Adiabatic approximation in atomic three-body systems

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We investigate the reliability of the adiabatic approximation in the hyperspherical harmonics formalism. It has been applied to a number of two-electron systems, both compact and loosely bound, with the interaction between the constituent particles being purely Coulombic. The results are compared with the exact ones obtained by solving the set of coupled differential equations numerically. The accuracy of this approximation for two-electron systems is compared with that for systems with nuclear interactions, and we find that the former is better. An explanation has been provided for better agreement with Coulombic systems, particularly for noncompact ones. [S1050-2947(97)07508-2]

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I. INTRODUCTION

Few-body problems in molecular, atomic, or nuclear systems are of special interest, since exact or near exact *ab initio* calculations are possible, which can shed light on the interactions and structure of such systems. With the choice of a suitable expansion basis, the Schrödinger equation reduces to an infinite set of coupled differential equations or equivalently an infinite-dimensional matrix eigenvalue equation. For practical purposes, the expansion basis is truncated, leading to a finite set of equations. Unfortunately the convergence trend is quite slow in most cases of physical interest (especially for long-range forces), so that for a sufficiently accurate calculation, one has to deal with a large number of coupled differential equations (CDE). Although numerical algorithms exist for solving a finite set of CDE up to a predetermined precision [1], numerical instabilities set in if the number (M) of coupled equations increases beyond 50. Besides, the computer time and memory requirements for such algorithms increase enormously as M increases. Thus for high precision, there are formidable computational difficulties. The situation can be salvaged by invocation of the adiabatic approximation [2], which drastically reduces the number of coupled equations, while taking almost the full effect of the M coupled equations. It is then important to study the accuracy and reliability of this approximation and the conditions for its applicability. Depending on the answer and the nature of the system under consideration, one can then make a choice between solving a relatively smaller set of CDE exactly and using the adiabatic approximation to a considerably larger set of CDE for the same computational facility available.

The adiabatic approximation, as the name implies, separates two or more motions adiabatically. In the hyperspherical harmonics expansion method (Sec. II), the hyper-angular motion is separated adiabatically from the hyperradial (ρ) motion [2], assuming the latter to be much slower than the former. This corresponds to diagonalizing the potential matrix for a fixed value of ρ to obtain the eigenpotential, and then solving one uncoupled differential equation with this eigenpotential, obtained as a parametric function of ρ (Sec. III). The computation labor is thus reduced considerably compared to solving the full set of CDE numerically. Hence the approximation is particularly useful when the rate of convergence is slow.

In this communication, we study the application of hyperspherical adiabatic approximation (HAA) to Coulombic three-body systems and compare it with the application to nuclear systems. We find the HAA to be unexpectedly reliable in the Coulomb case, including the systems that are not sufficiently compact. An attempt has been made to understand why the HAA works so well in diverse Coulombic systems.

The HAA has been used for nuclear three-body problems and compared with the corresponding exact results for a number of S-projected nucleon-nucleon potentials [2,3], realistic potentials [4], and also for the nuclear three-body force [5]. In all these cases it has been seen that the error in binding energy (BE) ranges from about 0.3% for the softest, smooth potentials without a repulsive core to about 4% for the potentials with a strong soft core repulsion. It was shown that the adiabatic approximation is expected to be reliable when the potential changes slowly as a function of its argument [3]. Thus it is not surprising that in nuclear applications, the HAA fares surprisingly well for the softest potentials having a gradual dependence on its argument, as the Baker potential [6], which has a pure Gaussian form. On the basis of this argument, one would not expect the HAA to be reliable for atomic systems, where the Coulomb potential has singularities as the interparticle separations go to zero. A singularity persists even in hyperspace as the global length vanishes. But straightforward HAA calculations for the ground states of various Coulombic systems show (see Sec. IV) that not only is the HAA applicable to such systems, but it produces results that are comparable in precision with the softest nuclear potentials. Furthermore, it is of interest to study how the HAA fares in relation to the compactness of the Coulombic system. Convergence of the hyperspherical expansion is slow for Coulombic bound systems, since the Coulomb force is a long-ranged one. For systems that are not sufficiently compact and extends to great global lengths (ρ), the convergence of hyperspherical expansion is even slower. At first thought, it may appear that the HAA would be worse for such systems. We have studied two such noncompact Coulombic systems (Ps^- and the first excited $^1S^e$ state of a

helium atom) and found that the HAA is quite reliable for such systems as well.

Several authors [7] have applied the hyperspherical adiabatic approximation to Coulombic three-body systems to calculate the ''channel'' potential, channel functions, BE, etc. Earlier, the adiabatic approximation was used for the singly and doubly excited states of atoms [8]. Although the convergence rate is quite slow (which is a typical feature of hyperspherical harmonic expansion), introduction of a correlation function or hydrogenic basis function in the asymptotic region in the wave function and a subsequent hyperspherical harmonics expansion produces very fast convergence and an excellent result for BE, as compared to accurate variational results [9,10]. However, no comparison of the HAA result is made with the corresponding exact one for the same number of hyperspherical partial waves. Thus earlier applications of HAA to Coulombic systems, although quite extensive, did not focus their attention on the accuracy of the HAA *vis à vis* the exact result and an attempt to understand the unexpected reliability of the approximation. It is our endeavor in this work to provide an explanation for this unexpected reliability in atomic systems as compared to nuclear systems.

