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The projected potential model: Exhausting two body correlations

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ABSTRACT

A solution of the Schrödinger equation written in terms of hyperspherical Jacobi coordinates is presented. The wave function and the potential are projected onto the space of a single reference pair Jacobi coordinate. The ground state binding energies and sizes obtained with the formalism, for an even number of bosons up to $A = 16$, and for the ^{6}Li, ^{12}C, ^{16}O and ^{40}Ca nuclei, are compared to the results in the literature.

The purpose of this work is to present a new approach to the solution of the Schrödinger equation.

The structure of this equation for identical particles of mass m,

$$\left\{-\frac{\hbar^2}{2m}\Delta + V(\vec{x}) - E\right\}\Psi(\vec{x}) = 0 \tag{1}$$

where Δ is the Laplace operator, $V(\vec{x})$ the interaction operating on all A particles, $\vec{x} = (\vec{x}_1, \ldots, \vec{x}_A)$, and E the energy, is rather simple for few-body systems.

The problem for heavier nuclei is related to the large number of independent coordinates $\vec{x}_i$ to be taken into account.

In the physical 3-dimensional space the Schrödinger equation, for a spherical potential, is solved in polar coordinates $\vec{x}_i(x_i, \omega_i)$ and the solution is the product of a radial function and a spherical harmonic. Here one intends to generalize the method to the whole space spanned by the particles coordinates.

Let $\vec{x}(r, \Omega)$ be the polar coordinates where the hyperradial and the center of mass coordinates are defined by

$$r^2 = 2\sum_1^A (x_i - X_{cm})^2 = \frac{2}{A}\sum_{i,j>i}^A r_{ij}^2$$

$$\vec{X}_{cm} = \sum_1^A \vec{x}_i/A, \quad r_{ij} = |\vec{x}_i - \vec{x}_j| \tag{2}$$

For translationally invariant coordinate system, in the center of mass frame, we consider a $D = 3(A-1)$-dimensional space (D-*space*).

Without interaction ($V(\vec{x}) = 0$) the eigenstates of (1) are harmonic polynomials.

When the potential is hypercentral, i.e. for $V(\vec{x}) = V_{HC}(r)$, the solution is the product

$$\Psi(\vec{x}) = Y_{[L]}(\Omega)u(r)/r^{(D-1)/2} \tag{3}$$

of a hyperspherical harmonic $Y_{[L]}(\Omega)$ (HH) defined by $D-1$ quantum numbers $[L]$ where L is the degree of the associated harmonic polynomial and $u(r)$ a solution of the radial equation

$$\left\{\frac{\hbar^2}{m}\left(-\frac{d^2}{dr^2} + \frac{\mathcal{L}(\mathcal{L}+1)}{r}\right) + V_{HC}(r) - E\right\}u(r) = 0 \tag{4}$$

with $\mathcal{L} = L + (D-3)/2$ for translational invariant hyperspherical harmonics. The ground state is for the weakest kinetic centrifugal barrier, i.e., the lowest available degree L which is $L = 0$ for bosons and some $L > 0$ for nuclei beyond ^{4}He.

At the beginning of the 1950s Mayer and Jensen discovered the shell structure of nuclei. For defining the shells they assumed that "each nucleon moves in an average field of force $V(r)$ of spherical symmetry and independent of the exact instantaneous position of all other nucleons" [1]. But "among all central potential wells the harmonic oscillator potential occupies a special position… it yields the order of single nucleon orbits which together with a strong spin orbit interaction give rise to the observed shells in nuclei" [2].

A sum of harmonic oscillator potential is itself a harmonic oscillator potential in the D-space which is a hypercentral potential. Then the general rule holds in this case where the eigenfunction is the product of an HH and a harmonic oscillator radial eigenfunction.

The HH is independent of the shape of the radial potential, therefore the independent particle HO eigenstates can be used to analyze the properties of the HH.

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Actually, the definition of the field of force proposed by Mayer and Jensen corresponds exactly to the hypercentral part $V_{HC}(r)$ of $V(\vec{x})$ inside which all nucleons move freely. This $V_{HC}(r)$ accounts for more than 75% of the total nuclear potential energy. The residual part which appears as a deformation, a lack of hyperspherical symmetry of the potential, generates the correlations.

For defining the HH states the hypercentral property of the HO potential is used. The states for identical fermions are defined by HO Slater determinants, where the motion of the center of mass in the 1s-state is factorized. This motion does not contribute to the calculation of translational invariant matrix elements. For the HO ground state, when all proportional columns of the HO determinant are eliminated and the Gaussian functions are factorized, the residual determinant $D_{[L_m]}(\vec{x}) = r^{L_m} D_{[L_m]}(\Omega)$ is a polynomial homogeneous in the $\vec{x}_i$ coordinates of minimum degree L_m and therefore harmonic and translational invariant. The element of the ith row and jth column is $x_i^{2n_j+\ell_j} Y_{\ell_j}^{m_j}(\omega_i)$ multiplied by a spin–isospin state.

From the birth of the Nuclear Shell Model the nuclear wave function was written as a product of an antisymmetric Slater determinant $D(\vec{x})$, and a correlation function $\Phi(\vec{x})$ symmetric for particle exchange. Traditionally $\Phi(\vec{x}) = \prod_{i,j>i} f(r_{ij})$ is the Jastrow function with $f(r_{ij}) = 1 + h(r_{ij})$. It is the product of pairwise functions in s-state. The Slater determinant $D(\vec{x})$ is constructed as in the Independent Particle Model (IPM), using a central potential well. The correlation function $h(r_{ij})$ is calculated variationally, looking for minimal ground state energy E in the integral

$$\langle \Psi | H - E | \Psi \rangle = 0, \quad \Psi = D(\vec{x})\Phi(\vec{x}) \tag{5}$$

Here H is the Hamiltonian.

