Asymptotic equations for two-body correlations

M. Fabre de la Ripelle

Abstract. An asymptotic equation for two-body correlations is proposed for a large numbers of particles in the frame work of the Integro-Differential Equation Approach. The quality of this equation is discussed with examples.

Adiabatic and asymptotic properties of the two-body correlations are investigated.

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Introduction

The integro-differential equation approach (IDEA) was proposed in 1984 [1] to avoid solving the large number of coupled differential equation of the Hyperspherical Harmonic Expansion Method (HHEM) needed to obtain an accurate converged solution for nuclei beyond systems of few bodies [2]. It already included the asymptotic expression of the projection function, which is the main ingredient in the equation for a large number of particles [1], and analytical solutions for bosons in an S-state were also derived [3].

In a recent paper [4] another derivation of the asymptotic equation has been published for bosons in the ground S-state. In order to obtain this asymptotic equation, the autor correctly deduced an equation (23) extracted from ref. [5]. But contrary to their allegation this equation cannot lead to their asymptotic equation (25). The asymptotic equation can be obtained directly from the asymptotic projection function already published in ref. [1], a reference quoted in [6] .The aim of the present paper is to establish the correct equation and to discuss the conditions for the validity of its utilization, as a substitute for the exact equation, for a large system of particles.

The method used in this paper to solve the Schrödinger equation $-\Delta + V(\vec{x}) - E \Psi(\vec{x}) = 0$ where 1 *A i* is the Laplace operator in the whole $D = 3 \times A$ dimensional space for A particles, $V(\vec{x})$ a function of all coordinates $\vec{x}(\vec{x}_1,...,\vec{x}_A)$ and E the eigenvalue related to the wave function $\Psi(\vec{x})$, proceeds step by step. First by assuming $V = E = 0$, the solutions are (\vec{x}) = (Harmonic polynomial in the \vec{x} coordinates = $Y_{[L]}(\vec{x})$). Since Harmonic polynomials are homogeneous polynomials the radial coordinate r with $r^2 = \sum x_i^2$ can be factorized and $(\vec{x}) = Y_{L}(\Omega) r^L$ written in polar coordinates (Ω, r) where $Y_{L}(\Omega)$ is a Hyperspherical Harmonic defined by the *D-*1 quantum numbers [*L*] including *L* the degree of the polynomial.

Introducing a Hypercentral Potential $V(r)$, i. e. depending only on the radial coordinate r , leads to a solution $\Psi(\vec{x}) = Y_{L}(\Omega)u(r)/r^{(D-1)/2}$ where $u(r)$ is an eigenstate of a standard Schrödinger radial equation.

In nuclear physics, more than 3/4 of the potential energy originates already from the Hypercentral part (invariant under rotation in the whole space of coordinates) of the nuclear interaction, and balances the contribution of the kinetic energy to the binding energy. To go further the structure of $V(\vec{x})$ must be known.

For a sum of two-body potentials , $(\vec{x}) = \sum V(\vec{r}_{ij}),$ $\overline{\overline{i,j}}$ *i* $V(\vec{x}) = \sum V(\vec{r}_{ij}), \ \vec{r}_{ij} = \vec{x}_i - \vec{x}_j$ the wave function

 $(\vec{x}) = Y_{[L]}(\Omega) \sum_{i,j>i} P(\vec{r}_{ij},r)$ $\sum_{i,j>i}$ \vec{x}) = $Y_{[L]}(\Omega) \sum P(\vec{r}_i, r)$ is a sum over all pairs of two-body amplitudes $P(\vec{r}_i, r)$ solutions of an Integro-Differential Equation (IDE) [1].

Traditionally the many-body bound states are defined by assuming that a state can be written as a properly symmetrised product of individual particle eigenfunctions of a one-body potential well, and a Jastrov function. This Jastrov function is the product over all pairs of variational functions $f(r_{ij})$, $r_{ij} = |\vec{x}_i - \vec{x}_j|$, where the pair variational function is selected to gives the strongest binding energy. This procedure suffers of several defects :

1/ Absence of an independent center of mass for a pair wise interaction.

2/ Inability to define the wave function out of the range of the potential, a defect of all variational methods.

3/ Inaccuracy in the computation of the wave function where it is small, since only the square of the wave function is significant in the variational procedure.

4/ Absence of an equation to define the correlations.

In contrasts another method has been proposed where, assuming the analyticity of the wave function, the state is defined by the polynomial of the lowest degree L_m occurring in an harmonic polynomial expansion of the wave function [1].

For bosons where all particles can be in 1s state this degree is $L_m = 0$. For identical Fermions it is given by the lowest degree antisymmetric polynomial homogeneous in the individual coordinates $\vec{x} = (\vec{x}_1, ..., \vec{x}_A)$ of the A-particle system, where the antisymmetry is provided by a Slater determinant.

This polynomial is translationally invariant since any scalar symmetrical operator seeking to decrease the degree of a homogeneous polynomial should give zero when applied to a polynomial of minimal degree.

Since the state is defined by a translationaly invariant harmonic polynomial [9], therefore it can be expressed in terms of Jacobi coordinates.

The radial equation

Let $D_{[L_m]}(\vec{x})$ be the antisymmetric harmonic polynomial written as a Slater determinant.

In a polar coordinates system $\vec{x} = (r, \Omega)$ where 1 $a^2 = 2\sum_{i=1}^{A} (\vec{x}_i - \vec{X})^2$ $r^2 = 2\sum (\vec{x}_i - \vec{X})^2$ and \vec{X} is the center of mass, is a set of $D-1$ angular coordinates in the $D = 3(A-1)$ dimensional space of the Jacobi coordinates. We can then write

$$
D_{L_m}(\Omega) = D_{L_m}(\vec{x}) / r^{L_m}
$$
 is a Hyperspherical Harmonic (HH). (1)

$$
\Psi_{L_m}(\Omega, r) = D_{L_m}(\Omega) u_{L_m}(r) / r^{(D-1)/2}
$$
\n(2)

The state is defined by the product of a HH and a (Hyper) radial wave solution of the radial equation

n
\n
$$
\left\{\frac{\hbar^2}{m}\left[-\frac{d^2}{dr^2} + \frac{\mathcal{L}(\mathcal{L}^2 + 1)}{r^2}\right] + V_{[L_m]}(r) + U_{\lambda}(r) - E\right\}u_{L_m}(r) = 0, \ \mathcal{L} = L_m + (D-3)/2
$$
 (3)

where $V_{[L_m]}(r)$ is a Hypercentral potential.