In Sec. II, we briefly review the hyperspherical harmonic expansion method. In Sec. III, the hyperspherical adiabatic approximation is introduced. Applications to Coulombic three-body systems and conclusions are presented in Sec. IV.

II. HYPERSPHERICAL HARMONICS EXPANSION

In the hyperspherical harmonics approach for an N-particle system, the $(N-1)$ Jacobi vector coordinates, defining the relative motions are

$$\vec{\xi}_i = a_i \left[\vec{r}_{i+1} - \left(\frac{\sum_{j=1}^{i} m_j \vec{r}_j}{\sum_{j=1}^{i} m_j} \right) \right] \quad (i=1,\, N-1), \tag{1}$$

and the center-of-mass coordinate is

$$\vec{R} = \frac{\sum_{i=1}^{N} m_i \vec{r}_i}{\mathcal{M}}, \tag{2}$$

where $\mathcal{M} = \Sigma_{i=1}^{N} m_i$ and m_i, $\vec{r}_i$ are the mass and the position vector of the ith particle. The mass-dependent constants a_i are so chosen that the Jacobian of the transformation (1) and (2) is unity and

$$\sum_{i=1}^{N} \frac{1}{m_i} \nabla_{r_i}^2 = \frac{1}{\mathcal{M}} \nabla_R^2 + \frac{1}{\mu} \sum_{i=1}^{N-1} \nabla_{\xi_i}^2. \tag{3}$$

The quantity μ is an effective-mass parameter obtained in terms of the individual masses of the particles. The structure of Eq. (3) shows that the center-of-mass motion is properly separated and the relative motion of the interacting particles is described by the Schrödinger equation in terms of the relative Jacobi coordinate $\vec{\xi}_i$ $(i=1,N-1)$.

$$\left[-\frac{\hbar^2}{2\mu} \sum_{i=1}^{N-1} \nabla_{\xi_i}^2 + \sum_{i<j=2}^{N} V_{ij} - E \right] \Psi(\vec{\xi}_1,\ldots,\vec{\xi}_{N-1}) = 0. \tag{4}$$

We next introduce the hyperspherical variables in the following manner. Define the hyperradius (ρ) as

$$\rho = \left[\sum_{i=1}^{N-1} \xi_i^2 \right]^{1/2}, \tag{5}$$

which is invariant under three-dimensional rotations as well as under all permutations of the indices of N particles. In addition, $(N-2)$ angular variables, ϕ_i $[i=2,3,\ldots,(N-1)]$ are defined in terms of ρ and the lengths of $(N-1)$ Jacobi coordinates $\vec{\xi}_i$ $(i=1,N-1)$ according to

$$\begin{aligned}
\xi_{N-1} &= \rho \cos \phi_{N-1}, \\
\xi_{N-2} &= \rho \sin \phi_{N-1} \cos \phi_{N-2}, \\
\xi_{N-3} &= \rho \sin \phi_{N-1} \sin \phi_{N-2} \cos \phi_{N-3}, \\
&\vdots \\
\xi_2 &= \rho \sin \phi_{N-1} \sin \phi_{N-2} \cdots \sin \phi_3 \cos \phi_2, \\
\xi_1 &= \rho \sin \phi_{N-1} \sin \phi_{N-2} \cdots \sin \phi_3 \sin \phi_2 \quad (\phi_1 \equiv 0).
\end{aligned} \tag{6}$$

Note that the transformation (6) automatically satisfies Eq. (5). The angle variables, $\phi_2,\ldots,\phi_{N-1}$, together with $2(N-1)$ ordinary polar angles (θ_i,φ_i) of $\vec{\xi}_i$ $(i=1,\ldots,N-1)$ constitute a set of $(3N-4)$ ''hyperangles,'' collectively denoted by Ω:

$$\{\Omega\} \rightarrow \{\phi_2,\phi_3,\ldots,\phi_{N-1},(\theta_1,\varphi_1),(\theta_2,\varphi_2),\ldots,(\theta_{N-1},\varphi_{N-1})\}. \tag{7}$$

