Accuracy of ground-state solutions of boson systems in the revised few-body integrodifferential equations approach

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In this work, the traditional two-variable few-body integrodifferential equations approach is reviewed. Boundary conditions are implemented in both the hyperradial and hyperangular domains. A novel procedure of including effects of higher partial waves of the interaction potential is introduced. The new approach reproduces results obtained by an exact method for boson systems. These results suggest that many-body correlations are negligibly small in systems with short-range interactions and that effect of higher partial waves are adequately accounted for by the revised hypercentral potential.

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I. INTRODUCTION

Many of the methods in few-body physics are capable of treating known features of the systems and degrees of freedom of constituents exactly. However, the implementation of their full capacity is prohibited by resulting complexities as the number of constituents increases. Examples of such methods are the widely used Faddeev formalism [1] and the hyperspherical harmonics expansion (HHE) method [2,3]. The exact implementation of the Faddeev formalism is limited to, at most, four-particle systems, while the HHE method is limited to less than seven-particle systems.

The few-body integrodifferential equations approach (IDEA) [4] circumvent shortcomings associated with few-body methods by considering two approximations. The IDEA [4,5] uses the Faddeev formalism to treat explicitly only two-particle correlations, and approximates effects of higher partial waves. These approximations reduce the many-body Schrödinger equation in hyperspherical coordinates to a system of coupled two-variable Faddeev-type integrodifferential equations, the form of which does not change as the number of constituents of the system changes. The system of coupled equations reduces to one two-variable equation in the case of systems of identical particles. This single integrodifferential equation can treat systems of up to a million particles [6]. The description of quantum few-body systems using this approach has shown considerable success in studies of various nuclear and atomic few-body as well as many-body quantum mechanical systems [7–9].

Although the IDEA is extensively discussed in the literature, an explicit implementation of boundary conditions in the angular domain [10] is still lacking. The direct solution of the integrodifferential equation explored in Ref. [11] for bound states reveals that the convergence of the numerical solution is sensitive to the boundary behavior of the amplitudes. This paper proposes a modification to the IDEA that accounts for boundary conditions of the amplitudes in both the hyperradial and hyperangular domains. This results in regularized integrodifferential equations for s-wave potentials.

In the IDEA, effects of higher partial waves are accounted for by introducing a zeroth order hypercentral potential multipole to the s-projected integrodifferential equations. Traditionally, the potential multipoles are determined using a parameter that depends on the size of the system. However, such a procedure faces challenges when the size of the system is large [12]. In this work, the procedure for determining the hypercentral potential is revised to be independent of the number of particles, and the procedure for the inclusion of the hypercentral potential in the s-projected integrodifferential equations is revised to be physically meaningful.

In Sec. II, the many-body Faddeev integrodifferential equations are presented. The derivation entails the elimination of first-order derivatives from the kinetic energy operator from the standard IDEA equations, introducing explicit boundary conditions in the angular domain. Test calculations with the new integrodifferential equations are conducted on A-boson systems with $A = 10$ at most. Results are presented and discussed in Sec. III. Conclusions are reported in Sec. IV.

II. FORMALISM

The derivation of the integrodifferential equations for few-body systems is now commonplace in the literature. In this section, only features of the derivation that are relevant to the goal of revising the equations are recalled.

A. Regularization

Consider a system of A identical bosons, each with mass m and position vector $\vec{r}_i$ $(i = 1, 2, \ldots, A)$. Internal properties of this system are extracted by eliminating the center-of-mass kinetic energy. That is achieved in the Jacobi coordinates defined by the vectors $\vec{\eta}_i = \sqrt{2\,i/(i+1)}\,(\vec{r}_{i+1} - \sum_{j=1}^{i} \vec{r}_j/i\,)$, where $\vec{\eta}_N = \vec{r}_1 - \vec{r}_2$ and $N = A - 1$. However, the dynamical equation for the system is more conveniently solved in hyperspherical coordinates (r, Ω_N) where $r \in [0, \infty)$ is the hyperradius and $\Omega_N \equiv \{\omega_1, \ldots, \omega_N; \varphi_2, \ldots, \varphi_N\}$ a set of angles, constituted by the spherical polar angles $\omega_i(\theta_i, \phi_i)$ of the Jacobi vectors and hyperangles $\varphi_i \in [0, \frac{1}{2}\pi]$. The definitions of these coordinates are readily found in the literature [3,10]. In hyperspherical coordinates, $\eta_N = r \cos\varphi_N$.

