Comparison of Born-Oppenheimer and hyperspherical adiabatic approximations in the trinucleon problem

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Ground state energies of the three-nucleon system interacting via standard S-projected potentials are studied using Born-Oppenheimer and hyperspherical adiabatic approximations. The extreme and the uncoupled hyperspherical adiabatic approximations, which are the lower and upper bounds for the exact ground state energy, are found to define a narrow band with the Born-Oppenheimer approximation lying close to it. While the hyperspherical adiabatic approximation conserves the basic symmetry requirements, the other does not. In spite of this, the Born-Oppenheimer approximation is found to be comparable to the other for potentials with a soft core repulsion.

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I. INTRODUCTION

The hyperspherical harmonics approach [1] has been in use since the early 1970s for the treatment of bound states of nonrelativistic few particle systems and has seen fairly widespread application in nuclear [2], atomic [3], and molecular [4] physics. This approach stems from a generalization of the textbook problem of two particles interacting via mutual interaction only, for which the space wave function can be expanded in ordinary spherical harmonics. The hyperangular functions spanning a $(3N-4)$-dimensional angular hyperspace of the relative coordinate system for a N particle system are called hyperspherical harmonics (HH) and constitute a generalization of the ordinary spherical harmonics spanning the two-dimensional angular space of a two-body system $(N=2)$. Complete analytical expressions for the HH can be obtained by solving the $(3N-3)$-dimensional Laplace equation. The wave function of a N particle system can be written as a sum of products of space and spin-isospin wave functions. The Pauli principle demands the imposition of a specified symmetry for the space wave function of each component, which depends on the symmetry character of the corresponding spin-isospin wave function. By a fairly straightforward procedure, one can construct the HH basis having a specified symmetry character. The space wave function of each component can be expanded in the appropriate HH basis. Substitution of this into the Schrödinger equation and projection on a particular HH give rise to an infinite number of coupled differential eigenvalue equations. A numerical solution can be realized only after a truncation of this set to a finite number of coupled equations. However, in many situations a truncation without valid physical justification leads to simplification at the cost of obtaining numerical results which are far from converged ones.

Recently an adiabatic approximation scheme in the hyperspherical harmonics approach, referred to as the hyperspherical adiabatic approximation (HAA), has been suggested [2–4] which allows a reduction in the dimensionality of the coupled set of equations without sacrificing precision in a completely uncontrolled way as in direct truncation. Two versions of this approximation, known as the extreme adiabatic approximation (EAA) and uncoupled adiabatic approximation (UAA), provide prescriptions for reducing a set of infinite—usually in practice a large finite—number of coupled differential equations to a single differential equation. The EAA and UAA are specially interesting because they are [5] an upper and a lower bound of the exact energy. In the three-nucleon problem, EAA and UAA have been found to define a very narrow interval which includes the exact energy [2,5]. In this case, the EAA and UAA produce results which are very close to the solution of the full set of equations and provide, respectively, lower and upper bounds for the exact energy [5].

A commonly employed tool in molecular physics is the Born-Oppenheimer [6] approximation (BOA), which has been successfully used over the last fifty years. This approach has been traditionally applied when some of the particles of a system are light (e.g., electrons) compared to others (nuclei). The motion of the light particles is expected to be fast compared to that of the heavy ones. As a result, the two types of motions can be thought of as approximately decoupled, which is the basic idea of the BOA. The motion of the light particle system for a fixed configuration of the heavy particles allows one to construct an effective potential for the heavy particle system. The Schrödinger equation for the heavy particle system is then solved with this effective potential. Brattsev has shown that the BOA provides a lower bound for the exact energy [7].

The EAA and UAA as well as the BOA have been successfully used in varied situations, although the reasons

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or conditions for the success have never been clear and explicit. The purpose of the present work is to study these approximation schemes and their applicability.

In an earlier work [8] we studied the ground state energies of a three particle system consisting of a distinct and two equal mass particles interacting via Gaussian S-wave potentials and investigated the applicability of the EAA, UAA, and BOA. Denoting the ratio of equal mass to distinct mass by m, the nuclear and molecular situations are simulated by $m \simeq 1$ and $m \gg 1$, respectively. It was found that all the approximations worked surprisingly well in all situations considered. Also in an earlier work, Fonseca *et al.* [19] treated ^{9}Be as a bound cluster of two α particles and a neutron and applied the BOA successfully. The earlier observations and the success of this BOA treatment of ^{9}Be motivates us to investigate how the BOA (which is normally expected to work for molecular situations only) fares in a typical semirealistic nuclear calculation.

