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N-body systems in the hyperspherical adiabatic approach

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Abstract A mathematical procedure called hyperspherical adiabatic approach (HAA), is presented to handle the solution of a coupled system of differential equations (finite or not) of Schrödinger type normally generated from N-body physical systems. We investigate the use of HAA in relatively simple but representative cases, in order to emphasize its broad range of applicability. The article derives a useful upper bound/lower bound theorem for the HAA. This proof clarifies a hitherto empirical estimate of the ground state energy based on different versions of the HAA: the extreme adiabatic approximation (EAA), uncoupled adiabatic approximation (UAA) and coupled adiabatic approximation (CAA). We finally discuss the familiar Born-Oppenheimer approximation where a similar inequality appears.

1. Introduction

The Schrödinger equation for a N-body system involving $(N-1)$ relative mass-weighted (Jacobi) coordinates can be written as an infinite set of coupled differential equations (CDE) in terms of a hyperradial variable, r. This system of equations has the form[1]

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

where $v_{\alpha\alpha'}(r)=\left(\frac{2m}{\hbar^2}\right)<y_\alpha|V|y_{\alpha'}>$, $\epsilon=-\left(\frac{2m}{\hbar^2}\right)E$ ($E<0$ for a bound state) and $y_\alpha(\Omega)$ are hyperangular basis functions (α characterizing all the necessary quantum numbers), in the $(3N-4)$ dimensional angular hyperspace (R). For example,

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$\{\mathcal{Y}_\alpha\}$ can be chosen as the hyperspherical harmonics[1]. The numerator of the centrifugal force term of Eq.(1) is related to the eigenvalue of the Casimir operator[1] of the system multiplied by a minus sign. For most few-body problems, the set of CDE for $\{\varphi_\alpha\}$ is a formidable one, even after reasonable truncation. Hence, it is greatly advantageous to further reduce the set. A mathematical scheme, called hyperspherical adiabatic approach (HAA), has been proposed and applied successfully to the three and four nucleon problems[2,3]. In this communication, we try to justify the HAA. The method furnishes a consistent mathematical procedure to reach higher accuracy in the numerical results. To achieve it, one initially starts with the extreme adiabatic approximation (EAA) where only one ordinary differential equation is necessary. The next step for higher accuracy is the uncoupled adiabatic approximation (UAA), also based on the solution of one single differential equation. To achieve even higher accuracy, one needs to solve a few coupled differential equations, whose number is somehow related to the desired accuracy. Certainly this number is still much smaller than that of the original CDE represented by Eq.(1). This approximate version of the HAA is called coupled adiabatic approximation (CAA).

A preliminary version of the HAA was presented earlier[2], but only for the three-body problem. For completeness, an extension for N-body systems[4] is reviewed here. An important point discussed in this work is the general proof of basic inequalitaties,

$$\epsilon_{EAA} \leq \epsilon \leq \epsilon_{CAA} \leq \epsilon_{UAA}, \tag{2}$$

where the binding energies, for a fixed a, are those in the EAA, the CAA and UAA, respectively. The ϵ means the exact result for the given Hamiltonian. The UAA provides an upper bound and EAA provides a lower bound to the ground state energy. This work thus clarifies a hitherto empirical estimate of the ground state energy based on different versions of the HAA (EAA, UAA and CAA). A preliminary proof of these inequalities was given by Ballot-Ripele-Levinger[3]. However, they made use of the approximate concept of the optimal subset making that proof not so general and unnecessarily complicated.

This paper complements ref.(4), with the inclusion of a general proof of the basic inequalities. It also discusses the deuteron, as a good academic illustration of the use of HAA. Two-body physical systems with non-central interactions normally generate a coupled system of differential equations of the form given by Eq.(1). The use of the HAA in such cases is also possible and advantageous. For instance, with the simple deuteron case this can be easily shown. With this example we also discuss how the mathematical nature of the interaction can affect the "goodness" of the various approximations. That can be used as an insight for the trinucleon problem also discussed in this article. Finally, the inclusion of a model system to simulate several physical systems is another important point in this paper. For this purpose, we idealized a simple three-body bound system composed of a distinct and two equal mass particles, interacting only via local pairwise S-wave potentials (Gaussian types) with their depth and range varying. Ground state energies are calculated using the HAA in the nuclear and molecular mass limits. The nuclear situation is simulated when the ratio m of equal to distinct particle mass is of the order of unity. The molecular case is simulated for $m \gg 1$, when the potential between the equal mass particles is switched off. The ratio m was varied between the limits $m = 1$ and $m \gg 1$ and the depths and ranges of the potentials were varied to simulate intermediate situations. In the physics literature there exist other types of adiabatic approximations, such as the classical Born-Oppenheimer approximation (BOA)[5]. We comment on the relation between HAA and BOA.

