

# ADIABATIC APPROXIMATION IN THE ATOMIC AND NUCLEAR SCALES

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## ABSTRACT

In this work we study an approximation method, called the adiabatic approximation (AA), based more on a mathematical foundation than a phenomenological physical basis. We investigate the application of AA to simple molecular and nuclear systems in order to extract insights into the criterion of validity of this approximation method. We also analyze the Born-Oppenheimer approximation and see if a correlation can be established between the two approximation schemes.

## 1. INTRODUCTION

The many-body problem, as well as the few-body problem, in quantum physics is still an area of intensive research. In particular in atomic, molecular, and nuclear physics there are many traditional many-body methods, such as the Hartree-Fock<sup>1</sup> calculation, but they are rather involved numerically, such that one loses the sight of what is really happening to the physics of the problem. For few-body problems, powerful and exact approaches, such as the hyperspherical harmonics (HH) formalism<sup>2,3</sup>, recently extended to many-body systems<sup>4</sup>, Faddeev<sup>5</sup> equations for three-body systems, later extended by other authors<sup>5</sup> to N-body systems, and Yakubowski<sup>6</sup> equations for four-body systems, were developed in order to handle the problem. If they are written in the configuration space involving differential equations, it is possible to find a connection among them, at least between the HH formalism and Faddeev equations<sup>7,4</sup>. All approaches will eventually result in difficult numerical calculations<sup>1-7</sup>. In configuration space they lead to an infinite system of coupled differential equations<sup>2-7</sup>. For practical purposes the system is truncated according to certain mathematical procedures leading to the solution of a desired accuracy<sup>1,2</sup>. Since the HH approach can be extended to many-body systems we will concentrate on it. Besides, this is an elegant and an essentially exact method being a natural extension of the two-body approach appearing in the standard text-books of Quantum Mechanics. Another advantage of the HH approach is to treat Coulomb interaction, which appears naturally in molecular systems, exactly, in contrast to the usual momentum space Faddeev approach<sup>5</sup> where Coulomb interaction is taken in an approximate way. Our purpose in this paper is to study an approximate method, called the adiabatic approximation (AA), which reduces the still

large system of truncated coupled differential equations, mentioned above, to a system of a few coupled differential equations. A preliminary version of AA was presented earlier<sup>13</sup> for the three-nucleon system, and extended here to many-body systems, including problems in atomic and molecular physics. We should notice that the adiabatic approximation is a common label which represents several classical approximations. The reason for choosing the name adiabatic approximation has its roots in a basically similar approximation used in molecular physics. In thermodynamics, as well, adiabatic states mean an approximation where each thermal state is generated from a previous one by neglecting the interaction with the environment. In a like manner the AA for a system of coupled differential equations reduces the system to a non interacting single differential equation. The difference between the AA presented here and the classical approximations, is the fact that in classical methods, the approximation is assumed in an ad hoc fashion, without any rigorous mathematical justification. This is the case for the Born-Oppenheimer approximation which, however, works fine for many Physical systems<sup>9-11</sup>. In reference (9) a mixture of Born-Oppenheimer with an old fashion HH is used.

In this paper we will investigate the application of AA to two rather simple situations. The aim is not just to show how well it works but rather to critically examine the conditions of its applicability in diverse situations. In particular the two applications – in nuclear and molecular physics – are so chosen as to be on the two extremities of the applicability criterion. In addition, the second application – for which the AA does not fare well – is chosen to be transparent enough to give an insight into the cause for this inadequacy, thus providing an understanding of the mechanism of the AA.

In section 2 the AA is presented together with a theoretical justification. In section 3 numerical results are given for selected physical systems in nuclear and molecular physics. Finally in section 4 we present our conclusions.

