Integro-differential equation for Bose-Einstein condensates

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We use the assumption that the potential for the A-boson system can be written as a sum of pairwise acting forces to decompose the wave function into Faddeev components that fulfill a Faddeev type equation. Expanding these components in terms of potential harmonic (PH) polynomials and projecting on the potential basis for a specific pair of particles results in a two-variable integro-differential equations suitable for A-boson bound-state studies. The solution of the equation requires the evaluation of Jacobi polynomials $P_K^{\alpha,\beta}(x)$ and of the weight function $W(z)$ which give severe numerical problems for very large A. However, using appropriate limits for $A \to \infty$ we obtain a variant equation which depends only on the input two-body interaction, and the kernel in the integral part has a simple analytic form. This equation can be readily applied to a variety of bosonic systems such as microclusters of noble gasses. We employ it to obtain results for $A \in (10\text{–}100)$ ^{87}Rb atoms interacting via interatomic interactions and confined by an externally applied trapping potential $V_{\rm trap}(r)$. Our results are in excellent agreement with those previously obtained using the potential harmonic expansion method (PHEM) and the diffusion Monte Carlo (DMC) method.

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I. INTRODUCTION

Broadly speaking, the A-particle bound-state problem can be solved using two families of approaches. The first is based on the assumption that the potential can be written as a sum of pairwise acting forces resulting in the wave function of the system being written as a sum of amplitudes for the pairs and fulfilling a Faddeev type equation; in the second family one may use correlation functions and employ one of the numerous variational approaches to solve the problem. In both types of approaches three-body correlations can also be included.

The Faddeev approach, introduced in the early 1960s [1], can be applied to systems up to $A = 4$ and it has been extensively used during the last few decades to study bosonic as well as fermionic systems in a rigorous way. Going beyond the $A = 4$ system, however, is not at present practical within the Faddeev scheme, as the resulting equations are too complicated to solve and therefore one has no option but to consider instead several assumptions and simplification such as clustering and effective interactions. An alternative to the Faddeev scheme is the use of the hyperspherical harmonics expansion method (HHEM) [2,3], which converts the Schrödinger equation into an infinite set of coupled second-order differential equations. This method is, up to a certain extent, variational since one has to truncate the expansion for numerical purposes and thus one limits the Hilbert space of the wave function, leading to an underestimate of the binding energy. It is therefore clear that any alternative method that includes the two-body (and three-body, if needed) correlations into account is welcome.

One such method in which the two-body correlations are taken into account exactly is the integro-differential equation approach (IDEA), valid for A-body systems suggested by Fabre de la Ripelle and collaborators [4–6]. It is based on the expansion of the Faddeev amplitudes into potential harmonics (PH) [7,8] and it can be used in a straightforward manner to calculate bound states of bosonic systems. The same procedure to take correlations into account can be used in fermionic systems, in which case spin (and isospin) is taken into account. This, however, results in some modifications stemming from spin-isospin projections (see, for example, Refs. [9,10]). The IDEA method has been successfully applied in few-body calculations [6,9], in realistic fermionic systems [10], in unequal mass particle systems [11–14], as well as in model calculations for the $A = 16$ system [15]. In all applications, the binding energies obtained are in good agreement with other results in the literature obtained by other methods.

When, however, the number of particles increases, the number of degrees of freedom also increases and the numerical complexity becomes intractable and one has no alternative but to seek methods or simplifications of existing ones suitable for handling many-body systems. The typical number of atoms involved in Bose-Einstein condensation (BEC), for example, is 10^3–10^6 [16], and consequently studies of the BEC phenomenon are naturally based on quantum Monte Carlo type methods, such as the diffusion Monte Carlo (DMC) [17,18], the variational Monte Carlo (VMC) [19], and the practically exact Green's-function Monte Carlo (GFMC) [20] methods.

A different approach to Monte Carlo methods in studies of BEC is the one employed by Das and collaborators [21–23], and it is based directly on the PH expansion of the Faddeev components resulting in a large system of differential equations. The scheme has been used to study the BEC phenomenon for ^{87}Rb atoms using repulsive interboson interactions. The method requires the evaluation of Jacobi polynomials $P_K^{\alpha,\beta}(z)$, where $\alpha = (D-5)/2$, $\beta = 1/2 + \ell$. D is the dimensionality of the A-boson system, $D = 3(A-1)$, and z is an angular variable. Furthermore, it requires the use of the so-called weight function $W(z) \equiv (1-z)^\alpha (1+z)^\beta$. It is clear that the accuracy in calculating the relevant quantities suffers with increasing A as the $P_K^{\alpha,\beta}(z)$ becomes highly oscillatory while the $W(z)$ has a spike similar to a δ function for $z \sim -1$, which is difficult to control numerically. As a result, the calculations become cumbersome and practically uncontrollable beyond certain A. A relevant discussion on this problem and how this can, up to a certain extent, be addressed is given in Ref. [23].