In section 2, the HAA is presented. In section 3, a proof of the basic inequalities is given. In section 4, numerical results are given for selected physical systems and in section 5, conclusions are outlined.

2. The Hyperspherical Adiabatic Approach

In order to obtain Eq.(1) we start with a wavefunction $\Psi(r,\Omega) = r^{-(3N-4)/2}\psi(r,\Omega)$ for the N-body Schrödinger equation

$$\left[-\frac{d^2}{dr^2} - \frac{\mathcal{L}^2(\Omega)}{r^2} + v(r,\Omega) + \epsilon\right]\psi(r,\Omega) = 0, \tag{3}$$

after elimination of the centre of mass. The operator $\mathcal{L}^2$ is given by[1]

$$\mathcal{L}^2(\Omega) = K^2(\Omega) - (3N-4)(3N-6)/4, \tag{4}$$

where $K^2(\Omega)$ is the Casimir operator of the system[1,4]. Expanding $\psi(r,\Omega)$ in a complete orthonormal set $\{\mathcal{Y}_\alpha(\Omega)\}$,

$$\psi(r,\Omega) = \sum_\alpha \varphi_\alpha(r)\mathcal{Y}_\alpha(\Omega), \tag{5}$$

and multiplying Eq.(3) from the left by $\mathcal{Y}^*_{\alpha'}(\Omega)$ and integrating over $d\Omega$, we obtain Eq.(1).

In the HAA procediire, an associated matrix eigenvalue equation (for a fixed *r)* is constructed as follows:

$$U(r,\Omega)\Phi_\lambda(r,\Omega) \equiv \left[-\frac{\mathcal{L}^2}{r^2} + v(r,\Omega)\right]\Phi_\lambda(r,\Omega) = u_\lambda(r)\Phi_\lambda(r,\Omega). \tag{6}$$

We can also expand $\Phi_\lambda(r,\Omega)$ in a complete orthonormal set $\{\mathcal{Y}_\alpha(\Omega)\}$,

$$\Phi_\lambda(r,\Omega) = \sum_\alpha \chi_{\alpha\lambda}(r)\mathcal{Y}_\alpha(\Omega), \tag{7}$$

and we obtain a simpler equation,

$$\sum_{\alpha'} U_{\alpha\alpha'}(r)\chi_{\alpha'\lambda}(r) = u_\lambda(r)\chi_{\alpha\lambda}(r), \tag{8}$$

with

$$U_{\alpha\alpha'}(r) = \frac{\Lambda_\alpha(\Lambda_\alpha+1)}{r^2}\delta_{\alpha\alpha'} + v_{\alpha\alpha'}(r), \tag{9}$$

which is solved to obtain the eigenvalues, $u_\lambda(r)$, and the eigenvectors, $\chi_{\alpha\lambda}(r)$, as parametric functions of r. Expanding now $\varphi_\alpha(r)$ in the complete orthonormal set $\{\chi_{\alpha\lambda}(r)\}$,

$$\varphi_\alpha(r) = \sum_\lambda \varsigma_\lambda(r)\chi_{\alpha\lambda}(r), \tag{10}$$

and substituting into Eq.(1), we finally obtain

$$\left[-\frac{d^2}{dr^2} + (u_\lambda(r) + \sum_\alpha |\frac{d\chi_{\alpha\lambda}}{dr}|^2) + \epsilon\right]\varsigma_\lambda(r) - \sum_{\lambda'(\lambda'\neq\lambda)} C_{\lambda\lambda'}(r) = 0, \tag{11}$$

where

$$C_{\lambda\lambda'}(r) = \left[2P_{\lambda\lambda'}(r)\frac{d}{dr} + Q_{\lambda\lambda'}(r)\right]\varsigma_{\lambda'}(r). \tag{12}$$

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

$$P_{\lambda\lambda'}(r) = < \chi_\lambda|\chi'_{\lambda'} > = \sum_\alpha \chi^*_{\alpha\lambda}(r)\frac{d\chi_{\alpha\lambda'}(r)}{dr},$$

$$Q_{\lambda\lambda'}(r) = < \chi_\lambda|\chi''_{\lambda'} > = \sum_\alpha \chi^*_{\alpha\lambda}(r)\frac{d^2\chi_{\alpha\lambda'}(r)}{dr^2}. \tag{13}$$