## 2. ADIABATIC APPROXIMATION

The Schrödinger equation for (N+1)-body system involving N-relative (Jacobi) coordinates  $(\vec{\xi}_i)$  has the form<sup>12</sup>, after the CM motion is removed,

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$$\left[ -\frac{\hbar^2}{2\mu} \sum_{i=1}^N \nabla_{\vec{\xi}_i}^2 + V(\vec{\xi}_1, \dots, \vec{\xi}_N) - E \right] \Psi(\vec{\xi}_1, \dots, \vec{\xi}_N) = 0, \quad (1)$$

where  $\mu$  is an appropriately defined effective reduced mass. The hyperradial variable ( $r$ ) defined through

$$r^2 = \sum_{i=1}^N \xi_i^2, \quad (2)$$

is invariant under ordinary rotations and all permutations. One can construct hyperangular basis functions ( $Y_\alpha$ ,  $\alpha$  characterizing all the necessary quantum numbers) in the (3N-1) dimensional angular hyper-space ( $\Omega$ ). For example,  $\{Y_\alpha\}$  can be chosen as the hyperspherical harmonics<sup>3</sup>. Expanding  $\Psi$  in  $\{Y_\alpha\}$ ,

$$\Psi = r^{-(3N-1)/2} \sum_{\alpha} \phi_{\alpha}(r) Y_{\alpha}(\Omega), \quad (3)$$

substituting in eq. (1) and finally projecting on a particular  $Y_{\alpha}$ , we get

$$\left[ -\frac{d^2}{dr^2} + \frac{\Lambda_{\alpha}(\Lambda_{\alpha}+1)}{r^2} + k^2 \right] \phi_{\alpha}(r) + \sum_{\alpha'} v_{\alpha\alpha'}(r) \phi_{\alpha'}(r) = 0, \quad (4)$$

where  $v_{\alpha\alpha'}(r) = \frac{2\mu}{\hbar^2} \langle Y_{\alpha} | V | Y_{\alpha'} \rangle$  and  $k^2 = -\frac{2\mu E}{\hbar^2}$

( $E < 0$  for a bound state) and  $\Lambda_{\alpha}(\Lambda_{\alpha}+1)$  is the eigenvalue of the hyperangular momentum operator,  $K^2(\Omega)$ . For most nuclear few-body problems, the set of coupled differential equations (CDE) for  $\{\phi_{\alpha}\}$  is formidable even after reasonable truncation. Hence it is greatly advantageous to reduce the set further. A scheme called uncoupled adiabatic approximation (UAA) for decoupling the CDE to a single equation has been proposed and applied successfully to the three nucleon problem in ref. (13, 14). In this communication, we try to justify the decoupling procedure and also examine under what conditions UAA is expected to be reasonable.

In the UAA procedure<sup>13</sup>, an associated matrix eigenvalue equation (for a fixed  $r$ )

$$\sum_{\alpha'} M_{\alpha\alpha'}(r) \chi_{\alpha'}(r) = \omega_{\lambda}(r) \chi_{\alpha}(r), \quad (5)$$

with

$$M_{\alpha\alpha'}(r) = \frac{\Lambda_{\alpha}(\Lambda_{\alpha}+1)}{r^2} \delta_{\alpha\alpha'} + v_{\alpha\alpha'}(r), \quad (6)$$

is solved to obtain the eigenvalue,  $\omega_{\lambda}(r)$ , and eigenvector,  $\chi_{\alpha\lambda}(r)$ , as parametric functions of  $r$ . For each fixed  $r$ , one can expand the column vector  $\phi_{\alpha}(r)$  in the complete set of eigenvectors  $\chi_{\alpha\lambda}(r)$  of the matrix  $M_{\alpha\alpha'}(r)$ :

$$\phi_{\alpha}(r) = \sum_{\lambda} \xi_{\lambda}(r) \chi_{\alpha\lambda}(r). \quad (7)$$

We should notice that the orthonormalization condition holds

$$\sum_{\alpha} \chi_{\alpha\lambda}^*(r) \chi_{\alpha\lambda'}(r) = \delta_{\lambda\lambda'}, \quad (8)$$