In terms of the hyperspherical variables (ρ,Ω), Eq. (4) takes the form

$$\left[-\frac{\hbar^2}{2\mu} \left\{ \frac{1}{\rho^n} \frac{\partial}{\partial \rho} \left(\rho^n \frac{\partial}{\partial \rho} \right) + \frac{\hat{\mathcal{K}}^2(\Omega)}{\rho^2} \right\} + V(\rho,\Omega) - E \right] \Psi(\rho,\Omega) = 0, \tag{8}$$

where $n=(3N-4)$ and $\hat{\mathcal{K}}^2(\Omega)$ is the square of the hyperangular momentum operator expressed in terms of the hyperangles. An expression for the operator can be found in Ref. [11]. The potential $V(\rho,\Omega)$ in Eq. (8) is the total interaction potential of Eq. (4) expressed in terms of ρ and Ω. For the expansion of the wave function, the basis is chosen as the complete set of hyperspherical harmonics (HH), $\{\mathcal{Y}_{K\alpha}(\Omega)\}$, which are the eigenfunctions of $\hat{\mathcal{K}}^2(\Omega)$:

$$\hat{\mathcal{K}}^2(\Omega)\mathcal{Y}_{K\alpha}(\Omega) = K(K+3N-5)\mathcal{Y}_{K\alpha}(\Omega), \tag{9}$$

where K is the hyperangular momentum quantum number [which is also the degree of the homogeneous harmonic polynomials, $\rho^K \mathcal{Y}_{K\alpha}(\Omega)$, in the Cartesian components of $\vec{\xi}_i$ $(i=1,\ldots,N-1)$] and α represents a set of $(3N-5)$ quantum

numbers. The set (K,α) together constitute $(3N-4)$ quantum numbers, associated with $(3N-4)$ hyperangular degrees of freedom. Complete analytical expressions for the HH can be found in Ref. [11]. The wave function Ψ is expanded in the complete set of HH,

$$\Psi(\rho,\Omega)=\sum_{K,\alpha}\rho^{-(3N-4)/2}\mathcal{U}_{K\alpha}(\rho)\mathcal{Y}_{K\alpha}(\Omega). \tag{10}$$

The factor $\rho^{-(3N-4)/2}$ is included so as to remove the first derivative term. Substitution of Eq. (10) in Eq. (8) and use of Eq. (9) result in a set of CDE in the hyperradial variable:

$$\left[-\frac{\hbar^2}{2\mu}\left\{\frac{d^2}{d\rho^2}-\frac{\mathcal{L}_K(\mathcal{L}_K+1)}{\rho^2}\right\}-E\right]\mathcal{U}_{K\alpha}(\rho)+\sum_{K'\alpha'}\langle K\alpha|V|K'\alpha'\rangle\mathcal{U}_{K'\alpha'}(\rho)=0, \tag{11}$$

where $\mathcal{L}_K=K+3(N-2)/2$ and

$$\langle K\alpha|V|K'\alpha'\rangle=\int\mathcal{Y}^*_{K\alpha}(\Omega)V(\rho,\Omega)\mathcal{Y}_{K'\alpha'}(\Omega)d\Omega \tag{12}$$

is the coupling matrix element.

Since ρ is invariant under three-dimensional rotations and permutations, the expansion basis of HH in Eq. (10) is chosen with appropriate symmetry required by the identity and nature of the interacting particles. Often this can easily be incorporated by restricting the set $\{\alpha\}$ to an appropriate subset. Furthermore, total angular momentum (for spin-dependent interactions) or total orbital angular momentum (for spin-independent interactions) is a good quantum number and restricts the set $\{\alpha\}$ further.

For a tractable calculation, the expansion, Eq. (10) is truncated to a maximum number (M) of terms leading to a finite set (M) of CDE in Eq. (11). The solution of this system of CDE, subject to appropriate boundary conditions on the partial waves, $\mathcal{U}_{K\alpha}(\rho)$, to determine the energy E and $\mathcal{U}_{K\alpha}(\rho)$, is a formidable numerical task. The numerical algorithm to solve Eq. (11) requires a large memory that increases as M^2. Sufficiently accurate calculation also takes a large CPU time, which increases as M^3. The truncation in the expansion basis is determined by the requirement of convergence in E up to a predetermined accuracy. The rate of convergence depends on the nature of the potential. It is fast for a short-ranged potential (e.g., in nuclear problems) and M is relatively small. But for a long-ranged potential (e.g., Coulomb potential in atomic and other Coulombic systems), the convergence is extremely slow and the value of M may run into three figures. The exact numerical solution of such a large system of CDE is a very tough numerical job. For this reason an approximate but sufficiently accurate solution of the truncated CDE is desirable.