The potential curves, $u_\lambda(r)$, similar to the molecular curves, contain essential information about the structure of the N-body system. When the derivatives of $\chi_{\alpha\lambda'}$ with respect to r are small, we expect to generate nearly decoupled equations. It results that the coupling terms, $C_{\lambda\lambda'}$(r), are small[4,6]. If truncation is performed in the system of equations (Eq.(11)), we get the coupled adiabatic approximation (CAA). Neglecting the coupling terms, in Eq.(11), we have the UAA,

$$\left[-\frac{d^2}{dr^2} + (u_\lambda(r) + \sum_\alpha |\frac{d\chi_{\alpha\lambda}}{dr}|^2) + \epsilon_{UAA}\right]\varsigma_\lambda(r) = 0. \tag{14}$$

The neglect of $\sum_a |\chi'_{\alpha\lambda}|^2$ in Eq.(14) leads to the EAA. We are able to define[4] a meaningful positive dimensionless parameter,

$$\delta = \left|u_\lambda(r_{min})/(u_{\lambda'}(r_{min}) - u_\lambda(r_{min}))\right|,$$

where r_{min} is the value of r at which $u_\lambda(r)$ has a minimum, that, together with the geometrical nature of the eigenpotential (u_λ(r)) plots, indicates the "goodness" of UAA. We found that only physical systems with no rapidly varying potentials, which generate smooth and well separated eigenpotentials, and in addition the condition $6 \ll 1$, make the UAA a good approximation scheme.

3. The Basic Inequalities

We can prove that the basic inequalities,

$$\epsilon_{EAA} \leq \epsilon \leq \epsilon_{CAA} \leq \epsilon_{UAA}, \tag{15}$$

hold for the ground state energies, for a given a, in the EAA, the CAA and the UAA, respectively. The inequalities for c, ϵ_{CAA} and ϵ_{UAA} follow immediately from the variational principle. By variational principle we mean here variational treatment of an integral expression such as $< \varphi|H - E|\varphi >$, where H is the Hamiltonin of the system. It remains to prove that $\epsilon_{EAA} \leq$ c. For that purpose, let us assume that the exact solution of Eq.(3), $\psi_x(r,\Omega)$, is known and for convenience is expanded in the complete set $\{\mathcal{Y}_\alpha(\Omega)\}$,

$$\psi_x(r,\Omega) = \sum_\alpha \varphi_{\alpha x}(r)\mathcal{Y}_\alpha(\Omega), \tag{16}$$

or equivalently, according to Eq.(10),

$$\varphi_{\alpha x}(r) \equiv \zeta_x(r)\chi_{\alpha x}(r), \tag{17}$$

where x labels the exact solution.

By substitution into Eq.(1), we obtain

$$\left[-\frac{d^2}{dr^2} + (u_x(r) + \sum_\alpha |\frac{d\chi_{\alpha x}}{dr}|^2) + \epsilon\right]\zeta_x(r) = 0, \tag{18}$$

where $u_x(r)$ is the eigenpotential in which $\lambda \to x$. Let us label $\lambda = 0$ the ground state. Clearly $u_0(r) < u_x(r)$ since $\chi_{\alpha 0}(r)$ is associated with the lowest eigenpotential $u_0(r)$. Therefore, the equation for the EAA, namely

$$\left[-\frac{d^2}{dr^2} + u_0(r) + \varepsilon_{EAA}\right]\zeta_0(r) = 0, \tag{19}$$

when compared with Eq.(18), implies the inequality $\varepsilon_{EAA} \leq \varepsilon$. Thus, the EAA provides a lower limit to the binding energy of the ground state. Hence, the basic inequalities are proved. The TJAA provides an upper boud to the ground state energy, while EAA provides a lower bound. A proof of these inequalities was

first discussed by Ballot, Fabre de la Ripelle and Levinger[3]. For that purpose, the authors used the approximate concept of the optimal subset, which made the proof unnecessarily complex and not so general.

4. Results

We applied the HAA and its different approximate versions (EAA, UAA and CAA) to simple well-chosen few-body systems, in order to extract insights into the criteria of validity of this approach. We start with a simple case in nuclear physics: the deuteron. For completeness, we also give results for triton, as a realistic calculation in nuclear physics. Following it, we idealized a model system to simulate various cases in physics.

Nuclear Scale

In the nuclear scale, we start with the deuteron as the simplest and pedagogical case of a two-nucleon bound system. It is known that hyperspherical (angular) states can be reduced to the usual $Y_{\ell m}(\hat{r})$ (angular) states for the two-body problem[1]. It is well known that due to the tensor form of the ineraction for the deuteron case we obtain a coupled system of two differential equations, similar to Eq.(1). Although being quite a simple example, it provides a nice illustration of the use of the HAA and its approximate versions (EAA, UAA, CAA). On top of it singular interactions (hard-core type) are considered to illustrate the "goodness" of the HAA. It also serves as an insight for the non-trivial three-body problem with hard-core type interactions. Four realistic nucleon-nucleon potentials, viz Reid soft-core (RSC)[7], Reid alternate soft-core (RSCA)[7], Reid hard core (RHC)[7] and Hamada-Johnston (HJ)[8] have been considered.