In the present work we also start by expanding the wave function for the A-body system into Faddeev components, which in turn are expanded in terms of PH. However, the resulting differential equations, as used by Das and coworkers [21–23], are first transformed into a single integro-differential equation which depends on two variables only, namely, the hyperradius r and an angular variable z, while the corresponding kernel is expressed in terms of Jacobi polynomials $P_K^{\alpha,\beta}(z)$, which also depend on α and the weight function $W(z)$. The aforementioned difficulties, however, can be removed by obtaining appropriate limits for $A \to \infty$. The obtained equation is quite simple, and the kernel depends on the much simpler associated Laguerre polynomials $L_K^{1/2}$ which are independent of α [24]. It can be even further transformed to have an analytical form, which does not depend on any polynomial, is independent of α, and only depends linearly on the number of particles A. We stress here that our scheme takes into account the two-body correlations exactly while three-body correlations can also be included, as described in Ref. [5].

In what follows, we describe, in Sec. II, how one can obtain from the IDEA the integro-differential equation suitable for a large number of particles A. We then apply it, in Sec. III, to obtain results: first for the hybrid nuclear model for the $A = 16$ particle system, where the particles are assumed to interact via short-range strong forces of the Wigner type; second, we apply it to ^{87}Rb atoms for various A and the results obtained are compared to those of the PHEM and DMC methods. Our conclusions are summarized in Sec. IV.

II. FORMALISM

In describing a system of identical bosons under the assumption that the interaction consists of a sum of pairwise acting central potentials, the A-body wave function can be written as a product of the harmonic polynomial $H_{[L_m]}(\mathbf{x})$ of minimal degree L_m characterized by the quantum numbers $[L_m]$ describing the state and a sum of two-body amplitudes:

$$\Psi(\mathbf{x}) = H_{[L_m]}(\mathbf{x}) \sum_{i<j\leqslant A} F(\mathbf{r}_{ij},r), \tag{1}$$

where $\mathbf{x}$ is the coordinate vector $\mathbf{x} = (\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_A)$, $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$ in terms of the particle coordinates $\mathbf{x}_i$, and r is the hyperradius, $r = [2/A\sum_{i<j\leqslant A} r_{ij}^2]^{1/2}$. The two-body amplitudes $F(\mathbf{r}_{ij},r)$ obey the Faddeev-type equation

$$\left[T + \frac{A(A-1)}{2} V_{[L_m]}(r) - E\right] H_{[L_m]}(\mathbf{x})\, F(\mathbf{r}_{ij},r) = -\left[V(r_{ij}) - V_0^{[L_m]}(r)\right] H_{[L_m]}(\mathbf{x}) \sum_{k<l\leqslant A} F(\mathbf{r}_{kl},r). \tag{2}$$

The hypercentral potential is the average potential $V(r_{ij})$ taken over the $[L_m]$ state on the unit hypersphere $r = 1$ of surface element $d\Omega$ in the D-dimensional space,

$$V_0^{[L_m]}(r) = \frac{\int H^*_{[L_m]}(\mathbf{x}) V(r_{ij}) H_{[L_m]}(\mathbf{x}) d\Omega}{\int |H_{[L_m]}(\mathbf{x})|^2\, d\Omega}. \tag{3}$$

We note that for ground states, the pairs are in an S state and the amplitude F is a function of $r_{ij} = |\mathbf{x}_i - \mathbf{x}_j|$, i.e., the amplitudes are now written as $F(r_{ij},r)$.