In the 1960s, a new method was proposed to solve the wave equation. In the Fermi gas model the nuclear kinetic energy amount to about three times the binding energy, therefore it seems legitimate to expand the wave function in terms of the eigenstates of the kinetic energy operator leading to the Hyperspherical Harmonic Expansion Method (HHEM) [3]. This method was developed using the Zernike and Brinkman polar Jacobi coordinates system [4] in the whole D-space.

A state is defined by the quantum numbers $[L_m]$ which are the (n_j, ℓ_j, m_j), $j = 1, 2, \ldots A$ and the associated spin–isospin individual states in an HO Slater determinant where the center of mass is in the 1s-state. The single particle coordinates are replaced by the Jacobi coordinates

$$\vec{\xi}_i = \sqrt{\frac{2i}{i-1}}(\vec{x}_i - \vec{X}_i), \quad \vec{X}_i = \frac{1}{i}\sum_{j=1}^{i} \vec{x}_j, \quad i = 2, \ldots, A \tag{6}$$

Here i is the number of particles involved ($\vec{x}_j$ is the jth particle position), and for example $i = 2$ for a particle pair. These coordinates are then transformed into the Zernike and Brinkman polar Jacobi coordinate system [4], $\vec{\xi}_i = \xi_i \vec{e}(\omega_i)$, where $\vec{e}(\omega_i)$ is a unit vector and the magnitude is defined in terms of the hyperspherical coordinates Φ_i through

$$\xi_2 = r\cos\Phi_2, \ldots, \xi_i = r\sin\Phi_2, \ldots \sin\Phi_{i-1}\cos\Phi_i$$

in such a way that the hyperspherical angular coordinates are $\Omega = [\Phi, \omega] = (\Phi_2, \omega_2, \ldots, \omega_A)$, ω_i are the angular coordinates of $\vec{\xi}_i$.

The magnitude of the vector $\vec{\xi} = (\vec{\xi}_2, \vec{\xi}_3, \ldots, \vec{\xi}_A)$ in the D-space $(\sum_2^A \xi_i^2)^{1/2} = r$ is the hyperradial coordinate.

A kinematic rotation vector, linear combination of $\vec{\xi}_i$ where φ_i are parameters

$$\vec{r}(\varphi) = \cos\varphi_2 \vec{\xi}_2 + \sum_{i=3}^{A} \sin\varphi_2 \ldots \cos\varphi_i \vec{\xi}_i, \quad \varphi = (\varphi_2, \ldots, \varphi_A) \tag{7}$$

is used for constructing combinations of Jacobi coordinates, e.g. for $\varphi_2 = 0, \pm 2\pi/3$ and $\varphi_i = 0$ for $i > 2$, one gets $\vec{r}_{12}, \vec{r}_{23}, \vec{r}_{31}$ while for $\varphi_2 = \pi/2$ one gets pairs disconnected with particles (12).

The differential elements are obtained by recurrence

$$\begin{aligned}
&d^{3N}\xi = r^{D-1} dr d\Omega, \quad d\Omega = d\Omega_N, \quad N = A - 1 \\
&d\Omega_{j+1} = (\sin\Phi_{j+1})^{D-4}(\cos\Phi_{j+1})^2 d\Phi_{j+1} d\omega_{j+1} d\Omega_j \\
&D_j = 3(j+1), \quad d\Omega_1 = d\omega_1
\end{aligned} \tag{8}$$

where j is the number of particles involved. In particular for the reference pair $(1, 2)$ with $i = 2$

$$\begin{aligned}
&d\Omega = W_0(z) dz d\omega d\Omega_{N-1}, \quad \omega = \omega_2 \\
&r_{12}/r = \cos\Phi_2, \quad z = \cos 2\Phi_2 = 2r_{12}^2/r^2 - 1 \\
&W_0(z) = (1-z)^{(D-5)/2}(1+z)^{1/2}/2^{D/2}, \quad D = 3(A-1)
\end{aligned}$$

The pair wise *hyperangular* kinetic energy operator for spherical nuclei is ([5], [6, eq. (A13)])

$$T(z) = -\frac{4}{r^2}\frac{\hbar^2}{m}\left(W_{[L_m]}(z)\right)^{-1}\frac{d}{dz}(1-z^2)W_{[L_m]}(z)\frac{d}{dz} \tag{9}$$

($L_m = 0$ for bosons in 1s-state) where $W_{[L_m]}(z, \omega)$ is the integral

$$W_{[L_m]}(z, \omega) = W_0(z)\int \left|D_{[L_m]}(\Omega)\right|^2 d\Omega_{N-1}, \tag{10}$$

with normalization $\int W_{[L_m]}(z, \omega) dz = 1$ independent of ω for spherical nuclei. This operator is similar in the D-space to the angular operator $\ell^2(\omega)$ in the physical space both associated with rotational motions. For more details refers to [5] and to the appendix of [6]. $W_{[L_m]}(z, \omega)$ is a two-body density function called the weight function. According to Erdelyi [7] it is associated with an orthogonal set of polynomials $P_K^{[L_m]}(z, \omega)$ of degree K, these are *eigenfunctions of the kinetic energy operator* $T(z)$ *with eigenvalue* $\lambda_K^{[L_m]}$. This basis is complete for the expansion of pair wise functions like the potential $V(r_{12})$ with $r_{12} = r\sqrt{(1+z)/2}$ and the two-body amplitude $P_\lambda(z, r)$ describing two body correlations.