When the interaction is a sum over all pairs of a two-body potential $V(r_i)$, the Hypercentral potential $V_{[L_m]}(r)$ is a sum over all pairs of the rotationally invariant part of the pair-wise

potential while
$$
U_{\lambda}(r)
$$
 is the contribution of the pairs correlation.
\n
$$
V_{[L_m]}(r) = A(A-1)/2 \times \int D_{[L_m]}(\Omega) V(r_{ij}) D_{[L_m]}(\Omega) d\Omega
$$
\n(4)

Contribution of the two-body correlations

This contribution is the eigenpotential in a two-variable Integro-Differential Equation obtained by writing that, for a sum of pairwise potentials, the wave function is the product

$$
\Psi(r,\Omega) = D_{[L_m]}(\Omega) \sum_{k
where $z_{k\ell} = \cos 2\phi_{k\ell} = 2r_{k\ell}^2 / r^2 - 1$ for $r_{kl} / r = \cos \phi_{kl}$, (5)
$$

of the state and a sum over all pairs of two body amplitudes [1].

Without correlations $U_2 = 0$ and the solution is given by (2) and (3).

"As A increases an important decoupling occurs between the variables z_{ij} and r, and a good approximation is obtained by taking for the solution the product

$$
P(r,z) = P_0(z,r) \times u_0(r),\tag{6}
$$

(for $z = 2r_i^2/r^2 - 1$) for a reference pair (i, j), where $P_0(r, z)$ is an eigenfunction for each r (r

is a parameter) of the Integro-Differential Equation (IDE).
\n
$$
-\frac{4\hbar^2}{mr^2} \frac{1}{W_{[L]}(z)} \frac{d}{dz} (1-z^2)W_{[L]} \frac{d}{dz} P_0(z,r) + (V(r\sqrt{\frac{1+z}{2}} - V_0(r))(P_0(z,r)) + \int_{-1}^{1} f(z,z)P_0(z,r) dz') = U_{\lambda}(r)P_0(z,r)
$$
\n(7)

with $[L] = [L_m]$ where $V_0(r)$ is the integral in (4), taken over all Hyperangular coordinates while $u_0(r)$ becomes a solution of (3).

The projection function $f(z, z')$ projects the amplitudes $P_0(r, z_{k\ell})$ in (5) on the space of the reference pair (i, j) . It is given by [1].

$$
f(z, z') = W_{[L]}(z') \sum_{K=0}^{\infty} (f_K^2 - 1) P_K^{[L]}(z) P_K^{[L]}(z')
$$
 (8)

where the $P_K^{[L]}(z)$ are the normalized polynomials associated with the weight function $W_{[L]}(z)$ while the coefficient are [1]

while the coefficient are [1]

$$
f_K^2 - 1 = 2(A-2)(P_K^{[L]}(-1/2) + \frac{(A-3)}{4}P_K^{[L]}(-1))/P_K^{[L]}(1)
$$
(9)

The weight function is [7, 8]

$$
W_{[L]}(z) = (1-z)^{\alpha} (1+z)^{1/2} Q(z)
$$
 with $\alpha = L + (D-5)/2 - 2\ell_m$. $Q(z) = \int |D_{[L]}(\Omega)|^2 d\Omega_1$

where the integral is taken over all Hyperangular coordinates Ω except z is a polynomial of degree $2\ell_m$ where ℓ_m refers to the last filled shell in nuclei with $\ell_m = 0, 1, 2, ...$ for the s, p, s-d… shells.

The asymptotic equation

For bosons in the ground state $L_m = 0$, $Q(z) = 1$ and the associated polynomials are the Jacobi polynomials $P_K^{\alpha,1/2}(z)$.

The weight function is

$$
W(x) = (1 - x^2 / r^2)^{\alpha} x^2
$$
 (10)

in terms of $x = r_{ij}$ with $dz = \frac{4}{3}$ $\overline{\mathbf{c}}$ $dz = \frac{4x}{2}dx$ *r* . where for a normalized $W(x)$ the first term evolves into a (x) function as $\alpha \rightarrow \infty$.

Analytical expressions for the sum in (8) have been already found : first in the case of threebodies where it leads to a Faddeev equation [9] and then for a large number of bosons when $\alpha \rightarrow \infty$ [1].

We now look back to details that were involved of the last calculation, to analyze the quality of the approximations.

The following are the main points :

1°/ One uses the asymptotic relation

$$
\lim 1 - Z^2 / \alpha^{\alpha} \xrightarrow[\alpha \to \infty]{} e^{-Z^2}
$$
\n(11)

this approximation is valid for *Z*²

2°/ The polynomials associated with the normalized weight function

$$
W_{[0]}(Z)dZ = 4/\sqrt{\pi}e^{-Z^2}Z^2dZ
$$
\n(12)

are the Laguerre polynomials $L_K^{1/2}(Z^2)$

$$
3^{\circ}\!/
$$

It can be proved easily from the asymptotic properties of the Jacobi polynomials used in ref [3] for z, n and fixed β ,