When the bosons interact only through two-body potentials $V(\vec{r}_{ij})$, where $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, the total interactions in the system are given by $\sum_{ij}^{A} V(\vec{r}_{ij})$. In the Faddeev formalism, the Schrödinger wave function for the system is expressed in the form [13]

$$\Psi(r, \Omega_N) = \sum_{ij}^{A} \psi_{ij}(r, \Omega_N), \tag{1}$$

where $\psi_{ij}(r, \Omega_N)$ are Faddeev-type two-body amplitudes. These $\frac{1}{2}A(A-1)$ amplitudes satisfy the coupled equations [4]

$$(\hat{T}_0 - E)\,\psi_{ij}(r, \Omega_N) = -V(\vec{r}_{ij}) \sum_{kl}^{A} \psi_{kl}(r, \Omega_N), \tag{2}$$

obtained from the Schrödinger equation for the system, where $\hat{T}_0$ is the internal kinetic energy operator and E is the energy of the system. The kinetic energy woperator has the general form

$$\hat{T}_0 = -\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial r^2} + \frac{3A-4}{r}\frac{\partial}{\partial r} + \frac{\hat{\mathcal{L}}^2(\Omega_N)}{r^2}\right), \tag{3}$$

where $\hat{\mathcal{L}}^2(\Omega_N)$ is the grand orbital angular momentum operator. This operator is constructed through the recurrence relation

$$\hat{\mathcal{L}}^2(\Omega_N) = \frac{\partial^2}{\partial \varphi_N^2} + [(3N-4)\cot\varphi_N - 2\tan\varphi_N]\frac{\partial}{\partial \varphi_N} + \frac{\hat{\ell}^2(\omega_N)}{\cos^2\varphi_N} + \frac{\hat{\mathcal{L}}^2(\Omega_{N-1})}{\sin^2\varphi_N}, \tag{4}$$

with $\hat{\mathcal{L}}^2(\Omega_1) = \hat{\ell}^2(\omega_1)$ and $\Omega_N = \{\omega_N, \varphi_N; \Omega_{N-1}\}$. The operators $\hat{\ell}^2(\omega_i)$ are orbital angular momentum operators associated with the Jacobi vectors $\vec{\eta}_i$.

It is noted that in (3) and (4), the first-order derivatives have singularities associated with them. To eliminate these first-order derivatives, one introduces the reduced two-body amplitudes

$$\psi_{ij}(r, \Omega_N) = \frac{\bar{\psi}_{ij}(r, \Omega_N)}{r^{(3A-4)/2}(\sin\varphi_N)^{(3A-7)/2}\cos\varphi_N} \tag{5}$$

and the corresponding reduced total wave function $\bar{\Psi}(r, \Omega_N) = \sum_{ij}^{A} \bar{\psi}_{ij}(r, \Omega_N)$. The reduced amplitudes satisfy the boundary conditions $\bar{\psi}_{ij}(r, \Omega_N) = 0$ for $r = 0$, $\varphi_N = 0$, and $\varphi_N = \frac{1}{2}\pi$. The condition $\bar{\psi}_{ij}(\infty, \Omega) = 0$ is also considered when determining bound states. The reduced amplitudes solve the coupled equations