For $L_m = 0$, $P_K^{[0]}(z)$ are the Jacobi polynomials $P_K^{\alpha,\beta}(z)$ with $\alpha = (D-5)/2, \beta = 1/2$, and $\lambda_K^{[0]} = K(K + \alpha + \beta + 1)$. The application of the kinetic energy operator $T(z)P_K^{[0]}(z) = \frac{\hbar^2}{mr^2}L(L + D - 2)P_K^{[0]}(z), L = 2K$ shows that $P_K^{[0]}(z)$ behaves like spherical harmonic polynomial of degree $L = 2K$ with $z = \cos 2\Phi_2$.

The set of properly normalized Jacobi polynomials $P_K^{[0]}(z)$ constitute the so called “Potential Harmonics” basis used for solving systems of particles in s-state, like bosons systems, trinucleons, or ^{4}He in ground state, with the HHEM [3]. For $L_m \neq 0$ they are “Potential Polynomials” associated with the $[L_m]$ state in D-space.

The overlap $\int_{-1}^{1} W_{[L_m]}(z) P_K^{[L_m]}(z) P_K^{[L_m]}(z') dz$ of two polynomials $P_K^{[L_m]}(z)$ and $P_K^{[L_m]}(z')$ for $z' = 2r^2(\varphi_2)/r^2 - 1$ is $f_K^{[L_m]}(\varphi_2) = P_K^{[L_m]}(\cos 2\varphi_2)/P_K^{[L_m]}(1)$, where $\cos 2\varphi_2 = -1/2$ ($\varphi_2 = \pm 2\pi/3$) for connected pairs, and $\cos 2\varphi_2 = -1$ ($\varphi_2 = \pi/2$) for disconnected pairs [8]. Here $\vec{r}(\varphi_2)$ is a parameterization of the pairs in terms of the Jacobi coordinates (7) with $\vec{r}(\varphi_2) = \cos\varphi_2 \vec{\xi}_2 + \sin\varphi_2 \vec{\xi}_3$ for $\vec{\xi}_2 = \vec{x}_2 - \vec{x}_1$ and $\vec{\xi}_3 = \sqrt{3}(\vec{x}_3 - \vec{X}_3)$.

The projection $\mathcal{P}^0$ of a function $F(r(\varphi_2))$ onto the space of r_{12} is obtained by an expansion of the function in a series of normalized polynomials $P_K^{[L_m]}(z(\varphi_2))$ with $z(\varphi_2) = 2r^2(\varphi_2)/r^2 - 1$ followed by a projection of each polynomial

Table 1
Projection coefficients of the connected (f_c) and disconnected (f_d) pairs for 16 and 40 particles where a (b) means $a \cdot 10^{-b}$.

K	16		^{16}O		40		^{40}Ca	
	f_c	f_d	f_c	f_d	f_c	f_d	f_c	f_d
2	2.24 (2)	8.11 (3)	2.64 (2)	7.11 (3)	4.67 (2)	1.13 (3)	4.87 (2)	9.31 (4)
3	3.34 (4)	−1.24 (3)	1.40 (3)	−8.98 (4)	8.08 (3)	−6.73 (5)	9.52 (3)	−4.10 (5)
4	4.37 (4)	2.31 (4)	2.36 (4)	1.36 (4)	1.12 (3)	5.04 (6)	1.70 (3)	2.14 (6)
5	2.27 (5)	−5.01 (5)	3.36 (5)	−2.58 (5)	1.11 (4)	−4.5 (7)	2.73 (4)	−1.29 (7)

$$\mathcal{P}^0\big(F\big(r(\varphi_2)\big)\big) = \int_{-1}^{1} f^{[L_m]}\big(z, z'\big) F\big(r\sqrt{(1+z')/2}\big) dz'$$

where the kernel

$$f^{[L_m]}\big(z, z'\big) = W_{[L_m]}\big(z'\big) \sum_{K=0}^{\infty} f_K^{[L_m]}(\varphi_2) P_K^{[L_m]}\big(z'\big) P_K^{[L_m]}(z) \tag{11}$$

is called projection function.

When $\varphi_2 = 0$ then $f_K^{[L_m]}(0) = 1$ generates a polynomial expansion of $F(r_{12})$. When $\varphi_2 = \pm 2\pi/3$ or $\pi/2$ it gives a projection of $F(r_{ij})$ for connected or disconnected pair like r_{1j} and r_{2j} or r_{jk} for j and $k > 2$ respectively.

When a projection of the sum over all pairs of pairwise functions is requested, the coefficients become

$$f_K^{[L_m]} = 2(A-2) f_K^{[L_m]}(2\pi/3) + (A-2)(A-3)/2 f_K^{[L_m]}(\pi/2) \tag{12}$$

for the $2(A-2)$ and $(A-2)(A-3)/2$ connected and disconnected pairs respectively.

An example of magnitude of the projection coefficients $f_K^{[L_m]}(\varphi_2)$ for the connected (f_c) and the disconnected (f_d) pairs is presented in Table 1 for 16 and 40 particles.

The coefficients decrease rapidly for growing K. It means that the pairs become independent for rather small values of K.