III. HYPERSPHERICAL ADIABATIC APPROXIMATION

A reduction of the set of CDE, Eq. (11), is provided by the hyperspherical adiabatic approximation method. This approximation scheme reduces the set of M coupled differential equations to a single (or at most a few coupled) differential equation(s). The physical picture underlying the HAA is the assumption that the hyperangular motion involving the $(3N-4)$ hyperangular variables (Ω) is fast compared to the hyperradial motion in terms of the hyperradial variable (ρ), and the former can be adiabatically separated from the latter. However, it is difficult to visualize the complete hyperangular motion. While one might expect the angular motion described by the polar angles $\{(\theta_i,\varphi_i),i=1,\ldots,N-1\}$ to be fast compared to the hyperradial motion (corresponding to breathing modes), it is not intuitively obvious why the hyperangular motion described by $\{\phi_i,i=2,\ldots,N-2\}$ is likely to be fast also. The HAA has the same adiabatic nature as in the Born-Oppenheimer approximation (BOA) [12], although in applications of BOA to molecular problems, the physical reason for the adiabatic decoupling of the motions is quite apparent, namely, that the motion of heavy nuclei is expected to be slow compared to the fast motion of the light electrons. Nevertheless, the HAA is applicable to both nuclear and atomic mass ratio limits and in fact is *better* than the BOA in both limits, for the same smooth potential [13].

In the adiabatic approximation procedure, one first solves an associated $M\times M$ matrix eigenvalue equation:

$$\sum_{K'\alpha'}\mathcal{M}_{K\alpha,K'\alpha'}(\rho)\mathcal{X}_{K'\alpha',\lambda}(\rho)=\omega_\lambda(\rho)\mathcal{X}_{K\alpha,\lambda}(\rho), \tag{13}$$

where

$$\mathcal{M}_{K\alpha,K'\alpha'}(\rho)=\frac{\hbar^2}{2\mu}\frac{\mathcal{L}_\mathcal{K}(\mathcal{L}_\mathcal{K}+1)}{\rho^2}\delta_{K\alpha,K'\alpha'}+\langle K\alpha|V|K'\alpha'\rangle \tag{14}$$

for each value of ρ, to obtain the eigenvalue $\omega_\lambda(\rho)$ and the corresponding eigenvector $\mathcal{X}_{K\alpha,\lambda}(\rho)$ as parametric functions of ρ. For a fixed value of ρ, Eq. (13) is equivalent to the matrix formulation of the hyperangular motion and $\mathcal{X}_{K\alpha,\lambda}(\rho)$ are the corresponding eigenfunctions. Considering M partial waves $\mathcal{U}_{K\alpha}(\rho)$ to form an M-component column vector, one can expand it in the set of M eigencolumn vectors $\{\mathcal{X}_{K\alpha,\lambda}(\rho),\lambda=1,\ldots,M\}$ of the matrix $\mathcal{M}_{K\alpha,K'\alpha'}(\rho)$ for a given parametric value of ρ:

$$\mathcal{U}_{K\alpha}(\rho)=\sum_\lambda\zeta_\lambda(\rho)\mathcal{X}_{K\alpha,\lambda}(\rho). \tag{15}$$

Substituting Eq. (15) in Eq. (11), making use of Eq. (13), and taking the inner product with $\mathcal{X}^*_{K\alpha,\lambda}(\rho)$ we have

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{d\rho^2}+\omega_\lambda(\rho)+A_\lambda(\rho)-E\right]\zeta_\lambda(\rho)-\sum_{\lambda'(\neq\lambda)}\left[B_{\lambda,\lambda'}(\rho)\zeta_{\lambda'}(\rho)+C_{\lambda,\lambda'}(\rho)\frac{d\zeta_{\lambda'}(\rho)}{d\rho}\right]=0, \tag{16}$$

where

$$A_\lambda(\rho)=\frac{\hbar^2}{2\mu}\sum_{K\alpha}\left|\frac{d\mathcal{X}_{K\alpha,\lambda}(\rho)}{d\rho}\right|^2, \tag{17}$$

$$B_{\lambda,\lambda'}(\rho)=\frac{\hbar^2}{2\mu}\sum_{K\alpha}\mathcal{X}^*_{K\alpha,\lambda}(\rho)\frac{d^2\mathcal{X}_{K\alpha,\lambda'}(\rho)}{d\rho^2}, \tag{18}$$

and

$$C_{\lambda,\lambda'}(\rho)=\frac{\hbar^2}{\mu}\sum_{K\alpha}\mathcal{X}^{*}_{K\alpha,\lambda}(\rho)\,\frac{d\mathcal{X}_{K\alpha,\lambda'}(\rho)}{d\rho}. \tag{19}$$

In the derivation of Eq. (16) use has been made of the orthonormality of the eigenvectors of Eq. (13), for each value of ρ:

$$\sum_{K\alpha}\mathcal{X}^{*}_{K\alpha,\lambda}(\rho)\mathcal{X}_{K\alpha,\lambda'}(\rho)=\delta_{\lambda,\lambda'}. \tag{20}$$

There is no approximation in Eq. (16). The uncoupled adiabatic approximation (UAA) consists of dropping the coupling terms of Eq. (16):