Letting

$$F(r_{ij},r) = P(z,r)/r^{\mathcal{L}_m+1}, \tag{4}$$

where $\mathcal{L}_m = L_m + (D-3)/2$ and $z = 2r_{ij}^2/r^2 - 1$, and projecting on the r_{ij} space, one gets the IDEA equation for an A-particle system [5]:

$$-\frac{\hbar^2}{m}\left[\frac{\partial^2}{\partial r^2} - \frac{\mathcal{L}_m(\mathcal{L}_m+1)}{r^2} + \frac{4}{r^2}T(z) + \frac{A(A-1)}{2} V_0^{[L_m]}(r) - E\right] P(z,r) = -\left[V(r_{ij}) - V_0^{[L_m]}(r)\right]\left[P(z,r) + \int_{-1}^{+1} F_{[L_m]}(z,z')\, P(z',r)\, dz'\right], \tag{5}$$

where $T(z)$ is the kinetic-energy term

$$\hat{T}(z) = \frac{1}{W_{[L_m]}(z)} \frac{\partial}{\partial z} (1-z^2) W_{[L_m]}(z) \frac{\partial}{\partial z} \tag{6}$$

and $W_{[L_m]}(z)$ is the weight function which, for bosonic systems, is given by

$$W_{[L_m]}(z) = (1-z)^\alpha (1+z)^\beta, \tag{7}$$

where $\alpha = (D-5)/2 + L_m - 2\ell_m$ and $\beta = 1/2 + \ell_m$. The kernel $F_{[L_m]}(z,z')$ is the projection function which is expressed in terms of the Jacobi polynomials $P_K^{\alpha,\beta}(z)$,

$$F_{[L_m]}(z,z') = W_{[L_m]}(z') \sum_K \frac{(f_K^2 - 1)}{h_K} P_K^{\alpha,\beta}(z) P_K^{\alpha,\beta}(z'). \tag{8}$$

The normalization h_K is given by

$$h_K = \int_{-1}^{+1} \left[P_K^{\alpha,\beta}(z)\right]^2 W_{[L_m]}(z)\, dz, \tag{9}$$

and the constant term $f_K^2 - 1$ is given by

$$f_K^2 - 1 = \frac{2(A-2)P_K^{\alpha,\beta}(-1/2) + [(A-2)(A-3)/2]P_K^{\alpha,\beta}(-1)}{P_K^{\alpha,\beta}(+1)}. \tag{10}$$

When the number of particles A is large, the calculations with the above formalism becomes time consuming and cumbersome. There are two main reasons for this, the first

one being the evaluation of the Jacobi polynomials $P_K^{\alpha,\beta}$, since the value of α becomes huge and the polynomials are highly oscillatory; the second reason stems from the behavior of the weight function which for $z \to -1$ is peaked close to 2^α, which gives rise to uncontrollable numerical problems.

In our approach we consider first the transformation

$$r_{ij} = r\zeta/\sqrt{\alpha} \tag{11}$$

with $z = 2\zeta^2/\alpha - 1$. It is noted that for $\ell = 0$, $\alpha = (D-5)/2 = [3(A-1)-5]/2$, i.e., $\alpha \sim 3A$ for large A. The purpose of this transformation is twofold: first to obtain, for $\alpha \to \infty$, the limit for the Jacobi polynomials $P_K^{\alpha,\beta}$,

$$\begin{aligned} P_K^{\alpha,\beta}\left(2r_{ij}^2/r^2 - 1\right) &\underset{\alpha\to\infty}{\longrightarrow} (-1)^K L_K^{1/2}\left(\alpha r_{ij}^2/r^2\right) \\ &\equiv (-1)^K L_K^{1/2}(\zeta^2), \end{aligned} \tag{12}$$

where $L_K^{1/2}$ are the Laguerre polynomials which are independent of α, and second, to remove the troublesome term $(1-z)^\alpha$ from the weight function, which now reads

$$W(z) = C_W \frac{2^{\alpha+\ell+1/2}}{\alpha^{1/2+\ell}} \zeta e^{-\zeta^2}, \tag{13}$$

where C_W is the normalization constant for the weight function. For $\ell = 0$

$$\begin{aligned} h_K &\underset{\alpha\to\infty}{\longrightarrow} \int_0^{\sqrt{\alpha}} \left[L_K^{1/2}(\zeta^2)\right]^2 e^{-\zeta^2} \zeta^2 d\zeta \\ &\simeq \frac{1}{2}\int_0^\infty \left[L_K^{1/2}(x)\right]^2 e^{-x}\sqrt{x}\, dx \\ &= \frac{1}{2}\frac{\Gamma(K+3/2)}{K!}. \end{aligned} \tag{14}$$