In the present work, we obtain the trinucleon binding energy when the nucleons interact via standard S-projected potentials with widely varying soft cores. We have calculated both the EAA and UAA results as well as the exact binding energy (BE), the truncation in the number of partial waves being determined by the requirement of convergence in BE to better than 4 keV (or about 0.05%). For strong soft core potentials like Afnan-Tang S3 potential [9], Malfliet-Tjon [10] MT-I/III or MT-V potentials, we need up to 20 partial waves to get a converged result for the totally symmetric S state of the trinucleon. We have also calculated the BE using the BOA to evaluate the effective potential between two nucleons kept at a fixed separation, while the motion of the third nucleon is governed by the chosen two-body potential between it and each of the fixed nucleons. Since in this case the three nucleons are identical and interact via the same two-body potential, one does not expect *a priori* that the BOA is applicable to this situation. But to our surprise, the BOA seems to fare reasonably well at least for the soft core potentials. This is in agreement with earlier works of Efimov [18] and Fonseca *et al.* [19].

In Sec. II we explain the various approximation schemes (EAA, UAA, and BOA). In Sec. III we present the numerical results and finally in Sec. IV we discuss the results and draw our conclusions.

II. ADIABATIC APPROXIMATIONS

Let us consider a three-body system formed by three particles of mass m. The Jacobi coordinates constituting the relative variables of the system are

$$\begin{aligned} \mathbf{x} &= \mathbf{r}_1 - \mathbf{r}_2 , \\ \mathbf{y} &= (2/\sqrt{3})[\mathbf{r}_3 - \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)] , \end{aligned} \tag{1}$$

where $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ are position vectors of the particles. We can eliminate the center of mass (c.m.) motion in the Schrödinger equation for the three particles. The resulting Schrödinger equation in the relative coordinate system is then

$$[-(\nabla_{\mathbf{x}}^2 + \nabla_{\mathbf{y}}^2) + v(\mathbf{x},\mathbf{y})]\Psi(\mathbf{x},\mathbf{y}) = \epsilon \Psi(\mathbf{x},\mathbf{y}) , \tag{2}$$

where

$$v(\mathbf{x},\mathbf{y}) = \frac{m}{\hbar^2}\left[V_{12}(x) + V_{13}\left(\left|-\frac{\mathbf{x}}{2} + \frac{\mathbf{y}}{a}\right|\right) + V_{23}\left(\left|\frac{\mathbf{x}}{2} + \frac{\mathbf{y}}{a}\right|\right)\right] , \tag{3}$$

V_{ij} is the pairwise interactions between particles i and j, and $a = 2/\sqrt{3}$. The quantity ϵ is related to the energy, E, of the system by $\epsilon = (m/\hbar^2)E$. We can now introduce the hyperspherical adiabatic approximation (HAA) and the Born-Oppenheimer approximation (BOA) for the three-body system.

A. The hyperspherical adiabatic approximation

In the hyperspherical formalism [1] one introduces six hyperspherical variables: a hyperradius, r, defined by $r^2 = x^2 + y^2$, and five hyperangles, concisely denoted here by Ω. They are the four angle variables which are the spherical polar angles $\hat{\mathbf{x}} \equiv (\theta_x, \varphi_x)$ of the vector $\mathbf{x}$ and $\hat{\mathbf{y}} \equiv (\theta_y, \varphi_y)$ of the vector $\mathbf{y}$, and one hyperspherical angle θ, defined in terms of the lengths of $\mathbf{x}$ and $\mathbf{y}$ by

$$x = r\cos\theta, \quad y = r\sin\theta, \quad 0 \le \theta \le \pi/2 . \tag{4}$$

As in the two-body case, the set Ω is the argument of hyperspherical harmonics [1], $Y_\alpha(\Omega)$ (for simplicity we keep the same notation of the two-body problem), defined below. The hyperradial variable r is invariant under ordinary rotations and all permutations. Equation (2) in hyperspherical coordinates is written as

$$\left[-\frac{d^2}{dr^2} - \frac{\mathcal{L}^2(\Omega)}{r^2} + v(r,\Omega) - \epsilon\right]\psi(r,\Omega) = 0 , \tag{5}$$

where $\Psi(\mathbf{x},\mathbf{y}) = r^{-5/2}\psi(r,\Omega)$. Notice that $v(r,\Omega) = v(\mathbf{x},\mathbf{y})$. The operator $\mathcal{L}^2$ is given by

$$\mathcal{L}^2(\Omega) = K^2(\Omega) - \tfrac{15}{4} , \tag{6}$$

where $K^2(\Omega)$ is the Casimir operator of the system [1], given by

$$K^2(\Omega) = \frac{\partial^2}{\partial\theta^2} + 4\cot g(2\theta)\frac{\partial}{\partial\theta} - \frac{\hat{l}_x^2}{\cos^2\theta} - \frac{\hat{l}_y^2}{\sin^2\theta} , \tag{7}$$

where $\hat{l}_x^2$ and $\hat{l}_y^2$ are the angular momentum operators. Thus the $Y_\alpha(\Omega)$ are eigenfunctions of $\mathcal{L}^2$

$$K^2 Y_\alpha(\Omega) = -K(K+4)Y_\alpha(\Omega) , \tag{8}$$

where K is an integer and α is the set of quantum numbers necessary to specify the system, which can be chosen as $\alpha \equiv \{K, L, M, l_x, l_y\}$, $\mathbf{L} = \mathbf{l}_x + \mathbf{l}_y$ is the total orbital angular momentum operator, and M is the quantum number corresponding to the z component of $\mathbf{L}$. Expanding $\psi(r,\Omega)$ in terms of the complete orthonormal set $\{Y_\alpha(\Omega)\}$,