The projection of the sum of all $F(z_{ij})$, $z_{ij} = 2r_{ij}^2/r^2 - 1$ onto the space of the pair 1, 2 where the coefficients $f_K^{[L_m]}$ in (12) are used in (11) is noted by $\mathcal{P}^0(F)$ with $r_{12} = r(\varphi_2 = 0)$.

For instance

$$\mathcal{P}^0(F) = F(z) + \mathcal{P}^0\big(F\big(z'\big)\big) = F(z) + \mathcal{P}^0\left(\sum_{i<j\neq 1,2}^{A} F(z_{ij})\right)$$

Since $\sum_{i,j>i}^{A} P_1^{[L_m]}(z_{ij}) = 0$ the term for $K = 1$ does not occur in the projection while $f_0^{[L_m]} = A(A-1)/2 - 1$. The coefficients $f_K^{[L_m]}$ for the projection of all pairs are shown Table 2 for ^{16}O and ^{40}Ca up to $K = 5$.

The ratio of the last $K = 5$ to the first $K = 0$ coefficients is in both cases $2.6 \cdot 10^{-5}$. It explains the rapid convergence of the projection in terms of the number of polynomials in the projection function [9, p. 26]. The converged solution of the Integro-Differential Equation Approach (IDEA) is reached with one polynomial for $K = 2$ and two with $K = 2, 3$ for ^{16}O and ^{40}Ca respectively [9] with the traditional MS3 test potential [10].

In nuclear physics, 2-body potentials are known to be of leading order, whereas 3- and 4-body forces are subleading and of lesser importance. A three body interaction including the product of two connected pairs of pairwise potentials can be approximated as a sum of density dependent $V_3(r_{ij}, r)$ potential [11], and can be incorporated into the present formalism. It can also be used with the HHEM [12].

Table 2
Projection coefficient $f_K^{[L_m]}$.

K	0	1	2	3	4	5
^{16}O	119	−1	1.385	$-4.23 \cdot 10^{-2}$	$5.788 \cdot 10^{-3}$	$-3.113 \cdot 10^{-3}$
^{40}Ca	779	−1	4.360	.6947	0.1307	$2.07 \cdot 10^{-2}$

For central potential the eigenstates are the product of a harmonic polynomial and a radial function. The states are the eigenstates originating from the coordinates missing in the interaction i.e. the spherical harmonics associated with the angular coordinates for a central potential.

The HHEM was proposed where the Schrödinger equation is projected onto a polynomial basis extracted from the eigenstates of the kinetic energy operator truncated to those polynomials needed to describe pairs in s-state. This method is applicable for bosons systems in s-state, the ground states of the trinucleon, and of ^{4}He [3,8,14].

In order to build the coupled equation of the HHEM one starts from the potential expansion in terms of the potential polynomials,

$$V(r_{ij}) = \sum_{K'=0}^{\infty} V_{K'}(r) P_{K'}^{[L_m]}(z_{ij}), \quad z_{ij} = 2r_{ij}^2/r^2 - 1$$

with

$$V_K(r) = \int_{-1}^{1} W_{[L_m]}(z) V\big(\sqrt{(1+z)/2}\big) P_K^{[L_m]}(z) dz$$

The basis symmetrical with respect to exchange of pairs $B_K^{[L_m]}(\Omega) = \sum_{i,j>i} P_K^{[L_m]}(z_{ij})$ is complete to expand the sum over all pairs of any pairwise functions in the s-state.

The coupled radial differential equations of the HHEM are obtained by projections onto this symmetrical basis

$$\begin{aligned} &\big\langle D_{[L_m]}(\Omega) B_K^{[L_m]}(\Omega) \big| H - E \big| \Psi(\vec{x}) \big\rangle = 0 \\ &\Psi(\vec{x}) = D_{[L_m]}(\Omega) \Phi(x). \end{aligned} \tag{13}$$

The $\Phi(x)$ is a symmetrical function which can be expanded with the symmetrical basis $B_{K''}^{[L_m]}(\Omega)$ and other orthogonals $B_{K''}^{\perp}(\Omega)$

$$\Phi(\vec{x}) = \sum_{K''} \big(B_{K''}^{[L_m]}(\Omega) u_{K''}(r) + B_{K''}^{\perp}(\Omega) u_{K''}^{\perp}(r)\big)$$

The matrix element with $V(\vec{x})$ and $B_{K''}^{\perp}(\Omega)$ in $\Phi(\vec{x})$ vanishes for $K = 0$ in (13) and operates only when K' and $K'' \neq 0$ bringing second order corrections with more than two-body correlations. It justifies the structure $\Phi(\vec{x}) = \sum_{i,j>i} P_\lambda(z_{ij}, r)$ fully expandable with the $B_{K''}^{[L_m]}(\Omega)$ basis. The $B_K^{\perp}(\Omega)$ is not coupled to the state $D_{[L_m]}(\Omega)$ by the potential for $K = 0$ and then contains many body (>2) correlations.

It is the structure chosen by Guardiola et al. [15] for their variational calculation

$$\left\langle D_{[L]}^{HO}(\vec{x}) \sum_{i<j} f(i,j) \middle| T + \sum_{k<\ell} V(k,\ell) - E \middle| \sum_{m<n} f(m,n) D_{[L]}^{HO}(\vec{x}) \right\rangle \\ = 0 \tag{14}$$

where $f(i,j)$ is similar to $P_\lambda^{[L_m]}(z_{ij},r)$.