Substituting eq. (7) into eq. (4), and taking the inner product with  $\chi_{\alpha\lambda}(r)$ , one obtains

$$\begin{aligned} & \left[ -\frac{d^2}{dr^2} + \omega_{\lambda}(r) + k^2 + \sum_{\alpha} \left| \frac{d\chi_{\alpha\lambda}}{dr} \right|^2 \right] \xi_{\lambda}(r) + \\ & + \sum_{\lambda' \neq \lambda} \left[ 2 \frac{d\xi_{\lambda'}}{dr} \sum_{\alpha} \chi_{\alpha\lambda}^* \frac{d\chi_{\alpha\lambda'}}{dr} + \right. \\ & \left. + \xi_{\lambda'} \sum_{\alpha} \chi_{\alpha\lambda}^* \frac{d^2 \chi_{\alpha\lambda'}}{dr^2} \right] = 0. \end{aligned} \quad (9)$$

In the derivation of eq. (9) we have used eq. (8), by first differentiating it with respect to  $r$ , and secondly differentiating once again for  $\lambda = \lambda'$ , which leads to the term

$\sum_{\alpha} \left| \frac{d\chi_{\alpha\lambda}}{dr} \right|^2$  in eq. (9). Neglecting the coupling terms in the coupling terms in eq. (9), one has the UAA equation

$$\left[ -\frac{d^2}{dr^2} + \omega_{\lambda}(r) + k^2 + \sum_{\alpha} \left| \frac{d\chi_{\alpha\lambda}}{dr} \right|^2 \right] \xi_{\lambda}(r) = 0. \quad (10)$$

By neglecting the last term in eq. (10) we get the so called extreme adiabatic approximation (EAA).

Depending on the system considered (this is a function of the potential nature, for example), UAA might not be an accurate enough approximation. In such a case we need to go to a higher order approximation. That is done by considering the coupling terms in eq. (9), with the next allowed value of  $\lambda'$  ( $\lambda' \neq \lambda$ ). As a result, we obtain a system of a few coupled second order differential equations, which is still simple enough to be quickly solved numerically. This procedure is called the coupled adiabatic approximation (CAA). As we will see below, for most applications the UAA is enough. To study the validity of UAA, we examine eq. (9) closely for various  $r$ .

a) *large r* - Many potentials are short ranged and the dominant asymptotic behavior of  $M_{\alpha\alpha'}(r)$  is

$$M_{\alpha\alpha'}(r) \xrightarrow{r \rightarrow \infty} f(r) m_{\alpha\alpha'}, \quad (11)$$

where  $m_{\alpha\alpha'}$  is a number and  $f(r)$  is either  $r^{-1}$  or  $r^{-2}$  (coming from centrifugal term) depending on whether Coulomb force is present or not. This can be understood as follows. In this limit, the  $\frac{1}{r}$  or  $\frac{1}{r^2}$  (depending on whether the Coulomb potential is present or not) fac-

tors out of the matrix element  $M_{\alpha\alpha}$ , leaving only hyperangular functions to be integrated over the hyperangles, which is thus independent of  $r$ . In this situation, eq. (5) shows that  $\omega_\lambda(r)$  has the same hyperradial dependence  $f(r)$  and  $\chi_{\alpha\lambda}$  is independent of  $r$ . Therefore, the coupling terms in eq. (9), which contain derivative of  $\chi_{\alpha\lambda}$ , are negligible.

b) *small r* – For nuclear, atomic or molecular potentials that go like  $r^{-n}$  for  $r \rightarrow 0$ ,  $M_{\alpha\alpha}(r)$  has the form (11) where  $f(r)$  is  $r^{-2}$  or  $r^{-n}$  according as  $n < 2$  or  $n > 2$ . Hence by the same argument the coupling terms in eq. (9) are expected to be small in this limit.

