\rho^2} \Delta_{\rho} \right), \quad n = 3A - 3
\]

- The eigenfunctions $Y_{K\gamma}(\hat{\rho})$ of the hyperangular part $\Delta_{\rho}$ are the hyperspherical harmonics. $K$ is a hyperangular momentum.

\[
\Delta_{\rho} Y_{K\gamma}(\hat{\rho}) = K (K + 3A - 5) Y_{K\gamma}(\hat{\rho})
\]

\[
Y_{K\gamma}(\hat{\rho}) = Y_{l_1,m_1}(\hat{\xi}_1) \prod_{i=2}^{A-1} \mathcal{N}_{K_{i-1}l_i} \left( \sin \phi_i \right)^{l_i} \left( \cos \phi_i \right)^{K_{i-1}}
\]

\[
\times P_{(K_i - K_{i-1})/2}^{l_i + 1/2, (3i - 5)/2} \left( \cos 2\phi_i \right) Y_{l_i m_i}(\hat{\xi}_i)
\]
Schrödinger equation in hyperspherical coordinates

The wave function A-body wave function is expanded onto complete set of hyperspherical functions.

$$\Psi(1, 2, \ldots, A) = \rho^{-(3A-4)/2} \sum_{K=K_{\text{min}}, \gamma}^{\infty} \chi_{K\gamma}(\rho) Y_{K\gamma}(\hat{\rho})$$

where $K = K_{\text{min}}, K_{\text{min}} + 2, K_{\text{min}} + 4, \ldots \infty$

$$\left( -\frac{d^2}{d\rho^2} - \frac{L_K(L_K+1)}{\rho^2} - \frac{2m}{\hbar^2}(E + V_{K\gamma,K\gamma}) \right) \chi_{K\gamma}(\rho) = \frac{2m}{\hbar^2} \sum_{K'\gamma' \neq K\gamma} V_{K\gamma,K'\gamma'}(\rho) \chi_{K'\gamma'}(\rho)$$

where $L_K = K + (3A - 6)/2$ and $m$ is the particle mass.

The hyperradial potentials $V_{K\gamma,K'\gamma'}(\rho) = \langle Y_{K\gamma}(\hat{\rho}) | \sum_{i<j} V_{ij} (r_i - r_j) | Y_{K'\gamma'}(\hat{\rho}) \rangle$ play the role of a self-consistent collective mean field created by all particles.
Acceleration of convergence

Pair-correlated HHs and Faddeev equations
Fractional parentage technique to construct HHs
(Barnea, Leidemann, Orlandini, Nucl.Phys. A 650, 427 (1999))

Binding energy of $^8\text{Be}(0^+)$ for various NN potentials

<table>
<thead>
<tr>
<th>$K_{\text{max}}$</th>
<th>$N_{HH}$</th>
<th>BI</th>
<th>MT-I/III</th>
<th>MTV</th>
<th>MS3</th>
<th>VV</th>
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<tr>
<td>4</td>
<td>1</td>
<td>56.71</td>
<td>52.82</td>
<td>134.29</td>
<td>31.19</td>
<td>147.42</td>
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<tr>
<td>6</td>
<td>4</td>
<td>65.39</td>
<td>59.31</td>
<td>137.72</td>
<td>38.08</td>
<td>148.70</td>
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<tr>
<td>8</td>
<td>15</td>
<td>70.03</td>
<td>60.64</td>
<td>137.80</td>
<td>42.11</td>
<td>148.49</td>
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<td>TICI$_{SI}$</td>
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<td>49.18</td>
<td>46.67</td>
<td>129.25</td>
<td>26.26</td>
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<td>TICI$_{SD}$</td>
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<td>61.30</td>
<td>52.67</td>
<td>130.23</td>
<td>37.30</td>
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TICI$_{SI}$ translation invariant configuration interaction (state independent) method
TICI$_{SD}$ translation invariant configuration interaction (state dependent) method
Effective interactions for Hyperspherical Harmonics (EIHH) method
(Barnea, Leidemann, Orlandini)

- Model space is split into P and Q: \( P + Q = 1 \)
- Schrodinger equation in hyperspherical co-ordinates is solved in the space P
- Effective interactions in the P-space are found using Lee-Suzuki similarity transformation
- Fractional parentage technique to construct HHs

Applications:

- Minnesota and Malfliet-Tjon NN potentials (PRC61, 054001 (2000))
- Phenomenological AV6, AV14 with non-central forces (NP A693, 565 (2001))
- Improved effective interactions and phenomenological NN potential AV8’ (PRC 67, 054003 (2003))
- EFT non-local potential (Idaho-N3LO) (PRC 81, 064001 (2010))
- Chiral low momentum interaction (S. Bacca, N. Barnea and A. Schwenk, PRC 86, 034321 (2012))
$^4\text{He}$ calculated with chiral $V_{\text{low }k}$ NN interaction

Ground-state energy

Point proton r.m.s. radius

S. Bacca, N. Barnea and A. Schwenk, PRC 86, 034321 (2012)
$^6$He calculated with chiral $V_{\text{low } k}$ NN interaction

Ground-state energy

Point proton r.m.s. radius

S. Bacca, N. Barnea and A. Schwenk, PRC 86, 034321 (2012)
Matter and proton radii of $^6$He in comparison to experiment
S. Bacca, N. Barnea and A. Schwenk, PRC 86, 034321 (2012)
Shell model approach to construction of hyperspherical harmonics

If the two-body interaction is harmonic oscillator:

\[ V_{ij}(|r_i - r_j|) = \frac{1}{2} m \omega^2 (|r_i - r_j|)^2 \]

then the Hamiltonian is

\[ H = -\frac{\hbar^2}{2m} \left( \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left( \rho^{n-1} \frac{\partial}{\partial \rho} \right) - \frac{1}{\rho^2} \Delta_{\hat{\rho}} \right) + \frac{1}{2} m \omega^2 \rho^2 \]

The eigenvalues are

\[ E_N = (2 \kappa + K + n/2) \hbar \omega = (N+n/2) \hbar \omega, \quad n = 3A - 3 \]

The eigenfunctions are

\[ \Psi_{NK\gamma}(\rho, \hat{\rho}) = R_{KK}(\rho) Y_{K\gamma}(\hat{\rho}) \]

On the other hand

\[ \Psi_{NK\gamma}(\rho, \hat{\rho}) = \Sigma_i C_i^{NK\gamma} D_i^{N}(r_1, r_2, ..., r_A) / \Phi_{000}(R_A) \]
The hyperspherical harmonic $Y_{K\gamma}(\hat{\rho})$ can be constructed with the help of the Slater determinants $D_i(r_1, r_2...r_A)$ with $K$ oscillator quanta:

$$Y_{K\gamma}(\hat{\rho}) = \frac{\sum_i C_i^K D_i^K (r_1, r_2...r_A)}{\Phi_{000}(R_A) R_{0K}(\rho)}$$

0s oscillations of the centre of mass

$$R_{0K}(\rho) = A_K \left(\frac{\rho}{b}\right)^K e^{-\rho^2/2b^2}$$

Algorithm to find the expansion coefficients $C_i^K$

- To construct the hyperspherical harmonics with hypermoment $K$, the Slater determinants of the oscillator shell model with the total number of quanta equal to $K$ are used. These Slater determinants are made of the single particle states with quantum numbers \{n, l, m, \sigma, \tau\}.

- To get well-defined LST values
  - Matrix $L^2$ is constructed and then diagonalised
  - Matrix $S^2$ is constructed and then diagonalised
  - Matrix $T^2$ is constructed and then diagonalised

- To get the states with well-defined permutational symmetry $[f]$, the second Casimir operator $\Sigma^A_{i<j} (i,j)$ of the symmetrical group is diagonalised.

- Matrix $R^2$ is diagonalised to get rid of centre-of-mass excitations.

- The hyperradial excitations are removed (two ways):
  - Hyperradial excitations are explicitly constructed and then removed (N.K. Timofeyuk, Phys. Rev. C65, 064306 (2002))
  - The matrix of angular part of multidimensional Laplacian expressed in individual nucleon coordinates is constructed and then diagonalised (N.K. Timofeyuk, Phys. Rev. C78, 054314 (2008))
Calculation of matrix elements

The HSFM matrix elements of an arbitrary operator $\hat{O}$ are related to the no-core shell model matrix elements

$$\left\langle Y_{K\gamma}(\hat{\rho}) | \hat{O} | Y_{K',\gamma'}(\hat{\rho}) \right\rangle = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} ds \ e^{s\rho^2} f_K(\rho, s) O_{K\gamma, K', \gamma'}^{SM}(s^{-1/2})$$