 $\lim \alpha^{-n} P_n^{\alpha,\beta}(z) \longrightarrow \frac{1}{n!} \left(\frac{z+1}{2}\right)^n, P_n^{\alpha,\beta}(1)$ $\frac{z}{\sqrt{2}}$ $P_n^{\alpha,\beta}(z) \longrightarrow \frac{1}{n!} \left(\frac{z+1}{2}\right)^n$, $P_n^{\alpha,\beta}(1) = \left(\frac{n!}{2!}\right)^n$ $P_n^{\alpha,\beta}(z) \longrightarrow \frac{1}{n!} \left(\frac{z+1}{2}\right)^n$, $P_n^{\alpha,\beta}(1) = \left(\frac{n+n}{n}\right)$ is a binomial coefficient, for $z = -1/2$

and $z = -1$ in Eq. (9) that asymptotically the coefficient $f_K^2 - 1$ become [10, Eq. (9.6)].

$$
\lim f_K^2 - 1 \xrightarrow[\alpha \to \infty]{} 2(A-2)/4^K
$$
\n(13)

4°/ If all the asymptotic relations are valid the formula [11]

$$
S = \sum_{n=0}^{\infty} \frac{n!}{\Gamma(n+\beta+1)} L_n^{\beta}(x) L_n^{\beta}(y) z^n
$$

= $(1-z)^{-1} \exp\left(-z \frac{x+y}{1-z}\right) (xyz)^{-1/2\beta} I_{\beta} \left[\frac{2(xyz)^{1/2}}{1-z}\right]$ (14)

can be used for $z = 1/4$, $\beta = 1/2$ associated with the weight function $x^{\beta}e^{-x}$.

Here one sets
$$
Z^2 = \frac{\alpha}{r^2} x^2
$$
 with $\alpha \xrightarrow{A \to \infty} 3A/2$ in (10) (15).

The radial function $u(r)$ is concentrated around the minimum at $r = r_m$ of the effective potential

$$
V_{eff}(r) = \frac{\hbar^2}{m} \frac{\mathcal{L}(\mathcal{L} + 1)}{r^2} + V_{[0]}(r) + U_{\lambda}(r)
$$
\n(16)\n
\n(3) where $\frac{d}{dr} V_{eff}(r_m) = 0$.

in Eq. (3) where $\frac{d}{dr}V_{\text{eff}}(r_m) = 0$ *dr*

The r.m.s. radius a is related to r_m by

$$
r_{m}^{2} \approx r^{2} \gg 2Aa^{2} \tag{17}
$$

and the validity of Eq. (11) is fulfilled for $x^2 \ll r_m^2 = 2Aa^2$. In the ground state, all bosons in the 1s state have the tendency to stay inside the range of the potential, in such a way that the r.m.s. radius should be either stationary or vary very slowly with the number of particles. Eq. (7) when solved exactly showed a stability of the r.m.s. radius a for growing A. For instance with the Afnan-Tang S3 potential [12], the r.m.s. radius $a = 1.34 \pm .01$ fm between $A = 6$ and *A* = 16 and $a \approx 1.4$ *fm* for *A* = 40 [7].

The behavior of the coefficients (9) with respect to K must now be investigated.

In table 1 the product $4^{k} (f_{k}^{2}-1)/2(A-2)$ is exhibited for $A=16,40,100,500,1000$ for $K \geq 2$.

Table 1

For $K = 0$ we have to deal with the weight function approximation where the projection function is the weight function itself, with f_0^2 $f_0^2 = A(A-1)/2$. The $K=1$ term generates a spurious component which must be eliminated [13]. It is clear from the table 1 that 4^{-K} over estimates the contribution of the terms of degree K in the projection functions. But we have shown previously [6] that nearly all the contributions to the binding energy originate from the few first terms in the expansion (8).

Since the weight function (12) with (15) is defined in terms of $x = r_{ij}$ it is appropriate to use the Integro-Differentiel Equation in the relative coordinates version [3] i.e. with the same variable *x* .

The sum (14) with $\beta = 1/2$, $z = 1/4$, $x = Z^2$, $y = Z'^2$ is

$$
S = \frac{4}{\sqrt{3\pi}} \frac{e^{-(Z^2 + Z^2)/3}}{ZZ} \sinh(\frac{4}{3}ZZ')
$$
 (18)

(note that in [4] the formula (15) of ref. [5] which gives 3/4 instead of 4/3 is flawed, indeed a term $t^{1/2}$ is missing in the last parenthesis).

It leads to the projection function [1]

to the projection function [1]
\n
$$
f(z, z')dz' = 2(A-2)/\sqrt{\pi} \left\{ \left[A-3 - \frac{2}{3} \left(Z^2 - \frac{3}{2} \right) \left(Z^2 - \frac{3}{2} \right) \right] e^{-Z^2} + \frac{4}{\sqrt{3}} \frac{1}{ZZ'} \left[e^{-(2Z'-Z)^2/3} - e^{-(2Z'+Z)^2/3} \right] \right\} Z'^2 dZ'
$$
\n(19)

which can be inserted as it is into (7) with $Z^2 = \alpha(1+z)/2$ (note $dz' = 4Z' dZ' \alpha$).

It can be easily transformed as well into an equation in the variable Z by using Eq. (38) of ref [3] which eliminates the first derivative in the variable $x = r_{ij}$ in the kinetic energy operator by writing $P_0(z, r) = g_{\lambda} / g_0$ with

$$
g_0 = \frac{\sqrt{\alpha}}{r} x \sqrt{1 - \frac{x^2}{r^2}} (1 - \frac{x^2}{r^2})^{\alpha/2} \xrightarrow{\alpha \to \infty} Z e^{-Z^2/2}
$$
 (20)

and thus $P_0(z,r) = e^{z^2/2}$ $P_0(z,r) = e^{z^2/2} / Z G_{\lambda}(z,r)$. By introducing this transformation together with the asymptotic weight function (12) in Eq. (7) one generates the asymptotic equation in the variable Z.