$$-\frac{\hbar^2}{m}\left[\hat{T}_r + \frac{1}{r^2}\left(\frac{\partial^2}{\partial \varphi_N^2} + \frac{\hat{\ell}^2(\omega_N)}{\cos^2\varphi_N} + \frac{\hat{\mathcal{L}}^2(\Omega_{N-1}) - \rho_A}{\sin^2\varphi_N}\right)\right]\bar{\psi}_{ij}(r, \Omega_N) - E\bar{\psi}_{ij}(r, \Omega_N) = -V(\vec{r}_{ij})\sum_{kl}^{A}\bar{\psi}_{kl}(r, \Omega_N), \tag{6}$$

where $\rho_A = (3N-4)(3N-6)/4 = (3A-7)(3A-9)/4$ and

$$\hat{T}_r = \frac{\partial^2}{\partial r^2} + \frac{1}{4r^2}. \tag{7}$$

Note that Eq. (6) do not involve any approximation. Approximations accounting for only two-body correlations are introduced, in the next subsection.

B. Two-body correlation

Two-body correlation are dominant in systems in which constituents are weakly interacting or interacting through short-range forces. The summation over $\{kl\}$ in (6) constitutes permutations of particles in, or kinematic rotations of, the system. When three-body and higher order correlations are neglected, the resulting wave functions of the system are invariant under rotations in the $D-3$ subspace spanned by the vectors $\vec{\eta}_1, \ldots, \vec{\eta}_{N-1}$ [14]. Such invariance is expressed by the property

$$\hat{\mathcal{L}}^2(\Omega_{N-1})\bar{\psi}_{ij}(r, \Omega_N) = 0, \tag{8}$$

which also implies that the amplitudes depend mainly on the global coordinate r and the local vector $\vec{r}_{ij}$. That is, the amplitudes can be expressed in the form $\bar{\psi}_{ij}(r, \Omega_N) = \mathrm{Y}_{[L]}(\Omega_N)F(r, \vec{r}_{ij})$, where $\mathrm{Y}_{[L]}(\Omega_N)$ are hyperspherical harmonics and $[L]$ a set of quantum numbers. However, $\mathrm{Y}_{[0]}(\Omega_N) =$ constant for states that satisfy (8). $F(r, \vec{r}_{ij})$ can be expanded in spherical harmonics $Y_\ell^{m_\ell}(\omega_N)$ as

$$F(r, \vec{r}_{ij}) = \sum_\ell F_\ell(r, r_{ij})Y_\ell^{m_\ell}(\omega_N), \tag{9}$$

were ℓ is the orbital angular momentum quantum number with azimuthal projection m_ℓ. Note that the same spherical harmonics arise in the case of the two-body interaction potentials.

The equations defining the amplitudes $F(r, \vec{r}_{ij})$ are obtained by applying condition (8) and the expansion (9) in (6), and then project the equations onto the $\vec{r}_{ij}$ space through the overlap integral $\langle \omega_N \Omega_{N-1})|$ Eq. (6)$\rangle$ to obtain

$$-\frac{\hbar^2}{m}\left[\hat{T}_r + \frac{1}{r^2}\left(\frac{\partial^2}{\partial \varphi_N^2} - \frac{\ell(\ell+1)}{\cos^2\varphi_N} - \frac{\rho_A}{\sin^2\varphi_N}\right)\right]F_\ell(r, \varphi_N) - EF_\ell(r, \varphi_N) = -V(r, \varphi_N)\left\langle \Omega_N' \middle| \sum_{kl}^{A}\bar{\psi}_{kl}(r, \Omega_N)\right\rangle, \tag{10}$$

where $\Omega_N' = \omega_N\Omega_{N-1}$ and $[\,\hat{\ell}^2(\omega_N) - \ell(\ell+1)\,]Y_\ell^{m_\ell}(\omega_N) = 0$ was used. The evaluation of the integral on the right-hand side of (10) is discussed, for example, in Refs. [14,15]. In terms of the new variable $z = \cos 2\varphi_N$, the integration leads to

$$G_\ell(r,z) = \left\langle \Omega_N' \middle| \sum_{kl}^{A} \bar{\psi}_{kl}(r,\Omega_N) \right\rangle \tag{11}$$