$$\psi(r,\Omega) = \sum_\alpha \varphi_\alpha(r) Y_\alpha(\Omega) , \tag{9}$$

and multiplying Eq. (5) from the left by $Y^*_{\alpha'}(\Omega)$ and integrating over $d\Omega$, we obtain the infinite set of coupled differential equations (SCDE) in terms of a hyperradial variable r,

$$\left[-\frac{d^2}{dr^2}+\frac{(K+2)^2-\frac{1}{4}}{r^2}-\epsilon\right]\varphi_\alpha(r)+\sum_{\alpha'} v_{\alpha\alpha'}(r)\varphi_{\alpha'}(r)=0 , \tag{10}$$

where $v_{\alpha\alpha'}(r)=\langle Y_\alpha(\Omega)|v(r,\Omega)|Y_{\alpha'}(\Omega)\rangle$. A well established procedure [2–4] to handle the SCDE is the HAA. Let us summarize it below.

In the HAA procedure, an associated matrix eigenvalue equation is constructed as follows:

$$U(r,\Omega)\Phi_\lambda(r,\Omega)\equiv\left[-\frac{\mathcal{L}^2}{r^2}+v(r,\Omega)\right]\Phi_\lambda(r,\Omega) =u_\lambda(r)\Phi_\lambda(r,\Omega) , \tag{11}$$

where λ labels the different $u(r)$ for a fixed r. We can now expand $\Phi_\lambda(r,\Omega)$ in the complete orthonormal set, $\{Y_\alpha(\Omega)\}$,

$$\Phi_\lambda(r,\Omega)=\sum_\alpha \chi_{\alpha\lambda}(r)Y_\alpha(\Omega) , \tag{12}$$

and obtain a matrix eigenvalue equation from Eq. (11)

$$\sum_{\alpha'} U_{\alpha\alpha'}(r)\chi_{\alpha'\lambda}(r)=u_\lambda(r)\chi_{\alpha\lambda}(r) , \tag{13}$$

which is solved to obtain the eigenvalues, $u_\lambda(r)$, and the eigenvectors, $\chi_{\alpha\lambda}(r)$ (column matrix), as parametric functions of r. The matrix elements $U_{\alpha\alpha'}(r)$ are defined as

$$U_{\alpha\alpha'}(r)=\langle Y_\alpha(\Omega)|-\mathcal{L}^2/r^2+v(r,\Omega)|Y_{\alpha'}(\Omega)\rangle . \tag{14}$$

The matrix $U_{\alpha\alpha'}(r)$ is just a real symmetric matrix (indeed, it has to be Hermitian, as it is the potential matrix). Expanding $\varphi_\alpha(r)$ in the complete orthonormal set $\{\chi_{\alpha\lambda}(r)\}$,

$$\varphi_\alpha(r)=\sum_\lambda \xi_\lambda(r)\chi_{\alpha\lambda}(r) , \tag{15}$$

using Eq. (9), and substituting into Eq. (5), we finally obtain [2]

$$\left[-\frac{d^2}{dr^2}+\left[u_\lambda(r)+\sum_\alpha\left|\frac{d\chi_{\alpha\lambda}(r)}{dr}\right|^2\right]-\epsilon\right]\xi_\lambda(r) -\sum_{\lambda'(\lambda'\neq\lambda)} C_{\lambda\lambda'}(r)=0 , \tag{16}$$

where

$$C_{\lambda\lambda'}(r)=[2P_{\lambda\lambda'}(r)+Q_{\lambda\lambda'}(r)]\xi_{\lambda'}(r) . \tag{17}$$

The nonadiabatic couplings $P_{\lambda\lambda'}$ and $Q_{\lambda\lambda'}$ are given by

$$P_{\lambda\lambda'}(r)=\left\langle\chi_\lambda\left|\frac{d}{dr}\chi_{\lambda'}\right\rangle\frac{d}{dr} ,\right. \qquad Q_{\lambda\lambda'}(r)=\left\langle\chi_\lambda\left|\frac{d^2}{dr^2}\chi_{\lambda'}\right\rangle .\right. \tag{18}$$

The potential curves, $u_\lambda(r)$, similar to the molecular potential curves, contain essential information about the structure of the three-body system. When the derivatives of $\chi_{\alpha\lambda'}$ with respect to r are small, we expect to generate nearly decoupled equations. The coupling term $C_{\lambda\lambda'}(r)$ turns out to be small in practical situations (as evidenced by the success of the HAA). If truncation is done in the still exact system of equations (16), we get the coupled adiabatic approximation (CAA). Neglecting the coupling terms in Eq. (16), we have the uncoupled adiabatic approximation (UAA). In the UAA, the neglect of $\sum_\alpha|\chi'_{\alpha\lambda}|^2$ leads to the extreme adiabatic approximation (EAA). The following basic inequalities

$$\epsilon_{\mathrm{EAA}}\leq\epsilon\leq\epsilon_{\mathrm{CAA}}\leq\epsilon_{\mathrm{UAA}} \tag{19}$$

hold for the ground state energies [5].