The kinetic energy operator becomes

etic energy operator becomes
\n
$$
-\frac{4\hbar^2}{mr^2} \frac{1}{W_0(z)} \frac{d}{dz} (1 - z^2) W_0 \frac{d}{dz} P_0(z, r) = \alpha \frac{\hbar^2}{mr^2} \frac{e^{z^2/2}}{Z} \left[-\frac{d^2}{dz^2} + Z^2 - 3 \right] G_\lambda(Z, r) \tag{21}
$$

And the wave equation (7) multiplied by $\frac{mr^2}{\lambda}Ze^{-Z^2/2}$ ² $\frac{mr^2}{\lambda^2}$ *Ze^{-Z2/2}* is transformed (with (19)) into

$$
\frac{d^{2}}{dt^{2}} = \text{Jshamiltonian} \text{ (a) } \frac{d^{2}}{dt^{2}}
$$
\n
$$
\left(-\frac{d^{2}}{dz^{2}} + Z^{2} - 3\right)G_{\lambda}(Z,r) + \frac{mr^{2}}{\hbar^{2}\alpha} \tilde{V}(Z,r) - U_{\lambda}(r) G_{\lambda}(Z,r)
$$
\n
$$
= \frac{mr^{2}}{\hbar^{2}\alpha} \tilde{V}Ze^{-Z^{2}/2} \int_{-1}^{1} f(z,z') \frac{e^{Z^{2}/2}}{Z} G_{\lambda}(Z',r) dz'
$$
\n(22)

One introduces $e^{-Z^2/2}$ inside the integral to produce an equation where the r. h. s. becomes

$$
\frac{mr^2}{\hbar^2\alpha}\tilde{V}\int_{0}^{\sqrt{\alpha}}F(Z,Z^{\prime})G_{\lambda}(Z^{\prime},r)dZ^{\prime}
$$
\n(23)

The projection function

The projection function
\n
$$
F(Z, Z') = 2(A-2)/\sqrt{\pi} \left\{ \left[A - 3 - \frac{2}{3} (Z^2 - \frac{3}{2}) (Z'^2 - \frac{3}{2}) \right] Z Z' e^{-(Z^2 + Z'^2)/2} + \frac{4}{\sqrt{3}} \left[e^{-(5(Z-Z)^2 + 2ZZ')/6} - e^{-(5(Z+Z')^2 - 2ZZ')/6} \right] \right\}
$$

is symmetrical in *Z* and *Z*['], $\tilde{V}(Z,r) = V(r_i) - V_0(r)$ for $r_i = r / \sqrt{\alpha Z}$, $V_0(r)$ is the hypercentral part of $V(r_{ij})$ and the boundary conditions $G(o,r) = G(\sqrt{\alpha}, r) = 0$ determine $U_{\lambda}(r)$.

Applications with comments

In the Hyperspherical Approach we obtain the wave function and binding energy from two semi independent equations : first from an equation where the contribution of the two-body

correlations to the binding energy appears as an eigen-potential $U_i(r)$ of the radial coordinate. This potential is then introduced in a radial equation generating a radial wave function and a total binding energy.

The Hypercentral potential $V_{L_m}(r)$ occurring in the radial equation can be easily computed from the original weight-function.

But in the other equation (22) only the residual potential $\tilde{V}(r_{ij}, r)$ where the Hypercentral part of $V(r_{ij})$ has been subtracted must occur. This Hypercentral part is calculated from the asymptotic weight function which differs from the exact one.

Therefore an inaccuracy, in the calculation of the correlations, originates first from the asymptotic weight function and then from the asymptotic projection function itself. In the projection function, when the number of terms needed to reach a requested accuracy for $U_i(r)$ is small, only the defect of the asymptotic weight function with respect to the original one should have an effect.

Here one presents a few computations for $A = 16$ and 40 with typical nuclear potentials.

The IDE can be easily and accurately solved numerically with a program [8] that uses the traditional algorithm to integrate for the Independent the Particle Model the radial Schrödinger equation (see ref. [14]).

Four potentials are chosen with an increasing strength of the repulsive core: the Gogny, Pire, de Toureil (GPDT) [15], Brink-Boeker B1 [16], Afnan-Tang S3 [12] and Malfliet-Tjon MTV [17] potentials.

First one recall a few results obtained with the Volkov [18], Afnan-Tang S3 [12] and Malfleit-Tjon MTV [17] potential for A=16 bosons, for which the binding energy were calculated with the Hypercentral Approximation (HCA), the Weight Function Approximation (WFA) and the IntegroDifferencial Equation Approach (IDEA).

Table 2

It is clear that the contribution to the binding energy, of the polynomials for $K > 0$ in the projection function, does not exceed a few Mev. Thus only the WFA, where the term $K = 0$ in the projection function is the weight-function itself, is actually significant.

Four different algorithms have been chosen to solve numerically the many body bound state problem.

In ref. [19, 20] the eigenfunction $P(z, r)$ is expanded in terms of some interpolating polynomials, thereby reducing the equation to a standard eigenvalueproblem. The B splines of order N have been chosen for this purpose.

In ref. [22] the Hyperspherical Harmonic Expansion Method (HHEM) was applied using up to 40 coupled equations.

In ref. [3] the solution of the I. D. E. is discretized by using a finite difference scheme and an appropriate inverse power method provides the requested eigenvalue by the diagonalisation of a large matrix.

In ref. [7] and in the present paper the I. D. E. in the variable $x = r_{ij}$ of ref. [3] is solved numerically by generating the amplitude with a standard shooting procedure [14] : the solution of $g''(x) = (W(x) - U_1) g(x)$ is generated by solution of $g''(x) = (W(x) - U_{\lambda})g(x)$ is generated by
 $g(x+h) = 2g(x) - g(x-h) + (W(x) - U_{\lambda})h^2$, for an interval h between two successive mesh points with the boundary conditions $g(0) = g(x = r) = 0$ reached for the eigenvalue $U_{\lambda}(r)$. The slope of the shoot $g(h) = Ph$ is chosen in order to normalize $P(x,r)$ to unity i. e. $P(x, r) = 1 + h(x, r)$, details are available in ref. [8]. All methods agree surprisingly well.