c) *intermediate r* – Since in this case,  $M_{\alpha\alpha}(r)$  does not have the simple form (11), the foregoing argument does not hold. Using eq. (5), together with the orthonormality of  $\{\chi_{\alpha\lambda}\}$  the coupling term in eq. (9) can be written as

$$\begin{aligned} \sum_{\lambda' \neq \lambda} [ \dots ] &= \sum_{\lambda' \neq \lambda} [ \omega_{\lambda'}(r) - \omega_\lambda(r) ]^{-1} \{ \\ &\{ \sum_{\alpha\alpha'} [ \chi_{\alpha\lambda}^* \chi_{\alpha'\lambda'} (2 \frac{d\xi_{\lambda'}}{dr} \frac{d}{dr} + \xi_{\lambda'} \frac{d^2}{dr^2}) v_{\alpha\alpha'}(r) ] + \\ &+ \sum_{\alpha\alpha'} [ 2\chi_{\alpha\lambda}^* \frac{d\chi_{\alpha'\lambda'}}{dr} \xi_{\lambda'} - \frac{dv_{\alpha\alpha'}}{dr} ] + \\ &+ \sum_{\alpha} [ 2\Lambda_\alpha (\Lambda_\alpha + 1) (\frac{3}{r^4} \xi_{\lambda'} - \frac{2}{r^3} \frac{d\xi_{\lambda'}}{dr}) \\ &\chi_{\alpha\lambda}^* \chi_{\alpha\lambda} ] - \sum_{\alpha} [ 2\xi_{\lambda'} (\frac{d\omega_{\lambda'}}{dr} + \\ &+ \frac{2\Lambda_\alpha (\Lambda_\alpha + 1)}{r^3}) \chi_{\alpha\lambda}^* \frac{d\chi_{\alpha\lambda'}}{dr} ] \} \quad (12) \end{aligned}$$

For intermediate values of  $r$ , assuming no rapidly varying potentials, the quantity within curly bracket in eq. (12) is finite and should vary smoothly. Hence in order that the coupling terms of eq. (9) are small,  $|\omega_{\lambda'}(r) - \omega_\lambda(r)|$  must be large in comparison with that quantity within curly bracket. An equivalent and more practical condition can also be obtained if one compares eqs. (9) and (12). Clearly the coupling term of eq. (9) (which are neglected in UAA) for each  $\lambda'$  is proportional to  $[\omega_{\lambda'}(r) - \omega_\lambda(r)]^{-1}$ , while the direct term (which is retained in UAA) of eq. (9) is  $\omega_\lambda(r) \xi_{\lambda'}(r)$ , hence the UAA will be good if  $|\omega_{\lambda'}(r) - \omega_\lambda(r)|$  is large compared to  $|\omega_\lambda(r)|$ . More specifically since  $\xi_{\lambda'}(r)$  will have a maximum in the neighbourhood of the position where  $\omega_{\lambda'}(r)$  has a minimum, this criterion is to be applied in the region where  $\omega_\lambda(r)$  has a minimum. Hence the criterion mentioned above can be better specified by a parameter  $\mu$  defined as

$$\mu = \left| \frac{\omega_\lambda(r_{\min})}{\omega_{\lambda'}(r_{\min}) - \omega_\lambda(r_{\min})} \right|, \quad (12')$$

where  $r_{\min}$  is the value of  $r$  at which  $\omega_\lambda(r)$  has a minimum.

Thus eq. (10) well approximates the exact eq. (4), in both the large and small  $r$  limits and for intermediate values of  $r$ , if the "eigenpotentials",  $\omega_\lambda(r)$ , are well separated and  $\mu \ll 1$ . In particular, for the ground state binding energy, eq. (10) is a very good approximation, if  $|\omega_1(r) - \omega_0(r)|$  is large in comparison with the quantity within curly bracket in eq. (12), especially in the region where the lowest eigenpotential,  $\omega_0(r)$ , has a minimum or equivalent  $\mu = |\omega_0(r_{\min})| / (\omega_1(r_{\min}) - \omega_0(r_{\min})) \ll 1$ . This condition is satisfied by many few-body systems. However if the potential involves rapid variations or singularities, the same nature will be reflected in  $v_{\alpha\alpha'}(r)$ . The quantity within braces in eq. (12) then will not be small, as it involves derivative of  $v_{\alpha\alpha'}(r)$ . Consequently UAA is not expected to be good for rapidly varying potentials.