B. The Born-Oppenheimer approximation

The usual way to introduce BOA [6] in Eq. (2) is to expand $\Psi(\mathbf{x},\mathbf{y})$ in the form

$$\Psi(\mathbf{x},\mathbf{y})=\sum_\lambda \hat{\varphi}^{(\mathbf{x})}_\lambda(\mathbf{y})\hat{\Phi}_\lambda(\mathbf{x}) , \tag{20}$$

where $\hat{\varphi}_\lambda$ satisfies the equation

$$[-\nabla^2_{\mathbf{y}}+\hat{v}^{(\mathbf{x})}(\mathbf{y})]\hat{\varphi}^{(\mathbf{x})}_\lambda(\mathbf{y})=\hat{\epsilon}_\lambda(\mathbf{x})\hat{\varphi}^{(\mathbf{x})}_\lambda(\mathbf{y}) , \tag{21}$$

and $\hat{v}^{(\mathbf{x})}(\mathbf{y})=v_{13}(|\mathbf{y}/a-\mathbf{x}/2|)+v_{23}(|\mathbf{y}/a+\mathbf{x}/2|)$. For each value of $\mathbf{x}$, $\hat{\epsilon}_\lambda(\mathbf{x})$ is obtained as an eigenvalue of Eq. (21). Substitution of Eq. (20) into Eq. (2) gives, with the help of Eq. (21),

$$[-\nabla^2_{\mathbf{x}}+v_{12}(x)]\Psi(\mathbf{x},\mathbf{y})+\sum_\lambda \hat{\epsilon}_\lambda(\mathbf{x})\hat{\varphi}^{(\mathbf{x})}_\lambda(\mathbf{y})\hat{\Phi}_\lambda(\mathbf{x})=\epsilon\Psi(\mathbf{x},\mathbf{y}) \tag{22}$$

which can be rewritten as

$$\sum_\lambda \hat{\varphi}^{(\mathbf{x})}_\lambda(\mathbf{y})[-\nabla^2_{\mathbf{x}}+\hat{\epsilon}_\lambda(\mathbf{x})+v_{12}(x)-\epsilon]\hat{\Phi}_\lambda(\mathbf{x}) =\sum_\lambda[\hat{\Phi}_\lambda(\mathbf{x})\nabla^2_{\mathbf{x}}\hat{\varphi}^{(\mathbf{x})}_\lambda(\mathbf{y})+2\nabla_{\mathbf{x}}\hat{\varphi}^{(\mathbf{x})}_\lambda(\mathbf{y})\cdot\nabla_{\mathbf{x}}\hat{\Phi}_\lambda(\mathbf{x})] . \tag{23}$$

Multiplying Eq. (23) by $\hat{\varphi}_{\lambda'}(\mathbf{y})^*$ from the left and integrating over the $\mathbf{y}$ variable, we finally obtain

$$[-\nabla^2_{\mathbf{x}}+\hat{\epsilon}_\lambda(\mathbf{x})+v_{12}(x)-\epsilon]\hat{\Phi}_\lambda(\mathbf{x})-\sum_{\lambda'}\hat{C}_{\lambda\lambda'}(\mathbf{x})=0 , \tag{24}$$

where

$$\hat{C}_{\lambda\lambda'}(\mathbf{x})=[2\hat{P}_{\lambda\lambda'}(\mathbf{x})+\hat{Q}_{\lambda\lambda'}(\mathbf{x})]\hat{\Phi}_{\lambda'}(x) . \tag{25}$$

The nonadiabatic couplings $\hat{P}_{\lambda\lambda'}$ and $\hat{Q}_{\lambda\lambda'}$ are given by

$$\hat{P}_{\lambda\lambda'}(\mathbf{x})=\langle\hat{\varphi}^{(\mathbf{x})}_\lambda|\nabla_{\mathbf{x}}|\hat{\varphi}^{(\mathbf{x})}_{\lambda'}\rangle\cdot\nabla_{\mathbf{x}} \tag{26}$$

and

$$\hat{Q}_{\lambda\lambda'}(\mathbf{x})=\langle\hat{\varphi}^{(\mathbf{x})}_\lambda|\nabla^2_{\mathbf{x}}|\hat{\varphi}^{(\mathbf{x})}_{\lambda'}\rangle . \tag{27}$$

If now the dependence of $\hat{\varphi}^{(\mathbf{x})}_\lambda$ on $\mathbf{x}$ is neglected, the terms contained in the sum on λ' in Eq. (24) drops out, and we obtain the BOA. It essentially consists in the

solution of the system of differential equations

$$[-\nabla_y^2+\hat{v}^{(x)}(\mathbf{y})-\hat{\epsilon}_\lambda(\mathbf{x})]\hat{\varphi}_\lambda^{(x)}(\mathbf{y})=0\ , \tag{28}$$

$$[-\nabla_x^2+\hat{\epsilon}_\lambda(\mathbf{x})+v_{12}(x)-\epsilon_{\mathrm{BOA}}]\hat{\Phi}_\lambda(\mathbf{x})=0\ . \tag{29}$$