The original Schrödinger equation [13] is for one particle. The extension to one pair is obvious by eliminating the center of mass coordinate. In order to find equations for solving the wave equation, for more than one pair, one needs first to treat the case of three identical particles in an s-state. The potential for each of the three pairs is expressed in terms of the kinetic rotation vector (7), $V(r,z,\cos\theta) = V(r\sqrt{(1+z(\varphi))/2})$ with $z(\varphi) = 2r^2(\varphi)/r^2 - 1 = z\cos 2\varphi + \sqrt{1-z^2}\sin 2\varphi\cos\theta$ where θ is the angle between the two Jacobi coordinates $\vec{\xi}_2$ and $\vec{\xi}_3$ and $\varphi = 0, \pm 2\pi/3$ for the reference and the two connected pairs respectively. The θ dependence determines the relative motion of the two Jacobi vectors in a plane. It is independent of the motion of the plane in the D-space which can be fixed by the three quantum numbers associated with the Euler angular coordinates.

The potential $V(\vec{x})$ can be expanded in Legendre polynomials $V(r,z,\cos\theta) = \sum_\ell V_\ell(r,z)P_\ell(\cos\theta)$ where according to the addition theorem $P_\ell(\cos\theta) = 4\pi/(2\ell+1)\sum_m Y_\ell^{m^*}(\omega_3)Y_\ell^m(\omega_2)$ with $P_0 = 1$.

The Legendre polynomial $P_\ell(\cos\theta)$ is associated with the states where the $Y_\ell^m(\omega_i), i = 2,3$ are coupled to give an $\ell, m = 0$ angular momentum with the kinetic energy operator $TP_\ell(\cos\theta) = \frac{\hbar^2}{mr^2}\frac{4\ell(\ell+1)}{1-z^2}P_\ell(\cos\theta)$.

By selecting the part of the potential operating on pairs in s-state when $\ell = 0$ one extracts the central part of $V(r, z(\varphi))$ given by the integral

$$V_0(r,z) = \frac{1}{2}\int_0^\pi V(r,z,\cos\theta)\sin\theta d\theta$$

which eliminates the $\ell \neq 0$ dependent terms [16, (2.15)].

A simple change of variable from $\cos\theta$ to $z' = z(\varphi)$ shows that

$$V_0(r,z) = \frac{1}{\sqrt{3(1-z^2)}}\int_{z-}^{z+} V\big(r,z'\big)dz'$$

$$z\pm = -1/2\big(z \mp \sqrt{3(1-z^2)}\big)$$

It is the projection $\mathcal{P}^0(V(r,z(\varphi)))$ of the potential [16]. The same result is obtained by summing the series in the projection function for three particles in the s-state [5].

This property is used to extract the central part $V_0(r,z)$ of the potential $V(\vec{x})$ by neglecting the effect of the Legendre polynomials for $\ell > 0$. The part of the solution originating from the relative rotation of the two Jacobi coordinates is missed.

It is the price we have to pay for avoiding to solve the system of coupled equations generated by the $\ell > 0$ terms. The choice of a reference pair is associated with the Jacobi coordinates.

The pair $(1,2)$ which correspondents to the two first rows of $D_{[L_m]}(\vec{x})$ is the easiest choice.

The kinetic energy operator (9) of the pair $(1,2)$ is applied to the amplitude $P_\lambda^{[L_m]}(z,r)$ with $z = 2r_{12}^2/r^2 - 1$.

The potential operating on the amplitudes where pairs are in the s-state is $\mathcal{P}^0(V)$ leading the equation

$$\big(T(z,r) - E\big)P_\lambda^{[L_m]}(z,r) + \mathcal{P}^0(V)\sum_{i,j>i} P_\lambda^{[L_m]}(z_{ij},r) = 0$$

By integrating this equation on θ the amplitudes for $i, j \neq 1,2$ are projected onto the space of the reference pair $(1,2)$ in s-state generating an equation where the sum of all amplitudes became the projection $\mathcal{P}^0(P_\lambda)$ and finally the equation

$$\big(T(z,r) - E\big)P_\lambda^{[L_m]}(z,r) + \mathcal{P}^0(V) \times \mathcal{P}^0(P_\lambda) = 0 \tag{15}$$

The kinetic energy operator

$$T(z,r) = \frac{\hbar^2}{m}\bigg(-\frac{\partial^2}{\partial r^2} + \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} \\ - \frac{4}{r^2}\frac{1}{W_{[L_m]}(z)}\frac{\partial}{\partial z}(1-z^2)W_{[L_m]}(z)\frac{\partial}{\partial z}\bigg) \\ \mathcal{L} = L_m + (D-3)/2 \tag{16}$$

includes the radial operator and $W_{[L_m]}(z)$ is the weight function associated with the state $[L_m]$.

When the projection of the potential is limited to the dominant term $V(r_{12})$ the equation is called the "S-state Integro-Differential Equation" (SIDE) [17].

When $V_{HC}(r) = 0$ and $\mathcal{P}^0(V) = V(r_{12})$ for three particles it is the Faddeev equation for an s-projected two-body potential. When the potential is local the radial equation (4) provides an exact solution for $V_{HC}(r)$ and the residual potential treated in the "Integro-Differential Equation Approach" (IDEA) operates on s-states [18]. It is an improvement with respect to the Faddeev equation when the terms $\ell > 0$ are neglected.