The variational methods of ref. [23] provide for the S3 Potential a binding energy of 1130.94 Mev from the Translationally Invariant Configuration Interaction (TICI2) method and 1234.86 Mev for the Translationally Invariant Coupled-Cluster (TICC2) method. In the last method the algebraic expression to be solved numerically covers more than one full page in ref. [23] while it takes one line in this paper !

The converged value for the binding energy is already reached with only four polynomials in the projection function, and the weight function approximation (WFA) for $K = 0$ gives an estimate of the binding energy with an accuracy better than half percent at the level of twobody correlations.

The WFA with $K = 0$ gives the largest increase of binding energy with respect to the Hypercentral Approximation, without correlations, where $U_i(r) = 0$.

On the other hand the WFA is independent of the polynomial occurring in the projection function since the first polynomial for $K = 0$ is $P_0 = 1$. Whatever the weight function used and when the amplitude $P(z, r)$ is normalized to one the integral in (7) becomes $A(A-1)/2-1$ obviously independent of *r*. Solving then the WFA, one test first the effect of the asymptotic weight function (alone) on the solution of the IDEA.

Near the minimum, at r_m of $V_{\text{eff}}(r)$ where $dV_{\text{eff}}(r)/dr = 0$, the effective Hypercentral potential behaves like an Harmonic oscillator and the m. s. radius 2 potential behaves like an Harmonic oscil
 $a^2 = \langle r^2 \rangle / 2A = (r_m^2 + \langle (r - r_m)^2 \rangle) / 2A$.

The r. m. s. radius a is given table 3 together with $a_m = r_m / \sqrt{2A}$.

Table 3

The very small difference between the a and a_m supports the estimate in eq.(17) and the condition for the validity of (11), assuming that the strong concentration of the radial function near the minimum of the effective potential is fullfilled.

The fully asymptotic binding energy obtained from eqs (22, 23) with $\alpha = 3A/2$ in the Asymptotic Kinetic energy and in the Asymptotic Weight Function is exhibited in table 4.

In the first line the exact WFA is given, then the exact Hyper Central Approximation HCA where $U_{\lambda}(r) = 0$, and next the same for the fully asymptotic energies where $\alpha = 3A/2$ in Eq. (22). Finally in the last line one finds the combination Test = exact $HCA - Asymptotic$ HCA + ASWFA, where ASWFA is the binding energy given by the Asymptotic Eq. (22).

Table 4. Contribution of the fully asymptotic approximation to the binding energy of 16 and 40 bosons in the ground state, AS is for asymptotic.

Table 4

 α

A comparison between the Test line and the exact WFA energy shows clearly that the asymptotic Eq. (22) provides a rather good estimate of the contribution of the correlations to the binding energy but that in order to obtain a binding energy similar to the one of the WFA, the HCA must be calculated with $V_{L_m}(r)$ obtained from the original weight function in the radial equation (3).

Nevertheless, the larger the difference between WFA and HCA, the larger is the difference between the test line and the exact WFA.

As a conclusion, the asymptotic weight function can be used to calculate $U_i(r)$, the contribution of the correlations to the binding energy, but in the radial equation the original weight function should be used to calculate $V_{[L_m]}(r)$.

One must stress that the calculation of $U_i(r)$ must be done with the asymptotic projection function, by starting from the residual potential $\tilde{V} = V(r_{ij}) - V_0(r)$ where the Hypercentral potential $V_0(r)$ is calculated with the asymptotic weight function.

Nevertheless one cannot avoid keeping in mind that for systems, like bosons in the ground state, where all particles interact together within the range of the potential, the many body correlations, and at first the three and four body correlations, have to be taken into account [21].

" For nuclear systems however, the increasing of importance of the high-order correlations is expected to be much less relevant, due to the role played by the Pauli principle" [21].

Another method can be used to generate asymptotic equations.

Our purpose is to substitute asymptotic expressions for the original equation, in the case of a large number of particles.

For this task it is easier to use the IDEA equation in term of $x = r_{ij}$ developed in ref. [3] and reproduced in Appendix. In this equation the kinetic energy term appears as g_0 ["]/ g_0 where

$$
g_0 = x(1 - \frac{x^2}{r^2})^{\alpha_0/2} P_{[L_m]}(x^2/r^2), \ \alpha_0 = \alpha + 1,
$$

and $P_{[L_m]}$ is a polynomial occurring for Fermion systems while $P_{[0]} = 1$ for bosons in their ground state and $\alpha_0 = (D-3)/2 + L_m - 2\ell_m$, with $L_m = \ell_m = 0$ for bosons.

The term

$$
g_0" / g_0 = -\frac{\alpha_0}{r^2} (\alpha_0 + 1 - (\alpha_0 - 2) / T) / T, \qquad (24)
$$

with $T=1-X$ for $X=x^2/r^2$ becomes a hard repulsive wall for $x \to r$, indeed with $\delta x = r - x > 0$.

$$
\frac{\alpha_0(\alpha_0 - 2)}{r^2 T^2} \xrightarrow{x \to r} \frac{\alpha_0(\alpha_0 - 2)}{4(\delta x)^2} \tag{25}
$$

behaves as a strong repulsive kinetic centrifugal barrier for $x \rightarrow r$.

One assumes in the asymptotic approximation that the significant values of $\frac{x^2}{x^2}$ $\overline{\mathbf{c}}$ *x r* occurring in the calculation of the wave function decreases for increasing number of particles which justifies the exponential approximation

$$
T^{\alpha} \xrightarrow[\alpha \to \infty]{} e^{-\alpha X} \tag{26}
$$

When the first order expansion

$$
\frac{1}{T} = (1 + X + X^2...)
$$
\n(27)

is used and $Xⁿ$ is neglected in (27) for $n>1$ the kinetic energy term (24) becomes $\frac{\alpha_0}{r^2}$ (α_0 -5)X-3 +O(X²) . It is an Harmonic oscillator potential in x^2/r^2 when X^2 can be neglected.