In order to evaluate the kinetic-energy term $\hat{T}P(z,r)$, we consider first the factorization

$$P(\zeta,r) = \frac{e^{\zeta^2/2}}{\zeta} Q(\zeta,r). \tag{15}$$

Then

$$\hat{T}P = \frac{1}{W}\frac{\partial}{\partial z}(1-z^2)W\frac{\partial}{\partial z}P \tag{16}$$

$$\equiv \frac{\alpha}{4}\frac{e^{\zeta^2/2}}{\zeta}\left[\frac{d^2}{d\zeta^2} + 3 + 2\ell_m - \zeta^2 - \frac{2\ell_m}{\zeta^2}\right] Q(\zeta,r). \tag{17}$$

Therefore, for bosons in the ground state where the harmonic polynomials $H_{[L_m]}$ correspond to $L_m = 0$, $\ell_m = 0$ [and thus $\mathcal{L}_m \equiv \mathcal{L} = (D-3)/2$], Eq. (5) becomes

$$\begin{aligned} &\frac{\hbar^2}{m}\left[H_r + \frac{\alpha}{r^2}H_\zeta + \frac{A(A-1)}{2}V_0(r) - E\right]Q(\zeta,r) \\ &\quad = -[V(r_{ij}) - V_0(r)] \\ &\qquad \times\left[Q(\zeta,r) + \int_0^{\sqrt{\alpha}} \mathcal{F}_E(z,z')Q(\zeta',r)d\zeta'\right], \end{aligned} \tag{18}$$

where

$$H_r = -\frac{\partial^2}{\partial r^2} + \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} \tag{19}$$

and

$$H_\zeta = \frac{\alpha}{4}\left[-\frac{\partial^2}{\partial\zeta^2} + \zeta^2 - 3\right]. \tag{20}$$

The kernel $\mathcal{F}_E$ is given by

$$\begin{aligned} \mathcal{F}_E(\zeta,\zeta') = \zeta e^{-\zeta^2/2} &\sum_K \frac{2\,K!}{\Gamma(K+3/2)} \\ &\times \left(f_K^2 - 1\right) L_K^{1/2}(\zeta^2) L_K^{1/2}(\zeta'^2)\zeta' e^{-\zeta'^2/2}. \end{aligned} \tag{21}$$

We see that Eq. (18) is free from the δ-function type peak and, apart from the easily evaluable constant $f_K^2 - 1$, the kernel $\mathcal{F}_E$ does not depend on α.

Equation (18) can be even more simplified by noting that

$$\begin{aligned} &\sum_K \left(f_K^2 - 1\right)\frac{K!}{\Gamma(K+3/2)} L_K^{1/2}(\zeta^2)L_K^{1/2}(\zeta'^2) \\ &\quad \underset{\alpha\to\infty}{\longrightarrow} 2(A-2)\sum_K \left(\frac{1}{4}\right)^K L_K^{1/2}(\zeta^2)L_K^{1/2}(\zeta'^2)/h_K \\ &\qquad - \; 2(A-2)\frac{1}{4}L_1^{1/2}(\zeta^2)L_1^{1/2}(\zeta'^2)/h_1 \\ &\qquad - \; L_1^{1/2}(\zeta^2)L_1^{1/2}(\zeta'^2)/h_1 - 2A(A-2)/h_0 \\ &\qquad + \; [A(A-1)/2 - 1]/h_0 \end{aligned} \tag{22}$$

and thus by making use of the relation [25]

$$\begin{aligned} &\sum_{K=0}^\infty \left(\frac{1}{4}\right)^K \frac{K!}{\Gamma(K+3/2)} L_K^{1/2}(\zeta^2)L_K^{1/2}(\zeta'^2) \\ &\quad = \frac{4}{\sqrt{3\pi}}\, e^{(\zeta^2+\zeta'^2)/3}\, \frac{\sinh(\frac{3}{4}\zeta\zeta')}{\zeta\zeta'} \end{aligned} \tag{23}$$

we obtain

$$\begin{aligned} &\frac{\hbar^2}{m}\left\{H_r + \frac{4}{r^2}H_\zeta + \frac{A(A-1)}{2}V_0(r) - E\right\}Q(\zeta,r) \\ &\quad = -[V(r_{ij}) - V_0(r)] \\ &\qquad \times\left[Q(\zeta,r) + \int_0^{\sqrt{\alpha}} \mathcal{F}_I(\zeta,\zeta')Q(\zeta',r)d\zeta'\right]. \end{aligned} \tag{24}$$