### 3. RESULTS FOR SEVERAL PHYSICAL SYSTEMS

In this section we will concentrate on applications to nuclear and molecular systems. The method in consideration can be applied, in principle, to any finite number of particles with the condition that the resulting Schrödinger equation can be put in the form of eq. (4). This can always be achieved, for instance, in the hyperspherical harmonic formalism<sup>2,3</sup>. For definiteness we choose three-body systems, which illustrate the use of AA. This application is already complex enough (involving time consuming numerical calculations) to be handled exactly<sup>14</sup>. As mentioned earlier, three-body problems can be solved exactly either by Faddeev equations<sup>5</sup> or by the HH approach<sup>14</sup> and in configuration space the two methods are somehow related<sup>4,7</sup>.

#### a) Three-nucleon system

In the nuclear scale let us choose the triton ( $^3\text{H}$ ) which is formed by two neutrons and a proton, bounded by a nuclear interaction<sup>14</sup>. Since we are only interested in showing the validity of the AA, we have chosen four relatively simple phenomenological nucleon-nucleon potentials (excluding tensor forces, three-nucleon forces, etc.). All the four two-nucleon potentials<sup>2,3</sup>, have the common form  $V(r) = (V_s(r) + V_t(r))/2$ , where  $V_s$  and  $V_t$  stand for the singlet and triplet parts, respectively. Both  $V_s$  or  $V_t$  have the form

$$V_{\{s,t\}} = \sum_{i=1}^3 a_i \exp(-r/b_i)^2, \quad (13)$$

where the parameter values ( $a_i$  and  $b_i$ ) are given in table 1.

In Table 2 the comparison between the results obtained by the UAA, EAA and the exact one is shown. The UAA seems already very good for the smooth Baker and Volkov potentials<sup>2,3</sup>, leading to a binding energy differing from the exact calculation by about 0.3% and 0.7% respectively. But even for potentials which have a rather strong soft core (i.e. a rather sharp change in a short range), like<sup>2,3</sup> S4 or S3, we find that the binding energy differs from the "exact" result<sup>2,15</sup> by 0.8% and 2.2% respectively. Furthermore, Table 2 shows that the convergence trend for the UAA and EAA is the same as the one of the exact calculation. The small discrepancies among

the results for  $N=1$  (which correspond to the eigenvalue  $K=0$  of the Casimir operator  $K^2(\Omega)$ ) are due to the choice of step size in the  $r$  mesh.

Besides  $\omega_0(r)$ , we have also calculated  $\omega_1(r)$ , the first excited eigenpotential (Fig.1). One immediately

notices that  $|\omega_1(r) - \omega_0(r)|$  is quite large compared to  $|\omega_0(r)|$  in the region where  $\omega_0(r)$  has an appreciable depth. According to our discussions in Section 2, one expects the UAA to be good in this case, which indeed turns out to be true.

TABLE I

Parameter values for the Baker, Volkov, S3 and S4 nucleon-nucleon potentials ( $a_i$  and  $b_i$ ) are given in MeV and fm, respectively.\*

Potential	i	Singlet		Triplet	
		$a_i$	$b_i$	$a_i$	$b_i$
Baker	1	-51.5	1.6	-51.5	1.6
Volkov	1	144.86	0.82	-83.34	1.6
S3	1	$10^3$	0.5774	$10^3$	0.5774
	2	-166.0	1.1180	-326.7	0.9759
	3	-23.0	1.5811	-43.0	1.2910
S4	1	880.0	0.4303	600.0	0.4264
	2	-70.0	1.25	-70.0	1.4142
	3	-21.0	1.4434	-27.6	1.6222

\* The space part of the S-state (space totally symmetric) wave function is expanded in the complete set of hyperangular functions,  $Y_{\alpha}$ , which are well known<sup>2</sup>. The spin-isospin part is then totally antisymmetric under exchange of any pair and is given in ref. 3.