The neglect of the sum in Eq. (24) can be justified physically from the assumption of smallness of the amplitudes of the motion in the **x** direction ($\nabla_x\hat{\varphi}_\lambda^{(x)}\approx 0$) in comparison with the motion in the **y** direction. Formally there exist certain resemblances between HAA and BOA [for instance, compare Eq. (16) with Eq. (24) and Eqs. (17) and (18) with Eqs. (25)–(27)]. Both approximations (HAA and BOA) are adiabatic in nature [small variations of $\chi_{\alpha\lambda}(r)$ and $\hat{\varphi}_\lambda^{(x)}(\mathbf{y})$] and thus based on the same physical ideas [11]. But they are mathematically different. HAA is developed in a hyperspherical space with O(6) symmetry while BOA is constructed in Cartesian space with O(3)×O(3) symmetry. In this work a comparison is made between HAA and BOA through a numerical calculation for the same model three-nucleon system.

As in the HAA, a basic inequality [7] holds for the BOA,

$$\epsilon_{\mathrm{BOA}}\leq\epsilon\ . \tag{30}$$

In general, $\epsilon_{\mathrm{BOA}}\neq\epsilon_{\mathrm{EAA}}$, although both are lower bounds of ϵ.

III. NUMERICAL CALCULATIONS

In the BOA, Eqs. (28) and (29) can be rewritten in a more convenient form for numerical calculations. Let us choose **x** along the Z axis and the center of mass of particles 1 and 2 at the origin. Then the angle between **x** and **y** is θ, resulting

$$\left|\frac{1}{a}\mathbf{y}\pm\frac{1}{2}\mathbf{x}\right|=\left[\frac{1}{a^2}y^2+\frac{1}{4}x^2\pm\frac{1}{a}xy\mu\right]^{1/2}, \tag{31}$$

where $\mu=\cos\theta$.

By expanding $\hat{\varphi}^{(x)}(y)$ in spherical harmonics, $Y_{lm}(\hat{y})$, and using the fact that there is azimuthal symmetry about the Z axis for the **y** motion, we have

$$\hat{\varphi}_\lambda^{(x)}(\mathbf{y})=\sum_{l_y'=0}^{\infty}\left[\frac{u_{\lambda l_y'}^{(x)}(y)}{y}\right]Y_{l_y'0}(\hat{y})\ . \tag{32}$$

Notice that m_y' is a good quantum number and since the potential [hence $\hat{\epsilon}_\lambda(x)$] does not depend on m_y', we can choose $m_y'=0$. Substitute Eq. (32) into Eq. (28), multiply by $Y_{l_y0}^*(\hat{y})$ and integrate over $d\Omega_y$, use orthogonality property of the spherical harmonics, and we obtain

$$\left[-\frac{d^2}{dy^2}-\epsilon_\lambda(x)\right]u_{\lambda l_y}^{(x)}(y)+\sum_{l_y'}\langle\hat{v}_{l_y l_y'}^{(x)}(y)\rangle u_{\lambda l_y'}^{(x)}(y)=0\ , \tag{33}$$

where

$$\langle\hat{v}_{l_y l_y'}^{(x)}(y)\rangle=\frac{l_y(l_y+1)}{y^2}\delta_{l_y l_y'}+[(2l_y+1)(2l_y'+1)]^{1/2}\int_0^1 P_{l_y}(\mu)\left[v_{13}\left(\left|-\frac{1}{2}\mathbf{x}+\frac{1}{a}\mathbf{y}\right|\right)+v_{23}\left(\left|\frac{1}{2}\mathbf{x}+\frac{1}{a}\mathbf{y}\right|\right)\right]P_{l_y'}(\mu)d\mu\ . \tag{34}$$

Similarly Eq. (29) can be written as

$$\left[-\frac{d^2}{dx^2}+\hat{\epsilon}_\lambda(x)+v_{12}(x)-\epsilon_{\mathrm{BOA}}\right]\hat{\phi}_\lambda(x)=0\ , \tag{35}$$

where we have essentially set $\hat{\Phi}_\lambda(\mathbf{x})=\hat{\phi}_\lambda(x)Y_{l_x0}(\mathbf{x})$. Since in this approximation $\hat{\epsilon}_\lambda(x)$ is taken as central, only $l_x=0$ contributes.

In this paper we restrict ourselves to the space symmetrical S state ($L=M=0\Longrightarrow l_x=l_y=$even) which implies fully antisymmetric spin-isospin states. The S state by itself is responsible for nearly 90% of the total probability [2].