In the next table various approximations of the kinetic energy are tested for $A=16$ and $A = 40$ bosons where $H0$, $AH0$, $T1$ and $T2$ refer to Harmonic oscillator (HO), Asymptotic *H0* where $\alpha = 3A/2$, *T*1 for $T^{-1} = 1 + X$ and *T2* for $T^{-1} = 1 + X + X^2$ in Eq. (24) with $X = x^2/r^2$ and exact without approximation. The computation is made with a space between mesh points of 0.1 fm for *x* and .05 fm for *r*.

It is worthwhile to notice that the asymptotic AHO approximation is very similar to the T1 approximation with a difference of around 1 Mev, or less, for *A*=16, and 2 Mev for *A*=40.

The good accuracy of the numerical program, each computation being independent, enables one to check the regular improvement between two successive approximations.

The next asymptotic approximation to be analyzed concerns the weight function in Eq. (A2) in Appendix with $g_0 = \sqrt{T} (1 - X)^{\alpha}$, $X = x^2 / r^2$ for bosons.

In the asymptotic approximation

$$
(1 - X)^{\alpha} = e^{-\alpha X} f(X) \tag{28}
$$

where $f(X) = (1 - X)e^{X}$ ^{*a*} and $f(X) = 1$ for an asymptotic exponential function.

The polynomial expansion

$$
(1-X)eX = (1-X2/2-X3/3-X4/8+...)
$$
 (29)

leads to an approximate formula

$$
(1-X)^{\alpha} = e^{-Z^2(1+\frac{X}{2}+\frac{X^2}{3}+\frac{X^3}{8}+\ldots)}
$$
\n(30)

 $X = x^2/r^2$, $Z^2 = \alpha \frac{x^2}{r^2}$ $\overline{\mathbf{c}}$ $Z^2 = \alpha \frac{x}{x}$ *r* limited to the third degree term.

The term of degree zero is for an asymptotic Gaussian weight function associated with Laguerre polynomials.

In the table 5, the convergence to the exact value is exhibited in terms of *N*, the degree of the polynomial in *X* in Eq. (30). *N*=0 for a Gaussian asymptotic weight function.

The difference between the approximate binding energy for $N=1$ and the exact value is about 10 Mev i. e. less than one percent and decreasing for increasing *A*.

The increase of binding energy WFA-HCA brought by the correlations is very similar for each potential for $N > 0$, in such a way that a nearly exact binding energy can be obtained by adding this increase to the exact HCA. When $N = 0$ the same procedure misses the binding energy by about 10 Mev, and even more for $A = 16$ and the MTV potential.

The IDEA is a two variables integro differential equation with one length r and one angle Φ defined by $\cos \Phi = r_{ij}/r$, $r_{ij} = |\vec{x}_i - \vec{x}_j|$ related to the description of the two-body correlations of a bound system of particles where pairs are in s-state.

This equation can be reduced to two one variable equations by assuming that the amplitude $P(z,r)$ can be written as the product $P(z,r) = u(r)P_{\lambda}(z,r)$ where $P_{\lambda}(z,r)$ is only

adiabatically *r*-dependent in such a way that the derivatives of P_{λ} with respect to r can be neglected. This approximation was first suggested for Atomic system [24] and then extended to Nuclei [27, 28, 29].

An upper and a lower bound to the binding energy can be derived in this adiabatic approximation [27, 28, 29].

The interval between upper and lower bound is less than about 1 Mev for 4 He, decreasing to 0.5 Mev for 16 bosons [30] and .2 Mev for *A* = 40, in such a way that by taking the middle of the interval for binding energy reduces the inaccuracy by half. It vanishes as $A \rightarrow \infty$.

When Eq. (7) is multiplied by r^2 the kinetic energy operator becomes independent of r and the variation with *r* of the kinetic energy should be adiabatic like $P_0(z, r)$.

Therefore one could expect that the eigenpotential $r^2U_i(r)$ might also vary adiabatically.

A potential where all the binding energy is generated by the correlations in nuclei was chosen for testing the behavior of the eigenpotential U_i in terms of r. The Argonne 14 potential [31] has a strong repulsive core which prevents any binding for both ¹⁶O and ⁴⁰Ca at the level of the Hyper Central Approximation without correlations (i. e. $HCA > 0$). Since the equation (7) does not include the treatment of the tensor forces, the Afnan-Tang S1 potential [12] which is adjusted to give the experimental triplet even ${}^{3}S_{1}$ Nucleon-Nucleon scattering phase-shifts is substituted for the V^{3+} + tensor force of the original Arg 14 potential. For bosons in ground state the Afnan-Tang S3 potential [12], already used in numerous test cases, is selected.

For the sake of comparison, the table is divided in three columns. In the first one $-U_1(r)$ is exhibited followed by the ratio $-U_{\lambda}(r) / Kin(r)$, where $Kin(r) = \frac{\hbar^2}{m} \mathcal{L}(\mathcal{L} + 1) / r^2$ is the Kinetic Centrifugal barrier in the radial equation, and then by the effective potential $V_{\text{eff}}(r)$ in the radial equation.