When the projection of the potential operates on the projection of the amplitudes onto the space of the reference pair it is the "Projected Potential Model" (PPM).

The radial vibrational motion and the hyperorbital motion are decoupled adiabatically very early for $A \to \infty$ [6, Tables 5, 6], in such a way that with $\Psi(\vec{x}) = D_{[L_m]}(\Omega)u(r)/r^{(D-1)}\sum_{i,j>i} P_\lambda^{[L_m]}(z_{ij},r)$ eq. (15) can be separated into two equations, a radial equation

$$\bigg\{\frac{\hbar^2}{m}\bigg(-\frac{d^2}{dr^2} + \frac{\mathcal{L}(\mathcal{L}+1)}{r^2}\bigg) + V_{HC}(r) + U_\lambda(r) - E\bigg\}u(r) = 0 \\ V_{HC}(r) = A(A-1)/2V_{[L_m]}(r) \\ V_{[L_m]}(r) = \int_{-1}^{1} V\left(r\sqrt{(1+z)/2}\right)W_{[L_m]}(z)dz \tag{17}$$

and an orbital equation

$$\bigg\{-\frac{4\hbar^2}{mr^2}\frac{1}{W_{[L_m]}(z)}\frac{d}{dz}(1-z^2)W_{[L_m]}(z)\frac{d}{dz} - U_\lambda(r)\bigg\}P_\lambda^{[L_m]}(z,r) \\ + \mathcal{P}^0(\tilde{V})\mathcal{P}^0\big(P_\lambda^{[L_m]}\big) = 0 \\ \tilde{V}(r_{ij},r) = V(r_{ij}) - V_{[L_m]}(r) \tag{18}$$

The last equation (18), called the "Integro-Differential Equation Approach" (IDEA), is first solved and the eigen-potential $U_\lambda(r)$ is utilized in the radial equation (17) to yield the total binding energy E. The radial $U_\lambda(r)$ and orbital wave function $P_\lambda^{[L_m]}(z,r)$ are obtained from (18) with the residual potential $\tilde{V}(r_{ij},r)$.

This two body amplitude is normalized to

$$\int_{-1}^{1} P_\lambda(z,r)W_{[L_m]}(z)dz = 1 \quad \text{with} \int_{-1}^{1} W_{[L_m]}(z)dz = 1 \tag{19}$$

The simplest version of the IDEA is when the projection function (11) is approximated by the weight function $W_{[L_m]}(z')$, then

$\mathcal{P}^0(P_\lambda^{[Lm]}) = A(A-1)/2-1+P_\lambda^{[Lm]}(z,r)$ and equation (18) becomes a simple a second order differential equation.

$$\big(T(z) - U_\lambda(r)\big)P_\lambda^{[Lm]}(z,r) + \tilde{V}(r_{12},r)\big(A(A-1)/2-1+P_\lambda^{[Lm]}(z,r)\big) = 0 \tag{20}$$

It is called “Weight Function Approximation” (WFA).

In the next approximation the projection of the potential $\mathcal{P}^0(\tilde{V})$ is substituted for $\tilde{V}(r_{12},r)$ in the WFA. It is the Without Projected Amplitude (WPA) approximation where $P_\lambda^{[Lm]}(z_{ij},r) = 1$ for $i, j \neq 1, 2$.

The solution of (17) and (18) provides the wave function everywhere. The equations are solved numerically in this paper with the program proposed in [9] used with the version of the IDEA where the variables are r and $x = r_{12} = r\sqrt{(1+z)/2}$ [19]. The trajectory $P_\lambda^{[Lm]}(x,r)$ starts from $P_\lambda^{[Lm]}(0,r) = 0$ where the slope $d/dxP_\lambda^{[Lm]}(0,r)$ is fixed by the normalization (19). For $A > 4$ it exhibits three zeros before vanishing for $x = r$. The position $r_m = 2Aa^2$ with $a^2 = m.s.$ radius where the effective radial potential $V_{eff}(r) = \frac{\hbar^2}{m}\frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + V_{HC}(r) + U_\lambda(r)$ in (17) is minimum is far out of the range of the potential $V(r_{12})$.

For applications, the Brink and Boeker B1 [20], Modified S3 [10], Afnan–Tang S3 [21], Malfliet–Tjon MTI-III [22], and MTV [23] potentials are used to calculate the $A = 6$ to 16 even boson systems, and the ^{6}Li, ^{12}C, ^{16}O and ^{40}Ca nuclei in their ground state.

The first equations by order of approximation occurring after the HyperCentral Approximation (HCA) where $U_\lambda(r) = 0$ are the Weight Function Approximation (WFA) (equation (20)) where in (11) $f^{[Lm]}(z,z') = W_{[Lm]}(z')$ and the (WPA) where $\mathcal{P}^0(\tilde{V})$ is substituted for $\tilde{V}$ in (20).

In Table 3 the binding energy of ^{16}O given by the WPA and the variational calculation of Guardiola et al. [15] are shown as test cases. The variational numbers are very similar to the WPA despite the extremely simple structure of the WPA.

Barnea and Viviani proposed a method for introducing the three and four body correlations in the solution of the IDEA [24]. An application was performed for A bosons in ground state with the S3 potential [21].

A comparison between the binding energies obtained with the Projected Faddeev–Yakubovsky (PF-Y) equation used in [24] and the PPM are presented in Table 4. The r.m.s. is stable for the IDEA at about 1.34 ± .01 fm while it decreases by .1 fm for A growing from 6 to 16 bosons for the PPM.