Several applications using AA have been considered by some authors to realistic calculations in few-body systems in nuclear physics (see references quoted in ref. 14). The results compare well with exact methods. Exact calculations (HH approach or Faddeev equations in coordinate space) involve a tremendously large number of coupled differential equations to be solved numerically and are very much time consuming. With the above example and some recent references<sup>13,14</sup> we have illustrated the efficiency and validity of AA in at least few-nucleon calculations.

#### b) Molecular system

The second case considered is the simplified hydrogen molecular ion  $H_2^+$  formed by two hydrogen nuclei A and B placed at fixed points on the z-axis, binding an electron "moving" in 3D space. A is located at R and B is located at -R, such that the Hamiltonian is (in atomic units).

$$H = -\frac{1}{2} \nabla^2 - \frac{1}{r_A} - \frac{1}{r_B}, \quad (14)$$

where  $r_A$  and  $r_B$  are the distances of the electron from A and B. In this context one can argue that due to the smallness of electron-proton mass ratio, the protons can be considered at rest as a first approximation. We could certainly treat the system exactly, resulting in a three-body problem. However the idea is to set up a system of coupled diffe-

rential equations involving the Coulomb potential in the atomic scale and compare the results of AA with the exact ones, rather than a correct treatment of the  $H_2^+$  ion. The potential in eq. (14) can be expanded in Legendre polynomials

$$r_A^{-1} + r_B^{-1} = 2 \sum_n (r_{<}^{2n} / r_{>}^{2n+1}) P_{2n}(\cos \theta), \quad (15)$$

where  $r_{<} = \min(r, R)$ ,  $r_{>} = \max(r, R)$  and  $\cos \theta = \hat{r} \cdot \hat{R}$ . For this simple example, eq (4) becomes

$$\left[ -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + 2k^2 \right] \phi_\ell(r) + \sum_{\ell'=|m|}^{\infty} v_{\ell'\ell}(r) \phi_{\ell'}(r) = 0, \quad (16)$$

where

$$v_{\ell'\ell}(r) = -4 \sum_{n=0}^{\infty} (r_{<}^{2n} / r_{>}^{2n+1}) \int Y_{\ell'm}^*(f) P_{2n}(\cos \theta) Y_{\ell'm}(f) df. \quad (17)$$

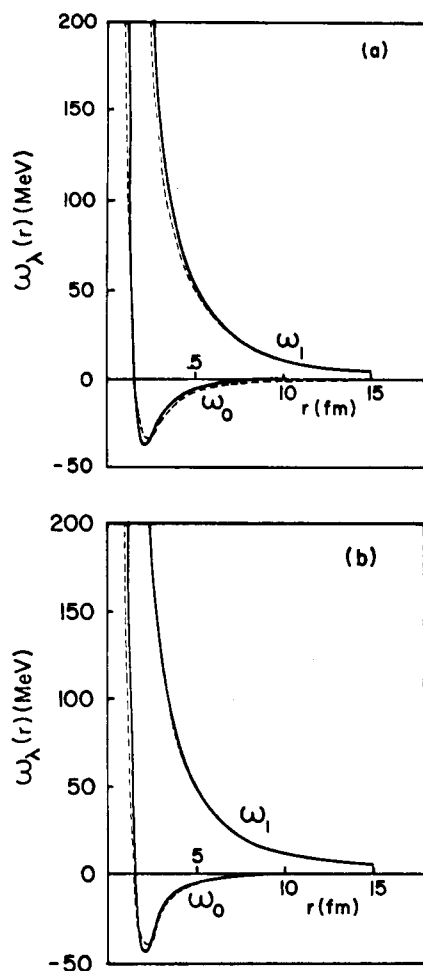


Fig. 1 - (a) Plot of the lowest ( $\omega_0$ ) and first excited ( $\omega_1$ ) "eigenpotentials" against  $r$  for a Baker potential (continuous curve) and a Volkov potential (dashed curve). (b) Same for the S3 potential (continuous curve) and the S4 potential (dashed curve). ( $N = 12$ ).