In Table 1, the comparison between the results obtained by the UAA, EAA and the exact one is given. We can see that the UAA seems to be very good for all the soft-core potentials. However for the hard-core nucleon-nucleon potentials (HJ and RHC), the UAA results are appreciably different from the exact ones. In Figs. 1 and 2 we plot the lowest eigenpotential, $u_0(r)$, and the next higher eigenpotential, $u_1(r)$, (see Eq.(14)). It is seen that $u_1(r)$ lies well above $u_0(r)$ for

the region of interest. In spite of this, the UAA appears not to work well for the hard-core potentials.

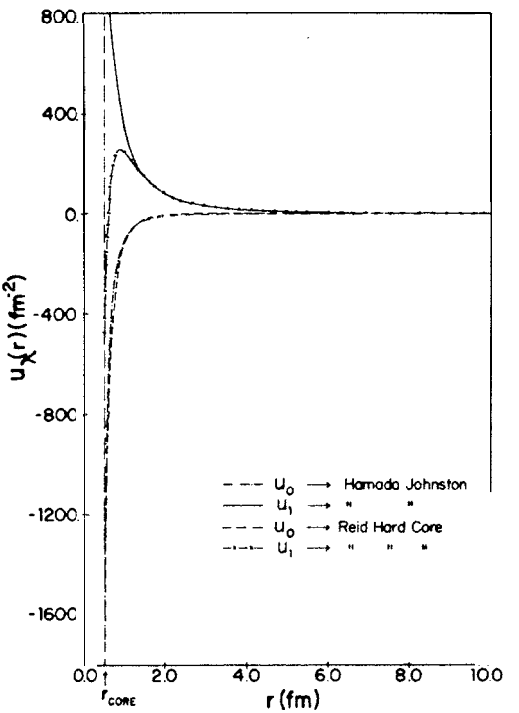

Fig. 1 – Plots of the ground and first excited states of $u_\lambda(r)$ for deuteron. The Hamada-Johnston and Reid hard-core were used for the nucleon-nucleon potential.

This can be understood from the fact that the derivatives of the potential are extremely large in the neighbourhood of the hard-core radius, whereas the $r \to 0$ part is outside the domain of the hard-core problem.

Table 2 illustrates a calculation for triton. We have used the Eikemeier-Hackenbroich (label **S4)** and the Afnan-Tang (label **S3) potentials**[9]. These potentials have a rather sharp change in a short range. They generate smooth and well separated eigenpotential curves[4] and $6 = 0.1$. The results show a good con-

Table 1 – Comparison of UAA and EAA with "exact" calculation for severa1 potentials (defined in the text) for deuteron. Energies are given in MeV. The values of the parameter 6 are given for the corresponding potentials.

Potential	UAA	EAA	Exact	6
HJ	**1.9722**	**2.8175**	**1.2690**	**0.53**
RHC	**1.9271**	**2.6211**	**2.2246**	**1.61**
RSC	**2.0930**	**2.4809**	**2.2246**	**0.17**
RSCA	**2.1068**	**2.4712**	**2.2246**	**0.26**

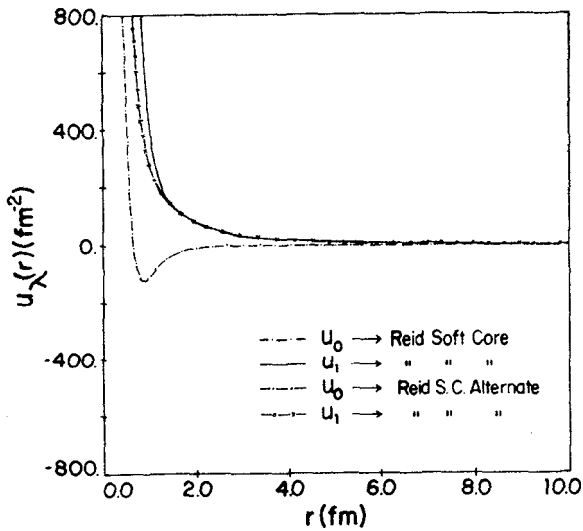

Fig. 2 – Plots of the ground and first excited states of $u_\lambda(r)$ for deuteron. The Reid soft-core and Reid soft-core alternate were used for the nucleon-nucleon potentials.

vergence trend. The binding energies obtained by the use of UAA differ from the "exact" results (CAA) by **0.8%** and **2.8%** respectively.

Several other applications using the HAA have been considered to realistic calculations in few-body nuclear physics[10]. The results compare well with exact methods. The validity criteria of UAA given above are basically satisfied for few-body nuclear systerns.