Table 3
Binding energy in MeV of ^{16}O with the Without Projected Amplitude (WPA) and a Variational calculation [15] for various potentials.

Potential	B1	MS3	S3	MTI-III	MTV
WPA	169.3	104.9	162.9	202.1	1020
Var. [15]	167.3	105.6	164.9	207.5	973.7

Barnea and Viviani in [24] calculated first the IDEA and found values in perfect agreement with those obtained with our numerical algorithm [9] and then included the three and four body correlations with the PF-Y.

A large amount of the increase of binding energy attributed to the three and four body correlations by Barnea and Viviani [24] are taken into account by the PPM. The increase of binding energy brought by the correlations is nearly proportional to $A(A-1)/2$ the number of pairs contributing to the bound state.

The energies obtained with the PPM missing the energy brought by the relative rotation of the two Jacobi coordinates neglected in the PPM are a little smaller than those of the PF-Y.

The 1234.86 MeV of the Translationally Invariant Coupled Cluster Method and the 1403 ± 1.5 MeV of the J-VMC for $A = 16$ [25] are in agreement with the IDEA and PPM respectively.

The next interesting potential is the Malfliet–Tjon MTV potential with a strongly singular hard core generating a large amount of correlations. It is often used for test case (Table 5).

The calculation of the PPM was performed by using the Extreme Adiabatic Approximation (EAA) which neglects the radial dependence of the amplitude and overbinds the bosons systems by about 0.5 MeV [26].

The size given by the IDEA is nearly constant but decrease slightly for the PPM and growing A.

For $A = 6$ the binding energy of the PPM agrees with the PF-Y = 125.68 MeV [24] but for $A = 16$ it cannot reach the Fermi hypernetted chain = 1584 ± 30 MeV (1.18) [27] neither the GFMC = 1605 ± 10 MeV [28] for 16 bosons. It might be related to the neglect of the contribution of the rotational motion of the Jacobi coordinates for $\ell > 0$.

The same MTV potential can be used without ambiguity for nuclei because it is a pure Wigner potential avoiding the occurrence of mixed symmetry states (Table 6).

For the ^{6}Li the PPM gives a binding energy similar to the 64.55 MeV of the Correlated Hyperspherical Harmonics 3 (CHH3) [29] but smaller than the 66.30 MeV of the Stochastic Variational Method (SVM) [30] and the 68.5 MeV of the Effective Interaction Hyperspherical Harmonic (EIHH) [31] but the r.m.s. radius agrees with the 1.52 fm and 1.512 fm of the two last methods.

The ^{12}C is calculated with the IDEA in the j–j coupling where the $1p^{3/2}$ shell is closed. In the Translationally Invariant Configuration Interaction (TICI2) [15] the L.S. coupling with $\ell = 1, m = \pm 1$ is used. It is not a $J = 0$ state and it gives an Esd binding energy of 429.44 MeV smaller than the IDEA.

Table 4
Binding energy in MeV and (r.m.s. radius in fm) for A-boson systems in ground state with the Afnan–Tang S3 potential [21].

A bosons	6	8	10	12	16
HCA	47.67	124.68	238.32	388.54	798.56
IDEA	111.16 (1.340)	247.41 (1.331)	430.68 (1.336)	657.57 (1.343)	1235.45 (1.358)
WPA	116.6 (1.328)	256.0 (1.312)	445.1 (1.309)	681.81 (7.308)	1291.7 (1.307)
PPM	115.07 (1.326)	257.38 (1.297)	455.0 (1.279)	708.88 (1.263)	1392.4 (1.236)
PF-Y [24]	114.98	260.20	457.17		
SVM [24]	115.06				

Table 5
Same as Table 4 with the Malfliet–Tjon MTV potential in the version defined by Zabolitzky [23].

A bosons	6	8	10	12	16
HCA	45.14	116.14	220.75	359.5	737.76
IDEA	124.0 (1.301)	274.9 (1.285)	477.6 (1.291)	729.3 (.1300)	1363.1 (1.322)
PPM	126.1 (1.287)	283.1 (1.253)	500.1 (1.239)	776.8 (1.229)	1512.5 (1.212)

Table 6
MTV potential. Binding energy in MeV and r.m.s. radius in fm.

	^{6}Li	^{12}C	^{16}O
HCA	11.4	189.6	506.9
IDEA	63.81 (1.537)	469.2 (1.351)	1026.7 (1.309)
PPM	64.88 (1.527)	503.7 (1.271)	1184.2 (1.182)

Table 8
MArg14 potential. Binding energy in MeV. The r.m.s. radius in fm is in parentheses.

	IDEA	PPM	PPM + Coul.
^{4}He	31.75 (1.337)		
^{6}Li	25.36 (1.998)	26.02 (2.006)	
^{12}C	53.72 (2.338)	60.33 (2.453)	
^{16}O	128.8 (2.235)	139.7 (2.38)	124.8 (2.41)
^{40}Ca	335.2 (2.882)	402.6 (3.09)	327.8 (3.119)

For ^{16}O the TICI2 with 973.67 MeV gives the smallest binding energy [15]. The 1024 ± 5 MeV of the Variational Monte Carlo (VMC) [28] is in agreement with the IDEA while the larger VMC [32] and [33] with 1103 ± 1 MeV and 1138.5 ± 2 MeV respectively are below the PPM which is in agreement with the 1194 ± 20 MeV of the Green Function Monte Carlo (GFMC) [28] and the 1189 ± 1 MeV of the Diffusion Monte Carlo (DMC) [33] values with a r.m.s. radius 1.30 ± .1 fm near the 1.18 fm of the PPM.