For our calculation, we have chosen several standard S-projected phenomenological potentials, namely Baker [13], Volkov [14], S4 [15], GPDT [16], and Malfliet-Tjon (in three versions MT-I/III [10], MT-II/IV [10], and MT-V [17]) potentials. Most of these potentials have explicit spin dependence while the Baker and MT-V potentials are spin independent. The behavior of these potentials at short distances have a wide variation starting from a finite attractive core for Baker to strongly repulsive core for MT-V and S3 potentials. The choice of these potentials thus allows us to investigate the effect of the core (i.e., the short separation behavior) of the potential on the applicability of a particular approximation method. The core behavior of these potentials has been displayed in Fig. 1. From this we find that in decreasing order of softness the potentials are MT-II/IV, Baker, Volkov, GPDT, S4, S3, MT-V, and MT-I/III.

The numerical procedure to handle the HAA can be found in Ref. [2] and will not be discussed here. The values of a cutoff radius (r_∞) and the truncation of hyperspherical partial waves ($K_{\max}$) have been obtained by the requirement that E_{exact} should converge up to a relative accuracy of 0.05% or better. The BE is nearly insensitive to the value of $r_\infty>10$ fm, as seen from Table I, for a few selected potentials. It is seen that the increase of r_∞ from 13 to 15 fm increases E_{exact} by less than 0.005%. Hence we fix $r_\infty=15$ fm for the rest of the cal-

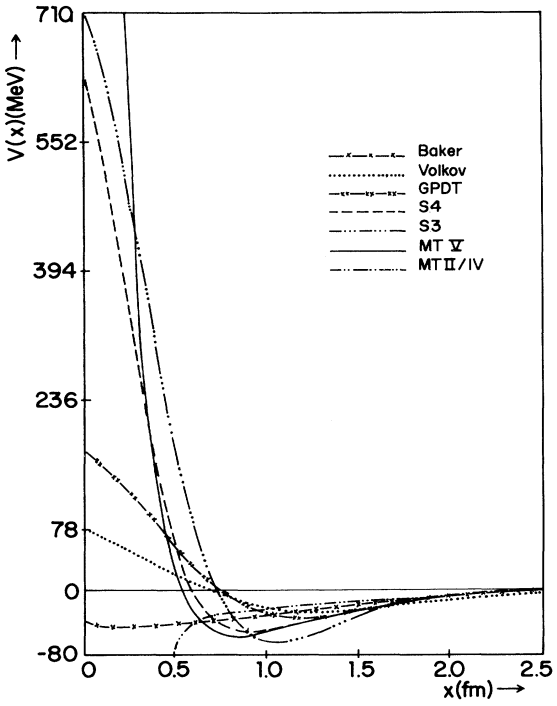

FIG. 1. Plot of two-body potentials against two-nucleon separation (x). Curve for MT-V is very close to MT-I/III, so it does not appear in the graph.

culations. The BE is much more sensitive to the choice of $K_{\max}$, as shown in Table II, where we present E_{exact} with $K_{\max}=14$, 16, 18, and 20 for three hardest potentials, viz., MT-I/III, MT-V, and S3 (for which convergence with respect to $K_{\max}$ is expected to be slowest). A clear convergence trend is discernible for each of the potentials. It can be seen from Table II that the relative change in E_{exact} from $K_{\max}=18$ to $K_{\max}=20$ is about 0.05%, 0.04%, and 0.005% for MT-I/III, MT-V, and S3, respectively. From this we conclude that a choice of $K_{\max}=20$ is sufficient to guarantee a relative precision in E_{exact} of better than 0.05% for all the potentials chosen.

For the BOA calculation we choose 301 mesh points with step size 0.05, extending up to 15 fm for both x and y variables. For a fixed value of x, the $\langle \hat{v}^{(x)}_{l_y l'_y}(y)\rangle$ matrix is calculated by a 32 points Gaussian quadrature. Note from Eq. (34) that $\langle \hat{v}^{(x)}_{l_y l'_y}(y)\rangle$ vanishes whenever l_y or l'_y is odd. This and the fact that $\langle \hat{v}^{(x)}_{l_y l'_y}(y)\rangle$ is a symmetric matrix have been used to optimize the calculation of the matrix. For each fixed value of x, we solve the coupled system of differential equations (33) in an exact numerical manner by the renormalized Numerov method [12], to obtain the eigenpotential $\hat{\epsilon}_0(x)$ (which is the effective potential in the x variable for the ground state). Once $\hat{\epsilon}_0(x)$ is obtained at each x mesh point we solve the x equation (35), which is an uncoupled second order differential equation, by the Runge-Kutta method to obtain the ground state energy eigenvalue ϵ_{BOA}.