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{d\rho^2}+\omega_\lambda(\rho)+\frac{\hbar^2}{2\mu}\sum_{\alpha}\left|\frac{d\mathcal{X}_{K\alpha,\lambda}(\rho)}{d\rho}\right|^2-E\right]\zeta_\lambda(\rho)=0, \tag{21}$$

which results in an uncoupled differential equation for each ''channel'' λ. The ground-state energy (E) is obtained by choosing the ''lowest eigenpotential'' $\omega_0(\rho)$ as a parametric function of ρ and solving Eq. (21) for $\lambda=0$. The approximate partial waves, corresponding to the ground state, are given by

$$\mathcal{U}_{K\alpha}(\rho)\approx\zeta_0(\rho)\mathcal{X}_{K\alpha,0}(\rho). \tag{22}$$

Dropping further the third term in Eq. (21), one has the extreme adiabatic approximation (EAA), which corresponds to the additional assumption that $\mathcal{X}_{K\alpha,\lambda}(\rho)$ is independent of ρ. Retaining a few of the coupling terms [corresponding to the lowest eigenvalues $\omega_\lambda(\rho)$] in Eq. (16) one has the coupled adiabatic approximation (CAA). The exact ground-state energy and the energy obtained by the three levels of the adiabatic approximation satisfy a basic inequality [14]:

$$E_{\rm EAA}\leqslant E_{\rm exact}\leqslant E_{\rm CAA}\leqslant E_{\rm UAA}, \tag{23}$$

where the subscript indicates the particular approximation or exact result.

IV. APPLICATIONS TO COULOMBIC THREE-BODY SYSTEMS

We have applied the HAA procedure to a number of Coulombic three-body systems: (a) ground states of two electron atoms (H^-,He,Li^+,Be^{2+},B^{3+}) and the first excited $^1S^e$ state of a He atom, in each of which the nuclear motion has been disregarded; (b) ground states of the positronium negative ion (Ps^-) consisting of three light equal mass particles ($e^-e^+e^-$) and the muonium ion ($ee\mu$). In these cases, the motion of the third dissimilar particle cannot be neglected and has been properly accounted for by separating the center-of-mass motion.

In these applications, we have chosen systems with widely varying mass ratios of the constituent particles. The interaction is purely Coulombic and the ρ dependence of $\langle K\alpha|V|K'\alpha'\rangle$ factors out as $1/\rho$. For the systems, consisting of two electrons (particles numbered 1 and 2) and a third dissimilar particle having a comparable mass and a charge $+Ze$, the total interaction potential is

$$V=\frac{e^2}{\xi_1/a_1}-Ze^2\left(\frac{1}{|\vec{\xi}_2/a_2-(\vec{\xi}_1/a_1)m_2/(m_1+m_2)|}+\frac{1}{|\vec{\xi}_2/a_2+(\vec{\xi}_1/a_1)m_1/(m_1+m_2)|}\right), \tag{24}$$

where

$$a_1=\left(\frac{m_1m_2M}{m_3}\right)^{1/4}\frac{1}{(m_1+m_2)^{1/2}},\qquad a_2=\frac{1}{a_1}. \tag{25}$$

The wave function must be antisymmetric under the exchange of the two electrons. Hence if the electrons are in the spin singlet (triplet) state, then l_1 [l_i is the orbital angular momentum associated with $\vec{\xi}_i$ motion ($i=1,2$)] should be an even (odd) integer. Since the third particle is distinct, there is no other symmetry requirement. The set of quantum numbers α is constituted by $\{l_1,l_2,L,M\}$, where L and M are the orbital angular momentum of the system and its projection, respectively, $\vec{L}=\vec{l}_1+\vec{l}_2$ and $K=l_1+l_2+2n$, n being a nonnegative integer. For the ground and the $^1S^e$ excited states, $L=0$ and $l_1(=l_2)$ takes only even values $\leqslant K/2$, K being an even integer.

In Table I, we present the binding energy ($-E$) calculated by UAA and compare it with the exact result [15] [obtained by solving Eq. (11) without approximation by the renormalized Numerov method [1]] for a few typical $K_{\rm max}$ values [$K_{\rm max}$ is the maximum value of K used in the truncated expansion, Eq. (10)]. It is seen that the calculated energies satisfy the inequality (23) in all cases. A common feature for the ground states of all the systems studied is that the error in UAA gradually increases with $K_{\rm max}$, and the error for the extrapolated BE [15] is slightly more than that for the largest $K_{\rm max}$ used for the extrapolation. This is not surprising since for larger $K_{\rm max}$, a larger number of CDE's are approximated by *only one* uncoupled differential equation. One further notices from Table I that the absolute error in the extrapolated BE increases with Z, while among the three $Z=1$ systems studied, H^- and muonium have comparable errors, but Ps^- has a markedly smaller error. Since the BE increases rapidly with Z, the relative error does not change much, varying from 0.26% (for Ps^- and Li^+) to 0.42% (for B^{3+}). The relative error is also quite small (0.28%) for the first excited state of the helium atom.