Table 2 - Comparison of UAA and EAA with "exact" calculation (CAA) for S3 and S4 potentials and various numbers (N) or CDE for ^{3}H.

Potential	N	Energy (MeV) UAA	EAA	CAA
S3	1	0.3647	0.3647	0.364
	2	2.0495	2.3952	2.120
	4	5.0712	5.6005	5.196
	6	6.0582	6.7123	6.208
	8	6.3153	7.0118	6.470
	10	6.4381	7.1549	6.5923
	12	6.4889	7.2132	6.6403
S4	1	3.6670	3.6669	3.667
	2	4.6958	4.9179	4.741
	4	6.1319	6.3986	6.182
	6	6.6793	6.9734	6.735
	8	6.8396	7.1514	6.898
	10	6.9217	7.2465	6.9820
	12	6.9583	7.2900	7.0182

The Model Three Particle System

To emphasize the broad range of applicability of HAA it is enough to idealize a three-body (bound) model system composed of two equal mass particles ($m_1 = m_2$) and a third one of mass m_3, interacting via pairwise (varying-range-depth) S-wave potentials. For most physical systems, the use of pairwise S-state is enough for the calculation of the ground state. For instance, in nuclear physics it is well known that $|V_{\ell=0}(r_{ij})| \gg |V_{\ell\neq 0}(r_{ij})|$, which means that the $\ell = 0$ channel contributes with more than 90% for the binding energy, as well as for the probability of the total wave function. For long range forces, the Coulomb interaction predominates. In this case, the interaction is ℓ-independent. For simplicity, we consider systems with the total angular momentum ($\vec{L} = \vec{\ell}_x + \vec{\ell}_y$) equal to zero and neglect spin complications. The angular momentum operator, $\vec{\ell}_x$, refers to the particle pair (12), and $\vec{\ell}_y$ to particle 3 and the center of mass of the pair (12). Notice that L = 0 implies & = ℓ_y = C. Because of the above arguments we consider only the $\ell = 0$ state in our calculations. The choice of the two-body potential has

the form

$$V(r_{ij}) = -V_0 \exp(-r_{ij}^2/\beta^2), \quad (i,j) = 1,2,3, \tag{20}$$

where V_0 is its depth and β the range of the interaction. We calculate the binding energies corresponding to UAA and EAA. From the basic inequalities, the "exact" values should lie between UAA and EAA. These results depend on the choice of the two parameters of the potential as well on the mass ratio, m $= m_1/m_3$.

We give below the matrix elements for the specific interaction (Eq.(20)) and important equations in order to use HAA. The quantum numbers needed here are $\alpha \equiv \{\mathrm{K}, \mathrm{L}, M, \ell_x, \ell_y\} = \{K, 0, 0, 0, 0\}$, K $= 0, 1, \ldots, \infty$, where K is the quanturn number associated with the Casimir operator[1]. As the hyperspherical harmonics, $\mathcal{Y}_\alpha(\Omega)$, are well known[1], we can calculate the matrix elements $U_{\alpha\alpha'}(r)$ which appear in Eq.(9). The result is

$$\begin{aligned} U_{KK'}(r) = {} & \frac{(K+3/2)(K+5/2)}{r^2}\delta_{KK'} + (2m_1V_0/\hbar^2)\left[\frac{(K+1)!(K'+1)!}{\Gamma(K+3/2)\Gamma(K'+3/2)}\right] \\ & \times \int_0^{\pi/2} d\theta \, \sin^2\theta \, \cos^2\theta \, P_K^{1/2,1/2}(\cos 2\theta) \, P_{K'}^{1/2,1/2}(\cos 2\theta) \times \\ & \mathrm{x} \, \{exp[-(r\sin\theta/\beta)^2] + \exp[-(\cos\theta/a - \sin\theta/2)^2 (r/\beta)^2] \\ & + \exp[-(\cos\theta/a + \sin\theta/2)^2 (r/\beta)^2]\} \, [(r/\beta)^2 (\sin 2\theta/2a)]^{-1}, \end{aligned} \tag{21}$$

where $P_K^{1/2,1/2}$ are Jacobi polynomials[1] and a $= 2/\sqrt{2m+1}$. By knowing $U_{KK'}(r)$, we can calculate $\chi_{K\lambda}$(r) (see Eq.(8)) and finally solve Eq.(11) to obtain the eigen-energies, in the different approximations, EAA and UAA.

In order to simulate both the nuclear and molecular situations, we varied m by two orders of magnitude and considered two distinct possibilities. In the first case, a typically nuclear one - all three pair potentials are taken to be of form (20); in the second - a typically molecular one - the pair interaction between the equal mass particles 1 and 2 is set equal to zero. In order to test the usefulness of the above approximation schemes under widely differing conditions, in addition to varying m, we also varied the potential depth V_0 and range β. The mass of the third particle is taken to be equal to that of a nucleon, so that $\hbar^2/m_3 = 41.47 MeV.\mathrm{f}\, m^2$.