The triton (^{3}H) binding energy calculated by the three approximation methods as well as an "exact" value [obtained by solving the exact equation (10) by the renormalized Numerov method] for each of the chosen potentials have been presented in Table III. We can compare our exact results with previous calculations using HHEM [21] or Faddeev method [20,22]. The agreement with previous HHEM calculation is excellent (note that our method is the same as that of Ref. [21], except that more partial waves have been used for harder potentials in the present work). For comparison with the latter method, we failed to find in the literature exactly the same calculation using any of the potentials used here. The BE calculated by Payne *et al.* [22] for the Faddeev calculation with MT-I/III, MT-II/IV, and MT-V are 8.535, 11.880, and 7.5403 MeV, respectively. The first two are appreciably higher while the last one is smaller than our E_{exact}. Note, however, that we retain only the space totally symmetric S state of the trinucleon, while Payne *et al.* included both S and the mixed symmetry S' states. The fact that our BE is lower than their value is consistent with the Ritz principle. The case with MT-V is different,

TABLE I. Dependence of E_{exact} on cutoff radius (r_∞) for representative potentials ($K_{\max}=18$).

r_∞ (fm)	E_{exact} (MeV) MT-I/III	MT-V	S3
11	7.9106	8.4301	6.7039
13	7.9107	8.4304	6.7040
15	7.9109	8.4307	6.7042

TABLE II. Convergence behavior of calculated E_{exact} for selected potentials (cutoff radius $r_\infty=15$ fm).

$K_{\max}$	E_{exact} (MeV) MT-I/III	MT-V	S3
14	7.8155	8.3325	6.6898
16	7.8973	8.4157	6.7006
18	7.9109	8.4307	6.7042
20	7.9148	8.4328	6.7045

TABLE III. Calculated binding energies (in MeV) of ^{3}H for several chosen potentials in different adiabatic approximations. Their values can be compared with the corresponding exact value.

Potential	E_{BOA}	E_{EAA}	E_{UAA}	E_{exact}
Baker	9.7386	9.8651	9.7547	9.7812
Volkov	8.5728	8.6227	8.4082	8.4648
GPDT	4.1166	3.8222	3.5723	3.6557
S4	7.7263	7.2901	6.9583	7.0182
S3	8.1302	7.2133	6.4889	6.7045
MT-II/IV	10.5191	10.6349	10.5731	10.5856
MT-I/III	8.8090	7.9602	7.5881	7.9148
MT-V	8.8001	8.4867	8.0997	8.4338

as the potential parameters used in Ref. [22] were those of Ref. [10] multiplied by a strength factor 0.9866 (to ensure a deuteron BE of 2.23 MeV), while the parameters of MT-V used by us are those of Ref. [17]. From Table III, it can be seen that the inequality (30) is obeyed by all potentials except the softest ones, viz., Baker and MT-II/IV, while the inequality (19) is obeyed by all potentials. The fact that the inequality (30) is not obeyed for the softest potentials (although the deviation $\epsilon_{\rm BOA}-\epsilon$ is small compared to ϵ in both cases) is puzzling. A possible explanation may be as follows. In our treatment of BOA only $l_x=0$ is retained; this gives higher BE compared to that for a nonvanishing effective l_x value. For potentials which are not so soft, the effective l_x value should be nonvanishing. Thus a chosen value $l_x=0$ gives relatively large overbinding. But for very soft potentials, the effective l_x value being close to zero (due to softness of the potential, the particles can approach each other without difficulty), the choice $l_x=0$ does not give a BE much different from the exact value. This is the reason for closer agreement with the exact value for the softer potentials (Table III). Now $\epsilon_{\rm BOA}$ obtained by solving Eq. (35) in which $\hat{\epsilon}_0(x)$ for each x mesh point is obtained by solving Eq. (33) with a relative error in $\hat{\epsilon}_0(x)$ of about 0.05%. Clearly the error in $\epsilon_{\rm BOA}$ is larger. Furthermore, an error in Eq. (35) arises due to the disregard of angular dependence of $\hat{\epsilon}_0(x)$ (the angular dependence is lost in the process of Born-Oppenheimer separation). Inclusion of additional degrees of freedom by way of angular dependence will result in higher BE. Although it is hard to estimate the magnitude of such errors, if the accumulated error is about 1%, it can well account for the lack of conformity with Eq. (30), for potentials for which $\epsilon_{\rm BOA}-\epsilon$ is small. One can notice from Table III that the BOA produces a good enough result for the softest potentials (namely, Baker, MT-II/IV, Volkov) which are better than the corresponding EAA and comparable with the UAA, while the disagreement with exact energies is worse (10% or more) for the potentials with stronger repulsive core and weaker binding. Although from these studies it cannot be said that the strength of the core repulsion is the only criterion for the validity of the BOA, it certainly seems to be a dominant deciding factor. In addition, it appears that the higher the binding, the closer is the agreement. Qualitatively, it then appears that the BOA provides a good results for softer core repulsion and stronger binding.

In contrast, the UAA result is much better than the BOA result for all the potentials considered. However, considering the mathematical nature of the BOA treatment, it should be compared with the EAA, as both are lower bounds for the exact ground state energy. Table I shows that the BOA result is comparable with the EAA result in most cases.

In Fig. 2 we plot the effective potential seen by particles 1 and 2 in the BOA, $V_{\rm eff}(x)=V_{12}(x)+(m/\hbar^2)\hat{\epsilon}_0(x)$, for some of the typical cases. Although this is physically very different from the "lowest eigenpotential," $u_0(r)$ of Eq. (16), both $V_{\rm eff}(x)$ and $u_0(r)$ [for a plot of $u_0(r)$, see Ref. [2]] have similar nature.