$O_{K\gamma, K', \gamma'}^{SM}(b)$ are the usual oscillator shell model matrix elements calculated for the oscillator radius $b$:

$$O_{K\gamma, K', \gamma'}^{SM}(b) = \sum_{ii'} C^K_i C_{i'}^{K'} \left\langle D^K_i (r_1, r_2...r_A) | \hat{O} | D^{K'}_{i'} (r_1, r_2...r_A) \right\rangle$$

and

$$f_K(\rho, s) = \sqrt{\Gamma(K + n/2)\Gamma(K' + n/2)} \rho^2 (s\rho^2)^{-(K+K'+n)/2}$$

where $n = 3A - 3$
**Link between the Hyperspherical Harmonics method (HHM) and the no-core oscillator translation invariant shell model (TISM)**

\[
\Psi_{\text{HHM}} = \sum_{K = K_{\text{min}}^- \gamma}^{\infty} \sum_{\kappa = 0}^{\infty} C_{K \gamma}^{\kappa} \Psi_{\text{TISM}}^{2 \kappa + K, \gamma}(\omega)
\]

\[
\Psi_{\text{HHM}} = \sum_{K = K_{\text{min}}^- \gamma}^{\infty} \int_{0}^{\infty} d\omega \ c_{K \gamma}(\omega) \Psi_{\text{TISM}}^{K, \gamma}(\omega)
\]

The probability \( P_K \) of the hyperharmonics with hyperangular momentum \( K \)

\[
P_K = \sum_{\gamma} \int_{0}^{\infty} d\rho \ \chi_{K \gamma}^{2}(\rho)
\]

gives an idea of how large is the probability of the \((K - K_{\text{min}}) \hbar \omega\) shell model configurations.
Superheavy hydrogen $^7$H

Proton separation energies
\[ S_p(^6\text{He}) = E(^6\text{He}) - E(^5\text{H}) \]
\[ S_p(^8\text{He}) = E(^8\text{He}) - E(^7\text{H}) \]
are relatively stable with respect to increase of model space

Estimation: \[ S_p(^8\text{He}) \approx 26 \text{ MeV} \]
Since \[ E(^8\text{He}) = 31.4 \text{ MeV} \]
\[ E(^7\text{H}) \approx 5.4 \text{ MeV} \] which is about 3 MeV above the t+4n threshold

\[ p(^8\text{He},pp)^7\text{H at } E(^8\text{He}) = 61.3 \text{A MeV (RIKEN)} \]
\[ \text{PRL 90, 082501 (2003)} \]

![Graph showing separation energies for different nuclei](image)

FIG. 4. Spectrum of $^7$H after subtraction of the polynomial fit to the empty-target background. Curves show nonresonant continuums explained in the text.

1 – 5-body (t+n+n+n+n+n) phase volume
2 – 3-body phase volume t + $^2n + ^2n$
3 – 2-body (t+$^4n$) phase volume
Application to $\alpha$-particle nuclei using the s-wave Ali-Bodmer $\alpha\alpha$ potential: 


All diagonal potentials $V_{K\gamma,K\gamma}(\rho)$ are purely repulsive. The binding in $N\alpha$ systems is a purely coupled-channel phenomenon for Ali-Bodmer potential.
Application to bosonic systems interacting by S3 two-body potential

PFY (Projected Faddeev-Yakubovskii approach),
N. Barnea and M. Viviani, PRC 61, 034003 (2002)
How do nuclear wave functions look like when one or several nucleons are far away from the rest?

\[ \Psi \sim \psi_1 \psi_2 \varphi_{12} \]

Cluster model:

\[ \Psi^{JM\pi} = \sum_{I_C U} A \left[ Y_l(\Omega_\rho) \otimes [\phi_C^I \otimes \phi_n]^I \right]^{JM} g_{ICU}^{J\pi}(\rho) \]

It is possible to take into account cluster degrees of freedom (or proper behaviour at large distances) without imposing cluster form of the wave function. Hyperspherical basis can be adapted to accommodate cluster degrees of freedom (\textit{N.K. Timofeyuk, Phys. Rev. C} \textbf{76}, 044309 (2007))

\[ A = (A-1) + n \]

\[ \rho_c, \theta_1, \theta_2, \ldots \theta_{3A-7} \quad \rho^2 = \rho_c^2 + \xi^2 \]

\[ \xi = \rho \sin \theta \]

\[ \rho_c = \rho \cos \theta \]
Hyperspherical Cluster Hahmonics (HCHs) for the same $K$ are not orthogonal

$$\langle \mathcal{Y}_{K'\gamma'}(\hat{\rho}) | \mathcal{Y}_{K\gamma}(\hat{\rho}) \rangle = \delta_{KK'} \mathcal{I}_{K\gamma \gamma'}$$
Link between the hyperspherical cluster model (HCM) and the microscopic cluster model