Previously, it was found that, in the nuclear situation for short range potentials with m $\approx$ 1, both **EAA** and **UAA** were good approximations to the exact ground state energies, so that **EAA** and **UAA** define a narrow band with the exact result lying in between[2-4]. The present study shows that **EAA** and UAA continue to define a narrow band even in widely varying situations ($0.2 \leq m \leq 100$) with diverse values of potential depths and ranges. In all the cases, both EAA and **UAA** were found to be good approximations to the exact ground state energy.

In Table **3,** we exhibit the results of the present calculation for $\beta = 1.6$, 2.4 and 4.0 fm when there is a potential between all three pairs. In Table **4** we exhibit the same results when there is no potential between the (equal-mass) pair (12).

In all cases the EAA and **UAA** are excellent approximations to the exact energy for $2 \leq m \leq 100$; for $0.2 \leq m \leq$ **1,** both EAA and **UAA** continue as excellent approximations. The inequalities (15) are never obviously violated.

We plot in Fig.3 the potential defined by Eq.(20), for different values of β and V_0. In Fig.4 we plot $\zeta_0(r)$ versus r for $\beta = 1.6$ fm and different values of ***m.*** Since the nature of the interaction given by Eq.(20) is mathematically well-behaved, it will of course generate smooth and well separated eigenpotential curves. It turns out that the parameter $\delta < 1.0$, making the UAA a good approximation scheme.

5. Conclusions

In this work we present results for binding energies only; and we know[11,12] that in the three-body problem the ground state binding energy is correlated with all low energy observables and, hence, is a reliable measure to assess the validity of the present approximations. In the quantum mechanical two-body problem, because of the existence of the effective range expansion, all low-energy bound state observables and scattering observables remain correlated with the binding energy. If a reasonable model calculation provides the correct binding energy and scattering length for the two-body system, it provides an excellent account of other low-energy observables. In the case of a three-body system, the ground state binding energy even constrains the scattering length for the three-body system. Consequently, for three bodies interacting via short-range pair potentials a correct

Table 3 – Results for the ground state energies for the model system in the UAA and EAA, respectively, when there is a potential between all three pairs.

β (fm)	m	$-V_0$ (MeV)	$-E_{UAA}$ (MeV)	$-E_{EAA}$ (MeV)
1.6	0.2	141.5	6.30	6.45
	0.5	76.5	9.02	9.06
	1	51.5	9.39	9.46
	5	40	26.62	27.28
	10	35	27.32	28.24
	20	30	25.29	26.27
	30	25	20.12	20.98
	50	20	15.25	15.94
	100	20	17.28	17.86
2.4	0.2	70	6.84	6.89
	0.5	40	8.92	8.95
	1	28	9.11	9.16
	5	20	15.16	15.47
	10	18	16.03	16.50
	20	16	15.57	16.11
	30	16	16.85	17.43
	50	14	14.70	15.20
	100	14	15.95	16.44
4.0	0.2	32	7.98	8.03
	0.5	19	8.16	8.18
	1	14	8.16	8.18
	5	14	17.54	17.82
	10	14	20.00	20.47
	20	14	21.80	22.39
	30	14	22.63	23.23
	50	14	23.46	24.07

ground state binding energy constrains, in a model calculation, almost all low-energy observables to yield the correct values. This is true, in general, in three as well as two dimensions[11]. Hence, though we present results only for binding energies, we have good reason to believe that the present approximation schemes will be valid for other low-energy observables.

In three-body systems in nuclear physics, only S-wave pair potentials are frequently used, as in the present study, not only to successfully model the three-nucleon system[2,10] but also complex systems such as ^{12}C, ^{9}Be, etc., treated as

Table 4 – Same as Table 3, but there is no interaction between the pair **(12).**

β (fm)	m	$-V_0$ (MeV)	$-E_{UAA}$ (MeV)	$-E_{EAA}$ (MeV)
1.6	1	51.5	0.24	0.29
	5	40	6.63	7.29
	10	35	6.59	7.31
	20	30	5.35	5.97
	30	25	3.10	3.49
	50	20	1.23	1.41
	100	20	1.70	1.90
2.4	1	28	1.76	1.86
	5	20	4.45	4.85
	10	18	4.69	5.14
	20	16	4.29	4.71
	30	16	4.79	5.22
	50	14	3.68	4.01
	100	14	4.13	4.42
4.0	1	14	2.93	3.03
	5	14	7.99	8.44
	10	14	9.30	9.81
	20	14	10.23	10.75
	30	14	10.65	11.14
	50	14	11.07	11.52