The MS3 [10] is commonly used as test potential (Table 7).

The ^{6}Li is underbound by about 10 MeV with respect to the experimental 32.0 MeV binding energy.

The TICI2 method gives 62.99 MeV for ^{12}C [15].

For the ^{16}O the 105.64 MeV of the TICI2 and the 105.3 MeV of the Fermi hypernetted chains [30] are near the IDEA, but the PPM is larger than the 118.6 MeV of the Bruekner–Hartree–Fock (BHF) value [10].

The PPM gives nearly the experimental binding energy 127.6 MeV but when the Coulomb potential is taken into account the energy becomes 114.8 MeV i.e. about 13 MeV below the experimental value.

The r.m.s. radii of 2.70 fm and 2.72 fm given by the PPM and the PPM + Coul. respectively must be compared with the experimental 2.7 ± .03 fm [35].

The numerical program computes together the investigated approximations and the monopolar excited states which is the eigenfunction with one node of the radial wave.

For the PPM + Coul. the monopolar excitation energy of ^{16}O with the MS3 potential is Mono = 20.7 MeV above the ground state.

For the ^{40}Ca the increase of binding energy brought by the PPM with respect to the IDEA is large but when the Coulomb potential is introduced the final binding energy of 330 MeV is near the 342 MeV experimental data, with a r.m.s. radius of 3.418 fm near the experimental 3.6 ± .1 fm [35]. By taking the nucleon charge structure into account the r.m.s. radius becomes 3.51 fm.

Once again the PPM is larger than the 354.0 MeV of the BHF [34].

The M.Arg.14 potential is the central parts of the Arg.14 potential [36] where the triplet even component of the Afnan–Tang S1 potential fitted to the deuteron and the N–N scattering phase-shifts is substituted for the V^{3+} + tensor of the original potentials for avoiding to solve the coupled equations generated by the tensor potential (Table 8).

The hypercentral potential does not give any bound state. The binding energy is fully provided by the correlations.

The binding energies obtained with this potential are larger than with the MS3 and the size is smaller but surprisingly this double effect by generating an increase of Coulomb energy leads to a final binding energy with Coulomb near the experimental data but with a r.m.s. radius smaller by about 10% for ^{16}O and ^{40}Ca.

It reproduces the effect in the ^{4}He where the r.m.s. radius given by MS3 is 10% larger than the one obtained with the MArg.14 potential.

In this paper the Schrödinger equation is written with hyperspherical Jacobi coordinates for central potential only.

The introduction of the tensor force was already treated for the three nucleons [37] and ^{4}He [38].

The extension to heavier nuclei is straightforward. The integration over $d\Omega_{N-1}$ leading to (18) for $L_m > 0$ generates two body density functions $W^{(\varepsilon)}(z,\theta)$ which enter in the construction of the effective potential [6, (120)]. The $W^{(t)}_{[L_m]}(z,\theta)$ function associated with the tensor operator is the one for the spin triplet state already known.

One modifies accordingly the equations of ^{4}He in [38, (2, 2)] to generate those for the $[L_m]$ state.

By projection of the interaction onto the space of a reference pair the contribution to the binding energy of the two-body correlations is exhausted when the contribution of the relative motion of the Jacobi coordinates is included.

The residual potential after the projection involves the contribution of three particles in interaction function of $\vec{\xi}_3$ which might be large for dense matter like for systems where all bosons are in 1s-states calculated in Tables 4 and 5.

But the contribution of the residual potential seems small in nuclei where for ^{16}O calculated with the MTV potential generating strong correlations, the GFMC, DMC and PPM binding energies are in agreement.

One can wonder whether the present method of projecting a local potential can be applied to other kinds of interactions. When the potential can be expressed in momentums space the projection of the plane wave in the Fourier transform is a solution. Otherwise it should be extracted from a method for solving the three body system.

In summary when the sum of all pairwise potentials is substituted for the single one of the reference pair used in the IDEA a new variable $\cos\theta$ where $\theta = (\widehat{\xi_2, \xi_3})$ is the angle between two first Jacobi coordinates appears in the potentials. It corresponds to the relative rotation of two Jacobi coordinates. When this motion is expressed in terms of a Legendre polynomial $P_\ell(\cos\theta)$ expansion the first term for $\ell = 0$ and $P_0 = 1$ only corresponds to a reference pair in s-state. The elimination of the other terms for $\ell > 0$ is performed by a projection of the potentials onto the space of the reference pair in s-state leading to the PPM model. The introduc-

Table 7
MS3 potential [10]. Binding energy in MeV and in the parentheses r.m.s. radius in fm. The contribution of the Coulomb potential is taken into account in the row PPM + Coul.

	^{4}He	^{6}Li	^{12}C	^{16}O	^{40}Ca
HCA	7.19	0	0	12.74	46.45
IDEA	28.15 (1.434)	21.64 (2.190)	44.65 (2.636)	103.6 (2.538)	273.3 (3.295)
PPM		22.79 (2.212)	58.29 (2.731)	128.1 (2.700)	402.25 (3.377)
PPM + Coul.				114.08 (2.72)	330.1 (3.413)

tion of terms for $\ell > 0$ generates a system of coupled equations neglected in the first order approximation where pairs are in s-state. The binding energies given by the PPM never exceed the known GFMC values.

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