It is interesting to compare the relative errors with those for the trinucleon system interacting via short-range forces [16]. The relative error in UAA depends strongly on the nature of the potential: 0.27% for the smoothly varying Baker potential [6] having no repulsive part, 0.66% for the Volkov potential [17] having a soft smooth repulsive core, and 3.22% for Afnan-Tang S3 potential [18], which has a fairly strong soft core repulsion at short separations. None of these potentials has any singularity. But the peak value of the derivative of the potential (with respect to its argument) is

TABLE I. BE of atoms and ions obtained by UAA and exact HHEM.

Atom	K_{max}	BE (a.u.) UAA	BE (a.u.) Exact	Error in BE for $K_{max}=20$	Extrapolated BE (a.u.) UAA	Extrapolated BE (a.u.) Exact	Error in BE absolute (percentage)
	4	0.480 084	0.480 799				
	8	0.501 179	0.502 585				
H^-	12	0.510 843	0.512 577		0.524 741	0.526 681	0.001 94 (0.35%)
	16	0.515 853	0.517 726				
	20	0.518 812	0.520 737	0.001 925			
	4	2.781 300	2.784 369				
	8	2.844 757	2.850 214				
He	12	2.869 283	2.876 006		2.895 595	2.903 680	0.008 08 (0.28%)
	16	2.880 159	2.887 540				
	20	2.885 847	2.893 580	0.007 733			
	4	7.030 368	7.039 221				
	8	7.162 257	7.175 991				
Li^+	12	7.211 026	7.227 336		7.260 825	7.280 070	0.019 25 (0.26%)
	16	7.232 084	7.249 755				
	20	7.242 885	7.261 233	0.018 348			
	4	13.223 11	13.248 45				
	8	13.449 38	13.482 73		13.612 74	13.656 00	0.043 26 (0.32%)
Be^{2+}	12	13.531 26	13.568 88				
	16	13.566 39	13.606 18				
	20	13.584 09	13.625 08	0.040 99			
	4	21.344 96	21.412 46				
	8	21.691 85	21.770 82				
B^{3+}	12	21.815 97	21.900 98		21.938 82	22.031 92	0.093 10 (0.42%)
	16	21.868 94	21.957 09				
	20	21.895 51	21.985 35	0.089 84			
	4	0.477 778	0.478 188				
	8	0.498 772	0.499 934				
$ee\mu$	12	0.508 387	0.509 934		0.522 545	0.524 626	0.002 08 (0.39%)
	16	0.513 371	0.515 108				
	20	0.516 313	0.518 163	0.001 850			
	4	0.220 598	0.220 937				
	8	0.241 696	0.242 245				
Ps^-	12	0.249 791	0.250 464		0.261 715	0.262 395	0.000 68 (0.26%)
	16	0.253 586	0.254 306				
	20	0.255 986	0.256 723	0.000 737			
	24	0.257 494	0.258 231				
First	4	1.592 168	1.599 267				
excited	8	1.759 054	1.771 541				
$^1S^e$	12	1.864 526	1.878 540		2.133 01	2.138 95	0.005 94 (0.28%)
state	16	1.933 777	1.947 698				
of He	20	1.981 317	1.994 575	0.013 258			

smallest for the slowly varying Baker potential and largest for the strongly varying S3 potential, while it has an intermediate value for the Volkov potential. Thus the observed results are in agreement with the argument [3] that the error in UAA is likely to be large for potentials having a singularity or when its derivative has a large magnitude. On the other hand, the Coulomb potential (24) has singularities when each of the interparticle separation vanishes. The singularity survives in ρ space as $\rho\to 0$. For finite ρ, the potential is a smoothly varying function. It is seen from Table I that the relative errors for the Coulombic systems are comparable to those for the softest and smoothest nuclear potentials (e.g., the Baker potential) and appreciably smaller than those for Volkov or S3 potentials [16]. This calls for a better understanding.

For the Coulombic systems, ρ dependence of $\langle K\alpha|V|K'\alpha'\rangle$ factors out as $1/\rho$ and so from Eq. (14) one sees that $\mathcal{M}_{K\alpha,K'\alpha'}(\rho)$ is approximately proportional to $1/\rho^2$ for small ρ and to $1/\rho$ for large ρ. Whenever $\mathcal{M}_{K\alpha,K'\alpha'}(\rho)$ has its ρ dependence factorizable as $f(\rho)$ times a matrix independent of ρ, Eq. (13) shows that $\omega_\lambda(\rho)$ has the *same* functional dependence on ρ and $\mathcal{X}_{K\alpha,\lambda}(\rho)$ becomes independent of ρ, so that the coupling terms $B_{\lambda\lambda'}(\rho)$ and $C_{\lambda\lambda'}(\rho)$ [Eqs. (18) and (19)] vanish and