The new form of the kernel $\mathcal{F}_I$ is

$$\begin{aligned} \mathcal{F}_I(\zeta,\zeta') = &\frac{2(A-2)}{\sqrt{3}} \\ &\times\left\{\left[A - 3 - \frac{2}{3}\left(\zeta^2 - \frac{3}{2}\right)\left(\zeta'^2 - \frac{3}{2}\right)\right]\zeta\zeta' e^{-(\zeta^2+\zeta'^2)/2}\right. \\ &\left. + \frac{4}{\sqrt{3}}\left[e^{-[5(\zeta-\zeta')+2\zeta\zeta']/6} - e^{-[5(\zeta+\zeta')-2\zeta\zeta']/6}\right]\right\}. \end{aligned} \tag{25}$$

The kernel (25) has a simple form and its computation is straightforward.

In the presence of a trapping potential $V_{\rm trap}(r)$ which depends on the hyperradius only, the modifications needed are trivial and consist of replacing H_r by

$$H_r = -\frac{\partial^2}{\partial r^2} + \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + V_{\rm trap}(r). \tag{26}$$

TABLE I. Comparison of the two terms T_1 and T_2 of $f_K^2 - 1$ (see text) for $K = 0, \ldots, 7$ for $A = 20$ and $A = 1000$.

	$A = 20$			$A = 1000$		
K	T_1	T_2	$f_K^2 - 1$	T_1	T_2	$f_K^2 - 1$
0	36	153	189	1996.000 0000	497 503	499 499
1	7.5	−8.5	−1	497.500 0000	−498.500 0000	−1.000 0000
2	1.100 4464	0.758 9286	1.859 3750	123.501 8775	0.831 9426	124.333 8201
3	0.072 9391	−0.091 5948	−0.018 6557	30.534 5323	−0.001 9425	30.532 5898
4	−0.008 6754	0.013 7392	0.005 0638	7.518 5722	0.000 0058	7.518 5780
5	−0.001 6333	−0.002 4376	−0.004 0709	1.843 7195	−0.000 0000	1.843 7195
6	0.000 2636	0.000 4951	0.000 7588	0.450 2550	0.000 0000	0.450 2550
7	0.000 0479	−0.000 1125	−0.000 0646	0.109 5002	−0.000 0000	0.109 5002

The solution of the two-dimensional equations (18) and (24) can be readily obtained. However, the Extreme Adiabatic Approximation (EAA) can also be employed. In this case we may write, as usual, $Q(\zeta,r) = Q_\lambda(\zeta,r)u_\lambda(r)$ to obtain

$$\frac{\hbar^2}{m}\left[\frac{4}{r^2}H_\zeta + U_\lambda(r)\right]Q_\lambda(\zeta,r) = -\left[V\left(\frac{r}{\sqrt{\alpha}}\zeta\right) - V_0(r)\right] \times\left[Q_\lambda(\zeta,r) + \int_0^{\sqrt{\alpha}} \mathcal{F}_n(\zeta,\zeta')Q_\lambda(\zeta',r)d\zeta'\right], \quad n = E,\ I \tag{27}$$

and

$$u_\lambda''(r) + \left[k_\lambda^2 + V_{\text{eff}}(r)\right]u_\lambda(r) = 0, \tag{28}$$

where the effective potential V_{eff} is given by

$$V_{\text{eff}}(r) = \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + \frac{A(A-1)}{2}V_0(r) - U_\lambda(r) + U_{\text{trap}}(r). \tag{29}$$

In the above, λ corresponds to a specific eigenpotential $U_\lambda(r)$ having an eigenvalue k_λ^2. It is noted that the hypercentral part V_0 can be omitted, especially when the two-body interaction is repulsive, in which case the results are S projected. In this case, no effects stemming from higher partial waves are included. It is further noted that the $\mathcal{L}(\mathcal{L}+1)/r^2$ or the $V_{\text{trap}}(r)$ can be included in the first equation (27) without affecting the final results.