Bosons		$A = 16$		$A = 40$			
r (fm)	$-U$ ₁ (Mev)	$-U$ ₂ / Kin	V_{eff} Mev	$-U$ ₂ (Mev)	$-U$ ₂ / Kin	V_{eff} Mev	
$\overline{\mathbf{4}}$	1406	1.18	4758				
6	748	1.41	-824				
8	437	1.46	-1281	3191	1.49	7183	
10	288	1.50	-1224	2306	1.68	-5016	
12	205	1.54	-750	1728	1.82	-7817	
14	155	1.59	-548	1341	1.92	-6651	
16	122	1.63	-406	1072	2.00	-6651	
18	99	1.67	-306	872	2.06	-5560	

Pot S3

Pot. Arg. 14

Fermions		16 _O		^{40}Ca			
r (fm)		$-U_{\lambda}$ (Mev) $-U_{\lambda}$ / Kin V_{eff} (Mev)		r (fm)		$-U_{\lambda}$ (Mev) $-U_{\lambda}$ / Kin V_{eff} (Mev)	
8	524	.721	198	20	774	.542	-127
10	308	.664	-102	22	636	.538	-282
12	205	.636	-144	24	533	.537	-338
14	149	.628	-130	26	453	.536	-346
16	114	.629	-107	28	390	.534	-330
18	91	.634	-85	30	338	.533	-304
20	74	.640	-67	32	296	.531	-274
22	62	.647	-53	34	262	.529	-245
24	53	.654	-43	36	233	.528	-217
26	45	.662	-34	38	208	.526	-191
28	39	.669	-28	40	187	.524	-169

The ratio $-U_{\lambda}$ / Kin vary slowly, adiabatically, for growing r. The larger \mathcal{L} , the better is the adiabatic approximation. The most significant ratio is in the vicinity of the minimum r_m of

 $V_{\text{eff}}(r)$, in the domains of a few fermis where the radial function $u(r)$ is not negligible, where it does not change by more than a few percent or less.

In this range the effective potential can be written

$$
V_{\text{eff}}(r) = \frac{\hbar^2}{m} (1 + U_{\lambda}(r) / \text{Kin}(r)) \mathcal{L}(\mathcal{L} + 1) / r^2 + V_0(r)
$$

where the ratio U_{λ} / Kin is negative and nearly constant.

An important difference appears between bosons and fermions systems.

While the kinetic centrifugal barrier is repulsive for nuclei with the ratio $U_{\lambda}/Kin > -1$ it becomes strongly attractive for bosons with a ratio \lt -1 generating a strong attraction in r^{-2} and thus a collapse of the bosons which gather near the origin.

The similarity between the eigenpotential U_i and an attractive r^{-2} potential has double effect. When a strong repulsive core is introduced in a potential to increase the size of a nucleus, it create a large amount of correlations which decrease the kinetic centrifugal barrier and then balance the effect of the core.

For this reason the modified Arg. 14 Potential used in this paper which produces (without Coulomb potential) a IDEA binding energy of 128.5 Mev and 336 Mev for ${}^{16}O$ and ${}^{40}Ca$ respectively [20], in good agreement with the experimental data, generates a r.m.s. radius of 2.25 fm and 2.91 fm respectively, smaller than the experimental data.

The adiabatic property of U_{λ} / *Kin* suggests a change of variable where instead of $x = r_{ij}$ in Eq. (A3) a new variable defined by $x / r = X / \mathcal{L}_0$ with $\mathcal{L}_0 = \mathcal{L} + 1/2$ is chosen.

The small difference $\mathcal{L}_0^2 - \mathcal{L}(\mathcal{L} + 1) = 1/4$ and $\alpha + 1 - \mathcal{L}_0$ become rapidly negligible with respect to \mathcal{L}_0 for growing A.

The derivative $d^2/dx^2 = (\mathcal{L}_0/r)^2 d^2/dX^2$ while the term T in the kinetic energy Eq. (24) becomes $1 - X^2 / \mathcal{L}_0^2$ independent of *r*.

One renormalizes the residual potential $\tilde{V}(r_{ij}, r)$ and $U_{\lambda}(r)$ in Eq. (A3) according to

$$
\tilde{V}_\mathcal{L}(X,r) = \tilde{V}(r_{ij},r) / Kin(r)
$$

$$
U_\mathcal{L}(r) = U_\lambda(r) / Kin(r)
$$

" $g_0^{\dagger}/g_0 \rightarrow \chi X^2-3\mathcal{L}_0$ / r^2 (see Appendix) for bosons in ground state. One divides Eq. (A3) by \mathcal{L}_0^2 / r^2 to obtain the asymptotic adiabatic equation.

$$
\begin{aligned} &\left[\frac{d^2}{dX^2} - (X^2 - 3\mathcal{L}_0) / \mathcal{L}_0^2 - (\tilde{V}_{\mathcal{L}}(X, r) - U_{\mathcal{L}}(r))\right] G_{\mathcal{L}}(X, r) \\ &= \tilde{V}_{\mathcal{L}}(X, r) G_0(X, \mathcal{L}) I_{\mathcal{L}}(X, r) \end{aligned}
$$

Where r is a parameter and $G_0(X, \mathcal{L})$ is deduced from Eq. (A2) by substitution of X / \mathcal{L}_0 for x/r with $z = 2x^2/r^2 - 1$, $\alpha = \mathcal{L}_0$ and a similar transformation for I_λ to obtain $I_\mathcal{L}$.

The behavior in terms of r of the eigenpotential $U_{\mathcal{L}}(r)$ is adiabatic.

Comments and conclusion

The asymptotic equation (22, 23) were obtained first by a transformation where the basic equation (7) is expressed in terms of the relative coordinate $x = r_{ij}$ including an elimination of the first derivative d/dx [3]. Using then the asymptotic expression $(1-X)^{\alpha} \xrightarrow[\alpha \to \infty]{} e^{-\alpha X}$, together with the relation (14), to sum the series of Laguerre polynomials occurring in the projection function, Eq. (8) leads to an analytical expression (19) [1].

This expression can be used directly in Eq. (7) or transformed into Eq. (22) in the variable $Z = \sqrt{\alpha x / r}$, by a change of scale.

With respect to the calculation published in ref. [4] : the formula chosen to sum the series of Laguerre polynomials is taken from ref. [5] and is used correctly. It leads to a coefficient 3/4 in Eq. (23) of ref. [4] instead of the 4/3 of ref. [11] and in our Eq. (18) and cannot lead to our asymptotic eqs (22,23).