\[ \Psi = \mathcal{A} \left( \sum_n \mathcal{N}^{-1}_{KcYcnlLST} \frac{\chi_{KcYcnl}(\rho)}{\rho^{(3A-4)/2}} Y_{KcYc}(\hat{\rho}_c) \varphi_{Kcnlm\sigma}(\theta, \hat{\xi}_{A-1}) \right) \]

\[ \sum_i \left| \Psi^{(i)}_{KcYc}(\rho_c, \hat{\rho}_c) \right| \left| \Psi^{(i)}_{KcYc}(\rho_c, \hat{\rho}_c) \right| = 1 \]

\[ \Psi = \sum_i \mathcal{A}(\Psi^{(i)}_{KcYc}(\rho_c, \hat{\rho}_c) \phi^{(i)}_{KcYc}(\xi_{A-1})) \]

\[ \phi^{(i)}_{KcYc}(\xi_{A-1}) = \sum_n \mathcal{N}^{-1}_{KcYcnlLST} \left( \phi^{(i)}_{KcYc}(\rho_c, \hat{\rho}_c) Y_{KcYc}(\hat{\rho}_c) \right) \frac{\chi_{KcY}(\sqrt{\rho_c + \xi_{A-1}^2})}{(\rho_c^2 + \xi_{A-1}^2)^{(3A-4)/4}} \varphi_{Kcnlm\sigma}(\xi_{A-1}) \]
Overlap integral $\langle ^4\text{He} \mid ^5\text{He} \rangle$, $V1$ $m = 0.3$, $S_n = 2.09$ MeV

$\sqrt{5} I_l(r) \rightarrow -i C_l \kappa h_1^{(1)}(i\kappa r), \quad r \rightarrow \infty$

$C_l (\text{HCM}) = 0.72 \text{ fm}^{-1/2}$ \hspace{1cm} $C_l (\text{MCM}) = 0.73 \text{ fm}^{-1/2}$
Hyperspherical Harmonics Method in atomic physics

Structure of light atoms
Electron correlations
Atomic clusters
Harmonically trapped atoms
Efimov physics
Photo- and electron-ionization
Three-body recombination
Electron-atom collisions
Boson condensates
Multi-component Fermi-gases
Time-dependent hyperspherical studies
Spectra of helium clusters with up to six atoms using soft-core potentials


2-body system He-He:

B.E. = 1 mK and scattering length of 190 a.u.

He-He interaction potential has a strong repulsive core but He atoms stay far away from each other where this repulsion is not felt.

Hard-core interaction is replaced by phase-equivalent soft interaction presented by one gaussian.

3-body system He-He-He:

To get the energy of 3-body He-He-He system a phenomenological 3-body repulsion is introduced.
Binding energies of 4, 5 and 6 helium clusters calculated with soft 2-body interactions
Convergence improves with number of atoms

<table>
<thead>
<tr>
<th>( K )</th>
<th>( E_{4b}^{(0)} ) (mK) ( E_{4b}^{(1)} ) (mK)</th>
<th>( E_{5b}^{(0)} ) (mK)</th>
<th>( E_{5b}^{(1)} ) (mK)</th>
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Binding energies of 4, 5 and 6 helium clusters calculated with soft 2-body interactions and repulsive 3-body interactions. Convergence improves with number of atoms.

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<th>K</th>
<th>$E_{4b}^{(0)}$ (mK) [4]</th>
<th>$E_{4b}^{(1)}$ (mK) [4]</th>
<th>$E_{5b}^{(0)}$ (mK) [5]</th>
<th>$E_{5b}^{(1)}$ (mK) [5]</th>
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Calculations for N > 6 helium atoms with 2-body potential


\[ V(r) = -1.227 \exp\left(-\left(\frac{r}{10.03}\right)^2\right) \]

<table>
<thead>
<tr>
<th>$K_{\text{max}}$</th>
<th>$N = 4$</th>
<th>$N = 6$</th>
<th>$N = 8$</th>
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<td>0.751 37</td>
<td>3.8109</td>
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</table>
Why does convergence improve with $N$?

\[
\left( \frac{d^2}{d\rho^2} - \frac{L_K (L_K + 1)}{\rho^2} - \frac{2m}{\hbar^2} (E + V_{K,\gamma,\gamma}(\rho)) \right) \chi_{K,\gamma}(\rho) = \frac{2m}{\hbar^2} \sum_{K',\gamma' \neq K\gamma} V_{K,\gamma,\gamma'}(\rho) \chi_{K',\gamma'}(\rho)
\]