III. RESULTS

We first analyze the behavior of the term $f_K^2 - 1$ as $\alpha \to \infty$. In Table I we present the results for $A = 20$ and $A = 1000$ for the two terms, $T_1 = (A-2)2P_K^{\alpha,1/2}(-1/2)/P_K^{\alpha,1/2}(1)$ and $T_2 = (A-2)(A-3)/2P_K^{\alpha,1/2}(-1)/P_K^{\alpha,1/2}(1)$ for $K = 0,1,\ldots,7$. We see that both terms as well as the total term $f_K^2 - 1$ become very small as K increases. Consequently, only few terms in the expansion (21) are required to achieved convergence. Furthermore, the behavior of the second term (only the $K = 0,1$ are significant for large α) justifies our approximation (22).

We next present, in Fig. 1, the kernel $\mathcal{F}_I(\zeta,\zeta')$ for $A = 20$ and $A = 1000$ particles. We see that, apart from the strength, its shape and spread are not drastically changed and in both cases the kernel becomes insignificant beyond $\zeta \sim 4$.

We employed Eq. (24) to obtain the bound-state solution for the $A = 16$ particle system, in which the particles interact via strong forces. The reason for this endeavor is twofold: first, to compare the results obtained with our equation for this model problem with those previously obtained by the hyperspherical harmonics expansion method (HHEM) [3] and by using the exact IDEA method; second, as our method is based on the assumption of the dominance of two-body correlations, to test the formalism in the case where the correlations (especially the short-range ones) stem from strong forces. This will allow us to evaluate and eventually apply our approach to systems in which the particles interact via strong nuclear forces such as a gas of α particles, which is a bosonic system.

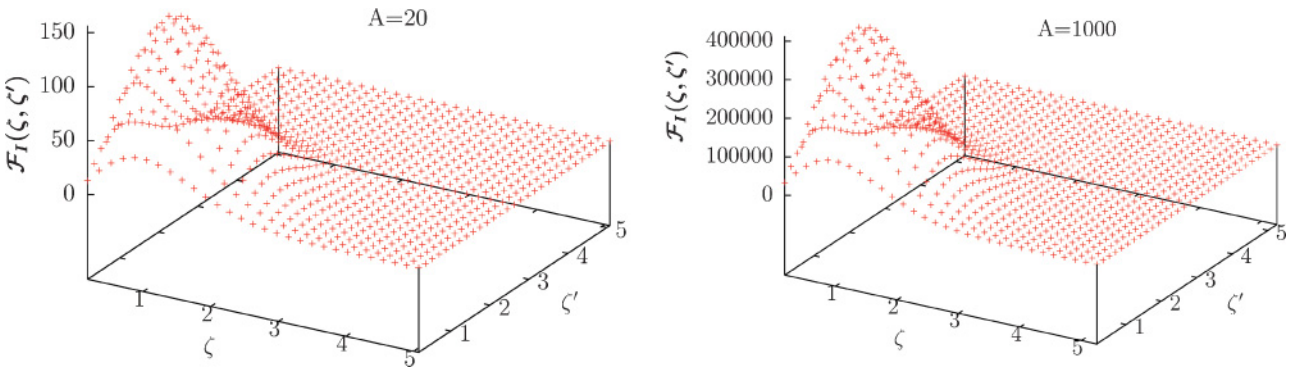

FIG. 1. (Color online) The kernel $\mathcal{F}_I(\zeta,\zeta)$ for $A = 20$ and $A = 1000$.

Three types of potentials were employed for this purpose that have different short-range characteristics. The first potential is the Volkov potential [26],

$$V(r_{ij}) = v_1 \exp[-(r_{ij}/b_1)^2] + v_2 \exp[-(r_{ij}/b_2)^2], \quad (30)$$

with $v_1 = -83.340\,02$ MeV, $v_2 = 144.843\,41$ MeV, $b_1 = 1.6$ fm, and $b_2 = 0.82$ fm, which has a soft repulsive core. The second is the Afnan and Tang $S3$ potential [27],

$$V(r_{ij}) = \sum_{i=1}^{5} v_i \exp\left[-b_i r_{ij}^2\right], \quad (31)$$

the strengths v_i being 1000.0, −163.345, −9.8025, −82.0, and −11.5 MeV, while the b_i are 3, 1.05, 0.6, 0.8, and 0.4 fm^{-2}, respectively. The third potential is the more realistic Malfliet-Tjon V potential (MT-V) employed in [28],

$$V(r_{ij}) = \frac{v_1}{r_{ij}} \exp[-b_1 r_{ij}] + \frac{v_2}{r_{ij}} \exp[-b_2 r_{ij}], \quad (32)$$

with $v_1 = -578.09$ MeV fm, $v_2 = 1458.05$ MeV fm, $b_1 = 1.55$ fm^{-1}, and $b_2 = 3.11$ fm^{-1}.