clusters[13]. In many situations in nuclear physics, Gaussian and linear combinations of Gaussian potentials are employed between nucleons[2] and clusters[13]. Such models give a good account of both the ground state energy and other low-energy observables. We are aware that in the molecular case a consideration of Gaussian pair potentials only is not realistic. However, we believe that, as in nuclear physics, linear combinations of Gaussian potentials should simulate qualitatively the molecular potential which should reproduce the basic vibration-rotation structure of molecular spectra. Also, as we studied the problem under diverse situations including wide variations of the mass ratio and potential and, as the approximations were accurate in almost all cases, we beiieve that our conclusions will hold in more realistic situations. We believe that the present pioneering study will shed important light on the validity of the adiabatic approximation schemes in general.

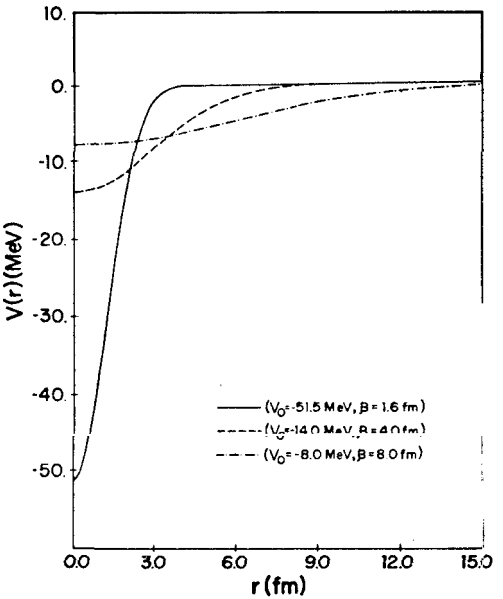

Fig. 3 - Plot of the two-body gaussian potential defined by Eq.(20).

An extension of the present study to more realistic situations will be welcomed in future studies. For nuclear systems, there are many publications[3,4,10] which confirm the use of HAA successfully. For realistic atomic and molecular systems this can be observed as well. References (4,6) (see also references there in) confirm it.

From an analysis of the results of our study we can safely conclude the following: 1) The HAA, in its different versions (EAA, UAA and CAA), is a good approximation scheme to handle the solution of non-relativistic N-body bound systems from the molecular to the nuclear scale. Other references[1-4,6,10] also confirm this statement, including atomic systems. It is true that in this article we have only used the HAA for $N=2,3$-body systems. However, since the mathematical structure of HAA presented in this paper is general for any N value, we can safely agree with the above statements. 2) The EAA and UAA are also good approximations to the exact result for the model three-particle system discussed here to simulate cases in the nuclear and molecular scales. A broad variation of

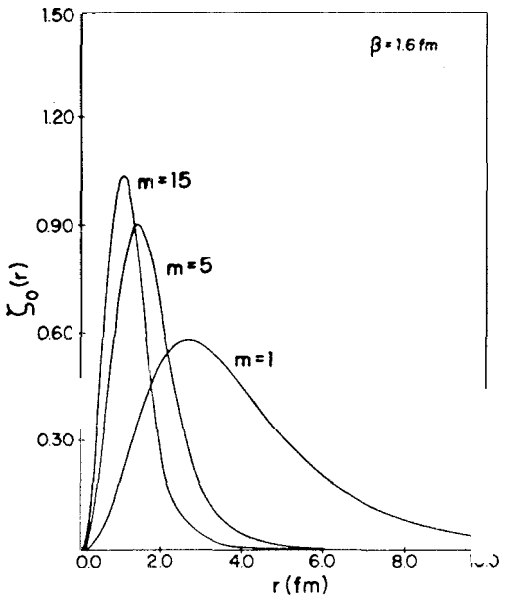

Fig. 4 – Typical plot of $\zeta_0(r)$ versus r for different values of m and $\beta = 1.6$ fm.

the parameters was considered ($0.2 < m < 100$, varying V_0 and β, and switching off the potential in pair 12). The EAA and UAA define a narrow band in the corresponding eigen-energies. **3)** In this article, we also clarified a hitherto empirical estimate of the ground state energy, bascd on different version of the HAA (EAA, UAA and CAA). For that purpose, we included a general proof of the basic inequalities. As mentioned before, a preliminary proof was given by Ballot et al. in ref. (3), but using the approximate concept of the optimal subset making that proof not so general and unnecessarily complex.

Formally there exists a certain resernblance between HAA and the Born-Oppenheimer approxirnation (BOA).