Because $U_{K,\gamma,K',\gamma'}(\rho) = \frac{V_{K,\gamma,K',\gamma'}(\rho)}{V_{K,\gamma,\gamma}(\rho)}$ decreases with $N$

For $V(r) = V_0 \exp(-\alpha r^2)$

$U_{K,\gamma,00} \sim N^{-1/2}$

at $\rho \to \infty$ and $N \to \infty$

$N^{-1/2}$ comes from normalization of the symmetric HHs and reflects small number of exchange terms that give non-zero contribution to $V_{K,\gamma,00}$

\[ V(r) = -5.134e^{-(r/10.03)^2} + 20e^{-(r/5)^2} \]

<table>
<thead>
<tr>
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<th>( N = 200 )</th>
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</table>
Two-body attraction + three-body repulsion

\[ W(\rho_{ijk}) = W_0 e^{-2\rho_{ijk}^2/\beta^2} \quad \text{where} \quad \rho_{ijk} = \frac{2}{3}[(r_i - r_j)^2 + (r_j - r_k)^2 + (r_i - r_k)^2] \]

The “Schrodinger equation” looks like

\[
\left( \frac{d^2}{d\rho^2} - \frac{L_K (L_K + 1)}{\rho^2} - \frac{2m}{\hbar^2} (E + V_{K\gamma,K\gamma} + W_{K\gamma,K\gamma}^{(3)}) \right) \chi_{K\gamma} = \frac{2m}{\hbar^2} \sum_{K'\gamma' \neq K\gamma} (V_{K\gamma,K'\gamma'} + W_{K\gamma,K'\gamma'}^{(3)}) \chi_{K'\gamma'}
\]

It can be proved that

\[ W_{K\gamma,00} / W_{00,00} \sim N^{-1/2} \quad \text{for} \ \rho \to \infty \text{ and } N \to \infty \]


\[ N^{-1/2} \text{ comes from normalization of the symmetric HHs and reflects small number of exchange terms that give non-zero contribution to } W_{K\gamma,00} \]
Many-body bosonic system in the lowest order approximation, $K = 0$, with Gaussian 2-body and 3-body forces

\[
\left( \frac{d^2}{d\rho^2} - \frac{L_0(L_0 + 1)}{\rho^2} - \frac{2m}{\hbar^2} (E + V_{00} + W_{00}^{(3)}) \right) \chi_{00} = 0
\]

$L_0 = (3N - 6)/2$

\[
V_{00}(\rho) = \frac{N(N - 1)}{2} V_0 M \left( \frac{3}{2}, \frac{n}{2}, -\frac{2\rho^2}{\alpha^2} \right)
\]

\[
W_{00}(\rho) = \frac{N!}{3!(N - 3)!} W_0 M \left( 3; \frac{n}{2}; -\frac{4\rho^2}{\beta^2} \right)
\]

$n = 3N - 3, \quad M$ is confluent hypergeometric function
## Ground state binding energy of N atoms of helium

<table>
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<tr>
<th>N</th>
<th>HH0</th>
<th>HH</th>
<th>DMC</th>
<th>MCH</th>
<th>GFMC</th>
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GFMC (Green’s Functions Monte Carlo) V.R. Pandharipande et al, PRL 50,1676 (1983)
Binding energies of N helium atoms obtained in K=0 HH calculations with two phenomenological potentials

Two-body potential

\[ V(r_{ij}) = V_0 \exp\left(-\frac{r_{ij}}{\alpha}\right)^2 \]

Three-body potential

\[ W(\rho_{ijk}) = W_0 \exp\left(-\frac{\rho_{ijk}}{\beta}\right)^2 \]

<table>
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With chiral low-momentum 2-body force convergence of HH expansion for $^8$He is not worse than for $^6$He and effective interactions do not give advantage.
Summary

HH expansion is an ab-initio method that uses dynamical equations for the wave function depending on only one degree of freedom – the hyperradius – which is determines the radius of the system.

HHM is linked to the no-core shell model and always contains larger model space than the NCSM for a fixed \( N_{\text{max}} \).

The HHM wave functions have better asymptotics than that given by harmonic oscillator employed in NCSM and does not contain centre-of-mass motion.

Cluster degrees of freedom can be naturally incorporated in HHM.

For bosonic systems, a theorem is proved that convergence of HH expansion for soft 2-body potentials improves with the number of bosons.

HHM is actively used to describe various properties of \( A \leq 6 \) nuclei and scattering in \( A = 3,4 \) system with the best interactions available.

Formalism for \( A > 6 \) is available and waiting for its applications to nuclear systems with modern NN forces.
2-body potential with a core

2-body potential without a core + 3-body repulsive potential