To obtain the solution of Eq. (24), we use the Galerkin method and B splines to reduce the problem, as usual, to an eigenvalue one. The results obtained using the analytic expression (25) and designated as IDEA-I are given in Table II. Despite the fact that the $A = 16$ case corresponds to a rather small number of particles, the accuracy achieved by our equation for strong nuclear forces is less than 1% of the exact values obtained by solving the IDEA method [15] or by using the HHEM [3]. The slightly higher deviation from the results of the HHEM can be attributed to the slow convergence rate of the hyperspherical harmonics expansion for the $S3$ [27] potential, which has a practically repulsive hard core, and for the Yukawa type MT-V [28] potentials.

We now turn our attention to the case where A bosons are confined in a magnetic trap approximated by a spherically symmetric harmonic oscillator potential,

$$V_{\rm trap}(r) = \sum_{i=1}^{A} \frac{1}{2} m\omega^2 x_i^2 = \frac{1}{4} m\omega r^2. \quad (33)$$

In our calculations we use oscillator units (o.u.), in which the energy and length are $\hbar\omega$ and $\sqrt{\hbar/m\omega}$, respectively, where ω is the harmonic oscillator circular frequency. In these units $\hbar^2/m = 1$.

As a first example we employ a Gaussian potential

$$V(r_{ij}) = V_0 \exp\left[-r_{ij}^2/r_0^2\right] \quad (34)$$

with $V_0 = 3.1985 \times 10^6$ o.u. and $r_0 = 0.005$ o.u. which corresponds to the Joint Institute for Laboratory Astrophysics (JILA) ^{87}Rb experiment [29] with $a_{\rm sc} = 100$ bohrs and trap frequency $\nu = 200$ Hz. The results obtained by employing the kernel (21), designated as IDEA-E, and the the kernel (25) are shown in Table III. The ground-state energy for $A = 3$ differs, as expected, from the corresponding value obtained within the PHEM [21] by 25%, and for $A = 5$ by 3.26%. For $A = 10$, however, the agreement is already within 0.2%. Going beyond $A > 10$, the differences from the results of PHEM are very small and can be mainly attributed to the overall numerical inaccuracies. It should be noted here that the binding energy per particle is of the order of $E_b/A \sim 1.50$. It should be further noted that the IDEA-E and the IDEA-I results are, for all practical purposes, identical and therefore we shall employ from now on only the kernel (25).

As a second example we use the semirealistic potential

$$V(r_{ij}) = V_0 \,\mathrm{sech}^2(r_{ij}/r_0). \quad (35)$$

Following Das *et al.* [23] we use $V_0 = 1.818\,47 \times 10^9$ o.u. and $r_0 = 0.001$ o.u. We present our results in Table IV and compare them with those of the PHEM and of the DMC results of Blume and Greene [30].

We endeavored to carry out calculations for up to $A = 100$, where a very good agreement is achieved in all cases for $A \geqslant 10$ with both the PHEM [23] and DMC [30] methods. Going beyond $A = 100$ requires more refined calculations and a rather exact solution of Eq. (24), the reason being that the extreme adiabatic approximation gives rise to a multitude of eigenpotentials $V_\lambda(r)$ very close to each other and the results, albeit not differing much, depend nevertheless on which eigenpotential $V_\lambda(r)$ is used. This is shown in Fig. 2, where two effective potentials, Eq. (29), corresponding to $\lambda = 1$ and $\lambda = 20$, are plotted for the case $A = 500$. This multitude of eigenpotentials close to each other does not appear in the case where forces having an attractive well are used.

TABLE II. Binding energies (in MeV) obtained for $A = 16$ with short-range forces and by using the kernel (25).

Potential	IDEA-I	IDEA (exact)	HHEM [3]
Volkov [26]	1643	1640	
$S3$ [27]	1247	1246	1235
MT-V [28]	1377	1376	1363

TABLE III. Results (in o.u.) obtained with IDEA-E [Eq. (18)] and IDEA-I [Eq. (24)] using the Gaussian potential (34).

A	IDEA-E	IDEA-I	PHEM
3	6.009	6.009	4.500
5	7.758	7.758	7.505
10	15.003	15.003	15.034
15	22.501	22.501	22.567
20	30.000	30.001	30.107
25	37.501	37.501	37.654
30	45.009	45.001	45.207
35	52.509	52.501	52.768

TABLE IV. Same as Table III using the sech potential (35).