An inequality similar to Eq.(15) was proved for the extreme BOA[14],

$$\epsilon_{BOA} \leq \epsilon. \tag{22}$$

Although EAA and BOA are similar in spirit and based on adiabatic approximatons, they are fundamentally distinct. The EAA is derived in a hyperspherical

space incorporating $O(3N\text{-}3)$ symmetry, while BOA is conceived in an independent particle coordinate, with $O(3) \times ... \times O(3)$ symmetry. As a result, they lead to different equations, giving in general $\epsilon_{EAA} \neq \epsilon_{BOA}$. A correlation between these two methods is established elsewhere[15]. 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 that 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 have to solve a coupled system of partial differential equations[5], without necessarily furnishing better results.

We should stress the generality of the basic inequalities which are independent of the nature of the interaction. The inequalities proved here hold for ground state energies. However the HAA can also be successfully used for excited states. Ref. (16) also diçcusses the above points in a general and elegant way.

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References

1. Yu. A. Simonov, The Nuclear Many-Body Problem, F. Calogero and C. Ciofi degli Atti, Ed., Editrice Compositori, Rome 1972, page 527; Yu. F. Smirnov, K. V. Shitikova, Sov. J. Part. Nucl. 8 (4), 344 (1977); F. Zermike, H. C. Brinkman, Proc. Kon. Ned. Acad. Wetensch. **33**, 3 (1935); for basic ideas on Casimir Operators see also ref. 5, Chapter 7.
2. T. K. Das, H. T. Coelho, M. Fabre de la Ripelle, Phys. Rev. C26, 2281 (1982).
3. J. L. Ballot, Proceedings oj the European Workshop on *Few-body* Physics, October 7-11, 1986, Edited by C. Ciofi degli Atti, O. Benhar, E. Pace and G. Salmé, page 140; J. L. Ballot, M. Fabre de la Ripelle, J. S. Levinger, Phys. Rev. C26, 2301 (1982).
4. V. P. Brito, H. T. Coelho, T. K. Das, Phys. Rev. A40, 3346 (1989).
5. L. I. Schiff, *Quantum* Mechanics, 3 rd. ed. (McGraw-Hill, New York, 1965), Chap. 12.

6. J. E. Hornos, S. W. MacDowell, C. D. Caldwell, Phys. Rev. A33, 2212 (1986).
7. R. V. Reid, Ann. Phys. (N.Y.) 50, 411 (1968).
8. T. Hamada, I. D. Johnston, Nucl. Phys. 34, 382 (1962).
9. H. Eikemeier, H. H. Hackenbroich, Zeitschrift Phys. 195, 412 (1966); I. E. Afnan, Y. C. Tang, Phys. Rev. 175, 1337 (1968).
10. T. K. Das, H. T. Coelho, M. Fabre de la Ripelle, Phys. Rev. **C26,** 2288 (1982); H. T. Coelho, T. K. Das, M. R. Robilotta, Phys. Rev. **C28,** 1812 (1983).
11. S. K. Adhikari et al., Phys. Rev. A37, 3666 (1988).
12. A. C. Phillips, Rep. Prog. Phys. 40, 905 (1977); V. Efimov, Nucl. Phys. **A362,** 45 (1981).
13. H. T. Coelho, T. K. Das, M. Vallières, Nucl. Phys. **A257,** 389 (1976); H. Kamada, S. Oryu, Nucl. Phys. **A463,** 347c (1987); A. C. Fonseca, J. Revai, A. Matveenko, Nucl. Phys. **A326,** 182 (1979); A. C. Fonseca, M. T. Pena, Proceedings of the International Workshop on *Few-body Approaches* to Nuclear *Reactions*, Ed. S. Oryu, T. Sawada, (World Scientific, Singapore, 1987), p. 247.
14. V. F. Brattsev, Sov. Phys. Doklady **10, 44** (1965) [Doklady Akademii Nank SSSR, 160, 570 (1965)].
15. S. K. Adhikari, V. P. Brito, H. T. Coelho, T. K. Das, Nuovo Cimento B, in print.
16. H. T. Coelho, J. E. Hornos, Phys. Rev. A, A43, 6379 (1991).

Resumo

Um procedimento matemático, chamado método adiabático hiperesférico (HAA), é apresentado para lidar com a solução de um sistema acoplado de equações diferenciais (finito ou não) do tipo Schrödinger, normalmente, gerado de sistemas físicos de N-corpos. Investigamos a utilização do HAA a casos relativamente simples, mas representativos, de modo a enfatizar sua larga aplicabilidade. O manuscrito deriva um teorema de "upper bound/lower bound" para o HAA. Esta demonstração esclarece uma estimativa, até aqui empírica, da energia do estado fundamental, baseada em diferente versões do HAA: a aproximação adiabática extrema, a aproximação adiabática desacoplada e a aproximação adiabática acoplada. Finalmente, discutimos a familiar aproximqão de Born-Oppenheimer, onde uma, estimativa similar ocorre.