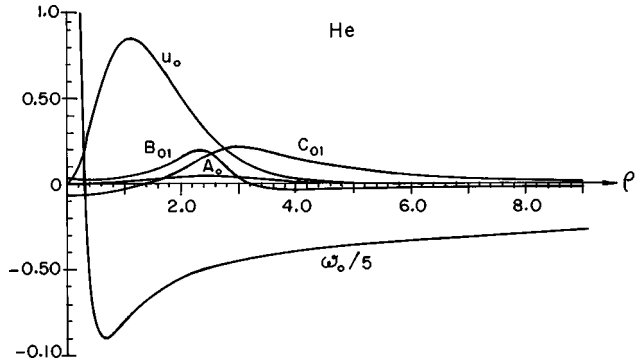

FIG. 1. Plot of $\omega_\lambda(\rho)$, $A_\lambda(\rho)$, $B_{\lambda,\lambda'}(\rho)$, $C_{\lambda,\lambda'}(\rho)$, and $\mathcal{U}_0(\rho)$ in appropriate atomic units (a.u.) against ρ (in a.u.) for the ground state of the helium atom; λ and λ' are chosen to be 0 and 1, respectively. $\omega_0(\rho)$ is properly scaled (as indicated in figure) so as to accommodate all the curves in the same figure; $\mathcal{U}_0(\rho)$ is in arbitrary units.

Eq. (21) becomes exact. Hence the coupling terms in Eq. (16) are small for large and small values of ρ. This is not true for intermediate values of ρ, where both terms of Eq. (14) compete with each other. However, in such regions the Coulomb potential is a smoothly varying function of ρ. Consequently $\mathcal{X}_{K\alpha,\lambda}(\rho)$ is slowly varying. Thus $B_{\lambda\lambda'}(\rho)$ and $C_{\lambda\lambda'}(\rho)$ are expected to be quite small for small and large ρ values and not too large in the intermediate region. Calculated values of $B_{\lambda\lambda'}(\rho)$ and $C_{\lambda\lambda'}(\rho)$ have been plotted against ρ in Fig. 1 for He atom, for $\lambda=0$ and $\lambda'=1$. For comparison we also plot $A_0(\rho)$ and $\omega_0(\rho)$ (suitably scaled to include in the same figure). As expected one finds that both B_{01} and C_{01} become negligibly small for large ρ ($\rho > 5$ a.u.); for $\rho\to 0$, C_{01} is not negligible, although quite small. Both these quantities peak around $\rho=2-3$ a.u., where the hyperradial wave function has already reached its tail part, the peak being at about 1.2 a.u. For comparison a plot of $\mathcal{U}_0(\rho)$ (corresponding to $K=0$, $l_1=0$, $l_2=0$, $L=0$, $M=0$) has also been included in Fig. 1. Smallness of both B_{01} and C_{01} over the entire domain is established by comparing them with $\omega_0(\rho)$. Thus we see that the coupling terms of Eq. (16) are small compared to $\omega_0(\rho)+A_0(\rho)$, which justifies the approximation procedure.

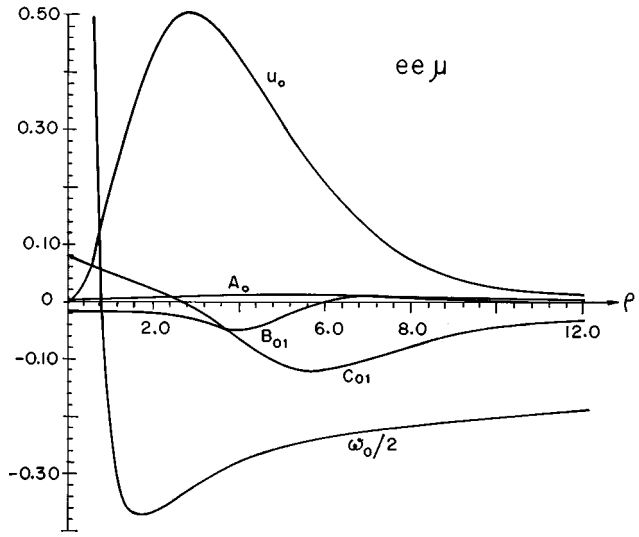

FIG. 2. Plot of the same functions as in Fig. 1 for the ground state of muonium.

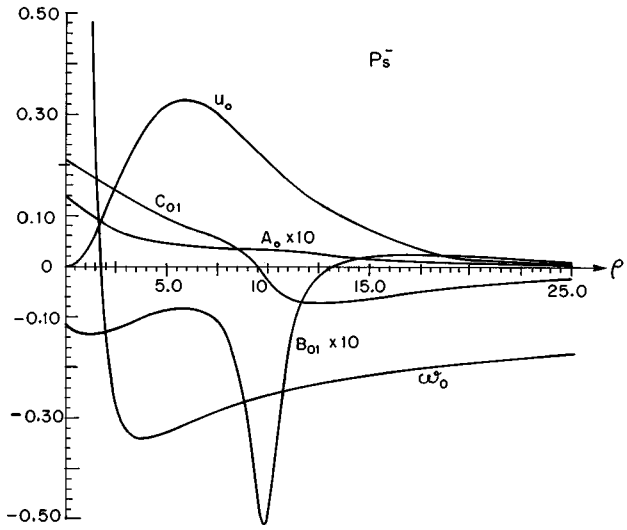

FIG. 3. Plot of the same functions as in Fig. 1 for the ground state of Ps^-. Scaling of $B_{0,1}(\rho)$, $A_0(\rho)$ is as indicated.