A	IDEA-I	PHEM [23]	DMC [30]
10	15.143	15.1490	15.1539
20	30.625	30.6209	30.639
50	78.701	78.8704	
100	165.038	164.907	

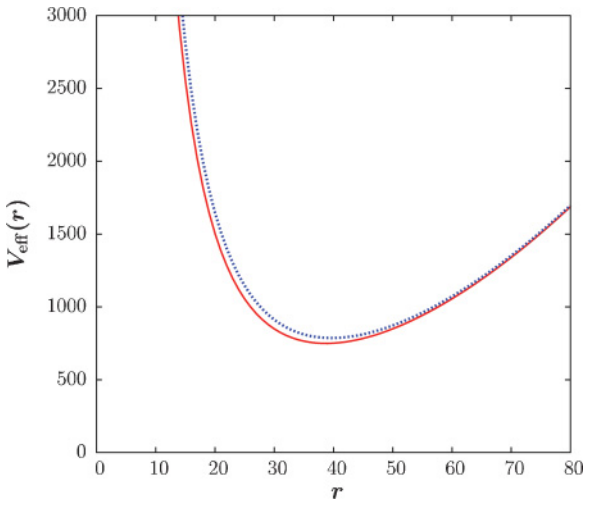

FIG. 2. (Color online) Two eigenpotentials $V_{\rm eff}(r)$ corresponding to $\lambda = 1$ and $\lambda = 20$ for $A = 500$.

IV. CONCLUSIONS

In conclusion, we obtained an integro-differential equation describing bound states of a large number of bosons. This has been achieved by using the transformation $r_{ij} = r\zeta/\sqrt{\alpha}$ and by using the asymptotic form of the Jacobi polynomials $P_K^{\alpha,\beta}(z)$, which for large A are approximated by the Laguerre polynomials $L_K^{1/2}(\zeta)$, which do not depend on α and thus are easier to evaluate. Furthermore, the above transformation simplifies the kinetic-energy term, the weight function, and the corresponding projection function. As a result the integro-diferential equation with a fully analytic and simple kernel can be easily applied to A-body bosonic systems.

It should be stressed that the IDEA formalism is, up to a certain extent, equivalent to the PHEM of Ref. [7] employed by Das and collaborators [21–23]. In the PHEM one has to solve a large number of differential equations, which in the IDEA are transformed, with the help of potential harmonics, into a single integro-differential equation. (Technical details on this transformation can be found in Refs. [5] and [14].) Therefore our equation can also be considered as a simplified version not only of the IDEA method but of the widely used PHEM as well. We note that the formalism takes the two-body correlations into account in an exact way and that three-body correlations can also be included, and thus it should be accurate enough in describing large numbers of bound bosonic systems.

We tested our equation by calculating the ground-state binding energy of the model nuclear problem for the $A = 16$ system where the short-range nuclear force was of Wigner type. The good agreement achieved, with the three different type forces having a soft core, a hard core, and that of Yukawa type, as compared to the results obtained using the IDEA and the HHEM methods, implies that our equation can be safely used to calculate binding energies of large number ($A \geqslant 10$) particles interacting via strong forces.

Turning now to the case of Bose-Einstein condensates consisting of A atoms trapped by an external field, we found that our equation gives results which are in excellent agreement with those of the PHEM and the diffusion Monte Carlo (DMC) method, at least up to $A = 100$. Going beyond this number requires improved numerical methods or a direct solution of the equation as a two-variable integro-differential equation without resorting to the EAA approximation, which gives rise to a plethora of eigenpotentials that are very close to each other. It is noted that when A increases, the centrifugal part $\mathcal{L}(\mathcal{L}+1)/r^2$ becomes extremely large and extends outward, while the interatomic potential is constant and restricted to smaller distances. Therefore the main contribution in the effective potential stems from the centrifugal and the trapping potentials, which generate a harmonic oscillator-type well which moves outward as the number of particles A increases.

The overall good results obtained indicate that the derived equation can be used in studies of bound A-boson systems as an alternative to competing methods such as the variational and hyperspherical harmonics methods. Our approximations should become better with increasing A, i.e., for $\alpha \to \infty$. However, to study their performance in particle systems with $A > 100$ one must address first the aforementioned numerical problems. Such work is under way.

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