The values quoted as exact, for the S3 potential and for 16 bosons in table 2 of ref. [4], are not in agreement with the five published values presented in table 2 in this paper, which are in common agreement.

We found, by application of the asymptotic equations, that for 16 and 40 bosons a rather fair binding energy can be obtained by adding the contribution $U_i(r)$ of the correlations, calculated from the asymptotic equation, to the exact hypercentral potential $V_0(r)$, in the radial Eq. (3).

It is, therefore, the asymptotic hypercentral potential which must be introduced in the asymptotic equation to calculate $U_i(r)$. We have shown that, thanks to the adiabatic approximation, $U_i(r)$ behaves like a r^{-2} attractive potential which reduces the strength of the hypercentral kinetic energy centrifugal barrier with a ratio $U_{\lambda}(r) / \hbar^2 / m(\mathcal{L}(\mathcal{L}+1))/r^2$ which is $>$ -1 for fermions and $<$ -1 for bosons. It generates a reduction of the strength of the kinetic energy and of the r. m. s. radius for bosons, producing a collapse, where all bosons gather inside the range of the potential.

This difference between bosons and fermions originates from \mathcal{L} in Eq. (3) which grows as 3A/2 for bosons in the ground state $(L_m = 0)$ and as $1/2(3/2)^{4/3}$ for nuclei [8] which makes the ratio smaller in absolute value for nuclei, than for bosons in the ground state.

In the asymptotic radial equation the eigenpotential energy $U_i(r)$ behaves like an attractive kinetic energy term, while the kinetic energy term in the amplitude equation Eq. (A6) becomes an Harmonic oscillator potential.

Finally the significative values of *r* stay in the neighborhood of the minimum of the effective hyperradial potential where $r_m^2 \approx 2Aa^2$ in terms of the r. m. s. radius *a*.

For bosons in ground state $\alpha \rightarrow 3A/2$ and $\sqrt{\alpha}/r \rightarrow \frac{\sqrt{3}}{2}$ 2 *r a* does not vary much when all particles stay inside the range of the potential.

For fermions $\alpha \rightarrow \frac{1}{2} (\frac{3}{2})^{4/3}$ 2^2A . Assuming a constant nuclear density $a^2 = \frac{3}{2} r_0^2 A^{2/3}$ $\mathbf 0$ $2 \approx \frac{3}{7}$ 5 $a^2 = \frac{3}{5} r_0^2 A^{2/3}$ for $r_0 \approx 1.2$ fm leads to $\sqrt{\alpha}/r_{m} \rightarrow .8458A^{-1/6}$ $/r_m \rightarrow .8458 A^{-1/6} / r_0$ decreasing slowly for increasing A.

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Appendix (see [3])

One starts from the transformation

(A1)
$$
P_0(z,r) = g_\lambda(x,r) / g_0(x,r)
$$
 with $z = 2x^2 / r^2 - 1, x = r_{ij}$,

(A2)
$$
g_0(x,r) = N \sqrt{(1 - x^2 / r^2) x W_{[0]}(z)}
$$

(note the misprint in ref [5] Eq. (30) where ζ must be substituted for ζ^2) where $W_{[0]}(z) = x(1-x^2/r^2)^\alpha$, $\alpha = (D-5)/2$ to get the equation in the variable x:

$$
(A3)\left(\frac{d^2}{dx^2} - \frac{g_0}{g_0} - \frac{m}{\hbar^2}(\tilde{V}(x,r) - U_{\lambda}(r))/(1 - \frac{x^2}{r^2})\right)g_{\lambda}(x,r)
$$

$$
= \frac{m}{\hbar^2}\tilde{V}(x,r)\frac{g_0(x,r)}{1 - x^2/r^2}(A(A-1)/2 - 1)I_{\lambda}(x,r)
$$

with $\tilde{V}(x,r) = V(x) - V_0(r)$

$$
(A4) I_{\lambda} = \int_{0}^{r} \frac{g_{\lambda}(x',r)g_{0}(x',r)}{1-x'^{2}/r^{2}} (1+\sum a_{K}^{[0]}P_{K}^{[0]}(x)P_{K}^{[0]}(x'))dx'
$$

$$
a_K^{[0]} = (f_K^2 - 1) / (A(A-1)/2 - 1)
$$

(A5) Asymptotically $g_0(x,r) \xrightarrow[\alpha \to \infty]{} Nxe^{-(\alpha+1)x^2/(2r^2)}$ with the normalization

$$
\int_{0}^{r} g_0^2(x, r)/(1 - x^2/r^2)dx = 1
$$
, i.e. $N^2 = \frac{4\alpha^{3/2}}{r^3 \sqrt{\pi}}$, $\int_{0}^{r} g_0(x, r)g_\lambda(x, r)/(1 - x^2/r^2)dx = 1$

and with the ratio
\n
$$
g_0^{\dagger}/g_0 = -\frac{\alpha}{r^2} (\alpha + 1 - (\alpha - 2)/T)/T \xrightarrow[\alpha \to \infty]{} (\alpha + 1) (\alpha + 1)x^2/r^2 - 3/r^2, T = 1 - \frac{x^2}{r^2}
$$

One makes the slight renormalization
$$
Z^2 = (\alpha + 1)x^2/r^2
$$
 to obtain the kinetic energy term
\n
$$
Ze^{-Z^2/2}Kin(x) = \frac{\hbar^2}{m} \left[-\frac{d^2}{dx^2} + (\alpha + 1)((\alpha + 1)x^2/r^2 - 3)/r^2 \right]
$$
\n(A6)
\n
$$
= (\alpha + 1)\frac{\hbar^2}{mr^2} \left[-\frac{d^2}{dZ^2} + Z^2 - 3 \right]
$$

(A7) with
$$
P_0(Z,r) = g_\lambda(x,r)e^{Z^2/2}/Z
$$
.

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