In Figs. 2–5 we plot $\omega_0(\rho)$, $A_0(\rho)$, $B_{01}(\rho)$, $C_{01}(\rho)$, and $\mathcal{U}_0(\rho)$ for muonium, Ps^-, B^{3+}, and the first excited state of He, respectively. In each of these cases, we find that the correction and the coupling terms are negligibly small for large ρ and they are peaked in the tail region of the hyperradial wave function (except for B^{3+} and first excited state of helium), the peak value being small compared to $|\omega_0(\rho)|$.

For two electron atoms with large Z, $\omega_0(\rho)$ has a sharp and very deep well located at a relatively smaller value of ρ. Thus the major part of the BE comes from small values of ρ, where $B_{\lambda,\lambda'}$ and $C_{\lambda,\lambda'}$ are not negligible. Hence as Z increases, the absolute error increases. On the other extreme, for Ps^- (Fig. 3), the well is shallow and extends to large ρ values; consequently the hyperradial wave function is not sharply peaked and spreads out to a greater distance. Hence a large contribution to the BE comes from larger ρ values. But the coupling terms are negligible in this region. Hence the absolute error in BE is small in this case. Thus the UAA becomes more reliable for weakly bound systems, whose wave function extends to great global lengths. This is also true for the first excited state of the helium atom.

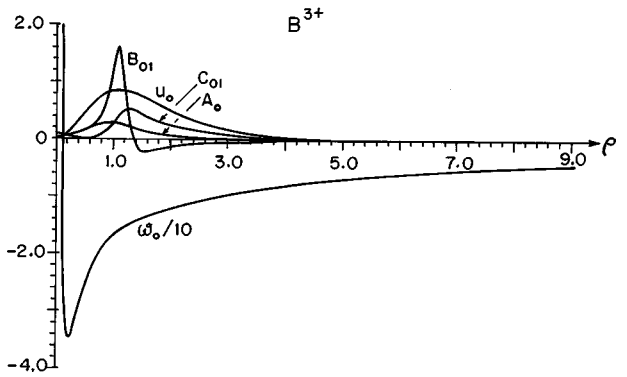

FIG. 4. Plot of the same functions as in Fig. 1 for the ground state of B^{3+}.

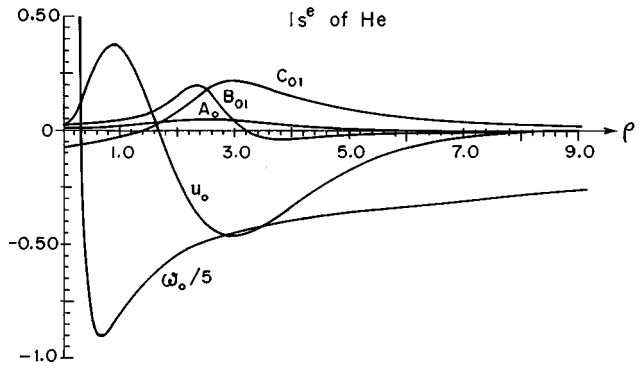

FIG. 5. Plot of the same functions as in Fig. 1 for the first excited state of a helium atom.

We conclude that the adiabatic approximation procedure is well justified for the Coulombic systems, in spite of the fact that the Coulomb force is a long-range force and has a singularity. The reliability is comparable to or better than that for the softest short-range nuclear forces. The error is particularly small in loosely bound systems, which extend to great global lengths. This makes the HAA especially useful in such cases. Since the convergence is very slow for loosely bound and well spread-out systems, an exact convergent calculation involving a large number of partial waves is very time and memory consuming. Using the HAA, which is comparatively more reliable for such systems, one can achieve convergence and a fairly accurate result with only a small fraction of the computational effort. The reason why the HAA works better than expected in Coulombic systems is due to the fact that the potential matrix of the Coulomb interaction alone is proportional to $1/\rho$. Whenever the matrix $\mathcal{M}_{K\alpha,K'\alpha'}(\rho)$ has a factorizable ρ dependence, the HAA becomes exact. Due to the centrifugal term ($\propto\rho^{-2}$), $\mathcal{M}_{K\alpha,K'\alpha'}(\rho)$ does not have an exactly factorizable ρ dependence over the entire interval of ρ even for Coulombic systems. But an approximately factorizable ρ dependence results both for large and small ρ values and a smooth ρ dependence for intermediate ρ values. This makes the coupling terms of Eq. (16) small, resulting in a high reliability of the HAA. By contrast in nuclear system, even the potential matrix alone does not have a factorizable ρ dependence. Consequently the HAA is less accurate for the nuclear systems.

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