$$= F_\ell(r,z) + \int_{-1}^{+1} u_\ell(z)\, f_\ell(z,z')\, F_\ell(r,z')\, w(z')\, dz', \tag{12}$$

where $u_\ell(z)\, f_\ell(z,z')$ is a projection kernel, $u_\ell(z) = (1+z)^{\ell/2}$, and $w(z) = (1-z)^\alpha (1+z)^\beta$ is the weight function with $\alpha = (3A-8)/2$ and $\beta = \ell + 1/2$. The nonlocal kernel has the form

$$f_\ell(z,z') = \sum_K^{\infty} \left[N_c \langle 0\ell|0\ell\rangle_{K\ell}^{c} + N_d \langle 0\ell|0\ell\rangle_{K\ell}^{d} \right] \times \frac{P_n^{\alpha,\beta}(z) P_n^{\alpha,\beta}(z')}{h_n^{\alpha,\beta}}, \tag{13}$$

where $K = 2n + \ell$, $\langle 0\ell \,|\, 0\ell \rangle_{KL}^{\nu}$ are Raynal-Revai coefficients, $N_c = 2(A-2)$ with $c = \pi/3$, and $N_d = \frac{1}{2}(A-2)(A-3)$ with $d = \pi/2$. Here N_c is the number of pairs of bosons when either k or l labels the same boson as either i or j, and N_d is the number of pairs when $\{kl\}$ and $\{ij\}$ label different pairs, i.e., $\{kl\} \neq \{ij\}$.

Equations (10) are now transformed by introducing the variable $z \in [-1,+1]$ and considering (12). This leads to the regularized two-variable integrodifferential equations

$$\left[-\frac{\hbar^2}{m} \left(\hat{T}_r + \frac{4}{r^2} \hat{T}_z \right) - E \right] F_\ell(r,z) = -V(r,z) G_\ell(r,z), \tag{14}$$

where the functional form of $V(r,z)$ is known and

$$\hat{T}_z = (1-z^2)\frac{\partial^2}{\partial z^2} - z\frac{\partial}{\partial z} - \frac{\alpha^2 - \frac{1}{4}}{2(1-z)} - \frac{\beta^2 - \frac{1}{4}}{2(1+z)} \tag{15}$$

is the parameterized angular kinetic energy operator. These equations are to be solved with the constraints

$$F_\ell(0,z) = F_\ell(\infty,z) = 0,$$
$$F_\ell(r,-1) = F_\ell(r,+1) = 0, \tag{16}$$

as indicated in (5). The solution to Eq. (14) is spatially symmetric [13] with respect to particle permutations, which is consistent with the symmetry requirement for systems of bosons. Equations (14) with the boundary conditions (16), which are here called regularized s-projected IDE (rSIDE), form part of the main results of this work. These results improve the traditional few-body s-projected IDE by incorporating angular boundary conditions explicitly. In the next subsection, the procedure of including effects of higher partial waves in (14) is discussed.

C. Effects of higher partial waves

Equations (14) hold for s-projected potentials where all the bosons, except the interacting pair, are in the s state [4]. Effects of higher partial waves of the potential are then taken into account by introducing the hypercentral potential multipole

$$V_0(r) = \frac{\int V(r_{ij}) d\Omega_N}{\int d\Omega_N} = \frac{\int_{-1}^{+1} V(r,z)(1-z)^\alpha (1+z)^\beta dz}{\int_{-1}^{+1} (1-z)^\alpha (1+z)^\beta dz} \tag{17}$$

in (14). This definition of $V_0(r)$ utilizes the parameter α which depends on the number of particles in the system. However, in weakly interacting systems, effects of two-body higher partial waves should be more significant in the interaction region than anywhere else in the system. That is, two-body higher partial waves are felt more by the spectator particles nearest to the interacting pair, as explained in Ref. [16]. This is to be expected when only two-body correlations are dominant.