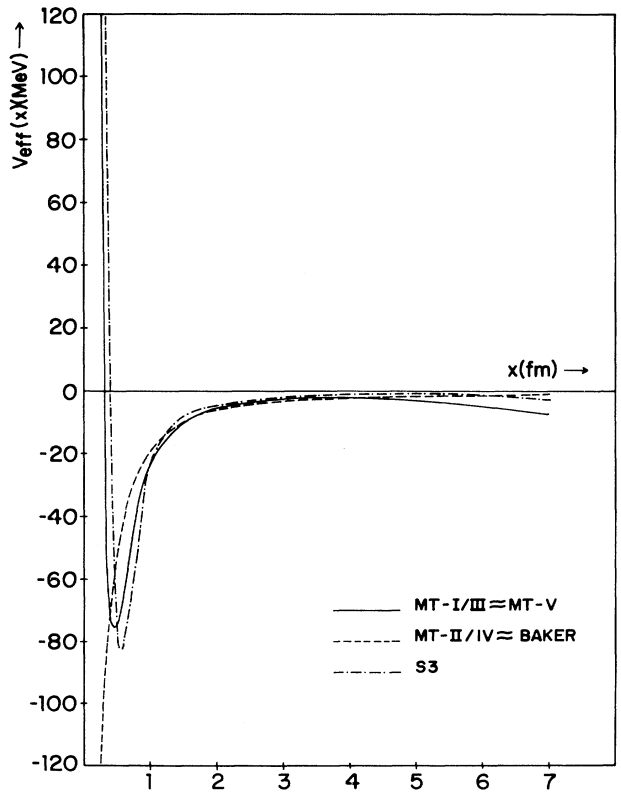

FIG. 2. Plot of the effective potential in x variable, $V_{\rm eff}(x)$, for the BOA, for several two-body potentials. Notice that the graph for MT-I/III is similar and very close to MT-V and does not appear in the figure.

IV. CONCLUSIONS

From the theoretical arguments justifying the approximation, one would expect the BOA to be good when two of the three particles are heavy compared to the third one. However, Fonseca *et al.* [19] profitably used the BOA for the low lying spectrum of ^{9}Be which was treated as a cluster of two α particles and a neutron. Thus it had been demonstrated that the BOA is useful even when the heavy to light particle mass ratio is ≈ 4. In the present work, we have been able to push this ratio to 1. Our calculations demonstrate that, at least for potentials with very soft cores, the BOA is reasonably good even in nuclear problems, where the three particles are of the same mass and interact via the same two-body interactions. The UAA, which is expected to be good in nuclear problems, is of course better, but the BOA is not much worse than the EAA, which from a mathematical point of view should be compared with the BOA.

Although EAA and BOA are similar in spirit and based on adiabatic approximations, they are fundamentally distinct. The EAA (or in general the HAA) is derived in a hyperspherical space, incorporating $O(3N-3)$ symmetry while BOA is conceived in an independent-particle coordinate, with $O(3)\times\cdots\times O(3)$

symmetry. As a result, they lead to different equations [the final equations have some resemblance; see for instance Eqs. (17), (18), and (25)–(27)], giving in general $\epsilon_{EAA} \neq \epsilon_{BOA}$. The richness of HAA is its simpler mathematical structure and the possibility to achieve in a simple and systematic way, higher-order accuracy, such as obtained from UAA and CAA. It is also important to mention that in order to obtain EAA and UAA we need only to solve a simple ordinary differential equation, while for BOA, we need to solve a coupled system of partial differential equations without necessarily furnishing better results.

It is important to note that in the BOA, the symmetry demanded from the physics of the problem is broken. Thus the total angular momentum is no more conserved properly. Note that the y equation of the BOA [Eq. (33)] does not conserve l_y, while l_x has been taken to be zero. Thus total $\mathbf{L}=l_x+l_y$ is not conserved. Furthermore, in the BOA, the imposition of the Pauli principle (antisymmetry of the full wave function under exchange of any pair) has been disregarded. In the HAA approach, both of these are properly satisfied, since the hyperspherical expansion basis is chosen appropriately and the adiabatic approximation is introduced only at a later stage, without disturbing these symmetries. In the light of this discussion, it is not surprising then that the HAA gives such a good agreement with the exact results, but the more intriguing question is why the BOA, which does not satisfy symmetry requirements and also lacks the usual arguments in favor of its applicability for the nuclear problems, fares not too badly in the nuclear case. A possible explanation of this phenomenon lies in the fact that for very soft core potentials, the contribution to the total wave function of the $l_x=l_y=0$ component is dominant. This component conserves the total angular momentum ($L=0$) and also has the appropriate symmetry.

In conclusion, we note that the BOA, although originally conceived for molecular problems, produces reasonably good results in the trinucleon, when the two-body interaction has a sufficiently soft core and the nuclear system has a strong binding. In such cases the BOA might serve as a valuable starting point for more accurate calculations.

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