The above argument suggests that the evaluation of (17) with $\alpha = \frac{1}{2} \equiv (A=3)$ and $\beta = \frac{1}{2}$, for any A, should adequately account for the effects of higher partial waves in the system. For this reason, the hypercentral potential is evaluated by

$$V_0(r) = \frac{(-1)^{\delta_{A3}}}{\pi} \int_{-1}^{+1} V(r,z)(1-z^2)^{1/2} dz, \tag{18}$$

where δ_{A3} is the Kronecker delta function, for $A \geqslant 3$, which is independent of variation of α and free of the challenges highlighted in Ref. [12]. This form of hypercentral potential is the zeroth multipole of the expansion of $V(r,z)$ in Chebyshev polynomials of the first kind, $T_n(z)\,(=\sqrt{1-z^2}\,U_{n-1}(z))$ relating to (15), where $U_m(z)$ are Chebyshev polynomials of the second kind.

Since the purpose of the hypercentral potential is to include effects of higher partial waves of the interaction potential, $V_0(r)$ should be added to the two-body potential and $V(r,z)$ should be replaced with $V(r,z) + V_0(r)$ in (14). One then can subtract the total $\frac{1}{2}A(A-1)\,V_0(r) = \sum_{ij} \int V(r_{ij})\, d\Omega_N / \int d\Omega_N$ from the left-hand side so that the resulting equations still sum up to the Schrödinger equation. Note that the opposite approach is implemented in the traditional IDEA [17]. The procedure outlined above leads to the regularized integrodifferential equations

$$\left[-\frac{\hbar^2}{m} \left(\hat{T}_r + \frac{4}{r^2} \hat{T}_z \right) - \frac{1}{2}A(A-1)V_0(r) - E \right] F_\ell(r,z)$$
$$= -[V(r,z) + V_0(r)] G_\ell(r,z). \tag{19}$$

Equations (19) revise the traditional few-body IDEA by incorporating angular boundary conditions explicitly as well as modify the incorporation of the hypercentral potential in the equations. Equations (19) are here called regularized IDEA (rIDEA).

These equations can be solved with any of the numerical methods that are applicable the Faddeev integrodifferential equations. In this paper, the Lagrange-mesh method [11,18–20] is used. Illustrative applications of (14) and (19) are discussed in the next section.

III. ILLUSTRATIONS

The integrodifferential equations (14) were solved directly using the Lagrange-mesh method [11]. Ground-state energies E_0 for A-boson systems interacting through the central Volkov

TABLE I. Calculated ground-state energy E_0(MeV) for few-boson systems with the central Volkov potential.

	$-E_0$(MeV)		
A	rSIDE	rIDEA	Ref.
3	8.430 9	8.460 2	
	8.430 9	8.464 6	[3]
4	28.845	29.844	
	30.252	30.418	[3]
5	66.831	68.340	
	66.893[a]	68.280	[3]
6	121.662	123.180	
	121.738[b]	122.776	[3]
7	193.129	194.453	
		200.136	[12]
8	281.176	282.253	
		285.808	[12]
9	385.809	386.649	
		386.640	[12]
10	507.064	507.698	
		512.193	[12]

[a]$K_{\max} = 6$ (all waves).
[b]$K_{\max} = 8$ (all waves).

nucleon-nucleon potential [21] with A ranging from 3 to 10 were calculated. The description of nuclear interactions with central potentials is not realistic [3,22] because it does not take into account significant degrees of freedom of the nucleons. However, this potential is widely used in the literature as a test case in many methods and provides benchmark results to compare with. The Volkov potential has the form

$$V(r_{ij}) = V_R e^{-r_{ij}^2/a_R^2} + V_A e^{-r_{ij}^2/a_A^2}, \tag{20}$$

where $V_R = 144.86$ MeV, $V_A = -83.34$ MeV, $a_R = 0.82$ fm, and $a_A = 1.6$ fm. The nucleon mass m such that $\hbar^2/m = 41.47$ MeV fm^2 was used and a maximum hyperradial range of $r_m = 30$ fm was adopted. Convergence was reached quite rapidly with a very low number of basis size ($N_r = N_z = 30$) for all the systems considered.

The calculated ground-state energies for boson systems with $A = 3$ to $A = 10$ are presented in Table I. In Table, it can be notice that the rIDEA results do not differ much (≈1 MeV) from the rSIDE results, in all the systems. This observation, also reported in Refs. [5,16], suggests that contributions of higher partial waves to ground-state energies do not appear to depend on the number of particles in the system when two-body correlations are dominant.

In Ref. [3], ground-state energies of boson systems with $A = 3$, 4, 5, 6 are presented for the Volkov potential. The results were obtained by solving the Schrödinger equation exactly for the systems using the HHE method. The "s-wave" results of this reference correspond to the rSIDE results while the "all waves" results correspond to the rIDEA results of this work. The results of this work are compared with those presented in the reference. As can be seen, the rIDEA reproduces the all waves exact results almost exactly (<1% differences) for all the $A \leqslant 6$ systems. On the other hand, the rSIDE and the s-wave results are identical for $A = 3$, but differ by about 5% for $A = 4$. However, the rSIDE results are 1% closer to the $K_{\max} = 0$ results. In the absence of the s-wave results for the $A = 5$ and $A = 6$ systems, it is tempting to compare the rSIDE results with the intermediate all waves results of Ref. [3]. The rSIDE results differ by <1% with those of the $K_{\max} = 6$ and $K_{\max} = 8$ all waves, respectively, for the $A = 5$ and $A = 6$ systems.

In general, it observed that there are small differences between the rSIDE and the rIDEA results. This could be an indication that effects of higher partial waves of short-range interaction potentials in few-body systems are small but significant. This agrees with the findings of Ref. [5]. Also, small differences are observed between the rIDEA results and the HHE method results. These small differences in the results of the two approaches can be confidently interpreted as an indication that the IDEA and the HHE method are equivalent and, therefore, generate similar solutions [13], and that A-body correlations ($A > 3$) are not significant in systems interacting via short-range potentials. These claims could not be made with confidence in the past because the comparisons were made with interpolated results from the adiabatic solutions of IDEA [5]. The results presented above are direct solutions of the rIDEA.

In Ref. [12], ground-state energies for $A = 7$, 8, 9, 10 bosonic systems are presented for the Volkov potential. The results are obtained by solving the integrodifferential equations using the perturbation method. As explained in the reference, the perturbation solution is not always reliable, but generates satisfactory solutions. On the other hand, the projection method, although exact, has convergence challenges. It should be noted that in both solution methods, the angular domain is not regularized, higher potential multipoles are employed, and the A-dependent weight function $w(z)$ is used. The results of this work are compared with the perturbation results of Ref. [12]. It is declared in the reference that the results from the projection method had not converged. Since the present results are converged and have been shown to consistently compare very well with exact results of Ref. [3], they provide a test of accuracy to the results of Ref. [12]. Whereas the energies for $A = 8$ and $A = 9$ are reproduced to within 1% and 0.01%, respectively, the energies for the $A = 7$ and $A = 10$ systems are overestimated by 3% and 1%, respectively. The perturbation solutions of the integrodifferential equation can be accepted as satisfactory.

IV. CONCLUSION

The traditional few-body integrodifferential equations approach has been reviewed. Dirichlet boundary conditions were implemented in the hyperradial and hyperangular domains. Procedures for the evaluation of the hypercentral potential and for the inclusion of effects of higher partial waves of the interaction potential have been revised. Results obtained with the modified integrodifferential equations approach converge rapidly and reproduce those obtained with the hyperspherical harmonics approach, an exact method, to within 5% for boson systems interacting through the

Volkov potential. These results suggest that contributions from effects of higher partial waves to the ground state of few-body systems are small, that many-body correlations are not significant in systems interacting through short-range potentials, and that the IDEA is equivalent to the HHE method. Work is under way to clarify the impact of these changes on other features of the integrodifferential equations approach.

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