The integral in eq (17) can be easily evaluated, and restricting our attention to the case  $m=0$ , we obtain

$$v_{\ell\ell'}(r) = -4 \left( \frac{-2\ell+1}{2\ell'+1} \right)^{1/2} \frac{\ell+\ell'}{2n=|\ell-\ell'|}$$

$$\left( \frac{r^{2n}}{2n+1} \right)_{r < R} \langle \ell 0 \ell' 0 | 2n, 0 \rangle^2. \quad (18)$$

We also restrict our calculations to the even parity solutions in order to compare to an exact solution given in reference 16.

We solved for the  $1s\sigma_g$  and  $2s\sigma_g$  states with  $R=1$  Bohr. The results of these calculations using UAA and EAA and their comparison with the exact ones are given in table 3.

We have calculated the binding energies with up to  $N=8$  coupled differential equations. The results using UAA differ from the exact ones by about 9% and 27% for the  $1s\sigma_g$  and  $2s\sigma_g$  respectively. We should notice that the results for the EAA are even closer to the exact ones since the positive last term of eq. (10) was neglected. Results can further be improved if one adds coupling terms in eq. (10), obtaining an approximation to eq. (9), which we called CAA. Since our intention is only to show how simple and efficient AA can be, we are at present, satisfied with the results of Table 3. In that table we also see the right trend of convergence of the results if they are compared which the exact ones.

In fig. 2 we have plotted  $\omega_0(r)$  and  $\omega_1(r)$  for this case. Again the two curves are smooth and well separated. However for this case the AA does not fare so well. This can be understood following the argument put forward as a justification of the method. Since we are faced only with a long range interaction (namely Coulomb interaction), the intermediate  $r$  region is quite critical. The particular choice of a demonstration case is also very well suited to bring out the lines of our justification transparently. From eq. (18) one sees that for  $r \gg R$  (for which  $r_{<}=R, r_{>}=r$ ) the sum over  $n$  for  $v_{\ell\ell'}$  is rapidly converging and only the  $n=0$  term dominates, leading to the effective matrix element being proportional to  $1/r$ , in agreement with case (a) of the justification (eq. (11), Section 2). On the other hand for  $r \ll R$  (for which  $r_{<}=r, r_{>}=R$ ), eq. (18) shows that again only the  $n=0$  term of the sum will dominate, making  $v_{\ell\ell'}$  approximately, independent of  $r$ , which again is in agreement with our foregoing justification (case (b), Section 2). But for  $r$  in the neighbourhood of  $R$ , a larger number of  $n$  values contribute to the sum in eq. (18), thereby making a factorization of  $v_{\ell\ell'}$  similar to eq. (11) impossible. This furthermore demonstrates how an a-priori evaluation of reliability of the UAA method is possible. The situation is worse for the excited state ( $2s\sigma_g$ ) as can well be expected, because being higher in energy, the interactions with other excited "eigenpotentials" ( $\omega_\lambda$  with  $\lambda \neq 0$ ) cannot be neglected altogether. The CAA with two or three terms is expected to work much better.

A final word should be said about Born-Oppenheimer (BO)<sup>8</sup> approximation. In this approximation we have two heavy centers, considered basically at rest, and separated by a parametric distance  $R$ , while the light particles (electrons for molecular systems and nucleons for nuclear systems) "surround" these two centers. One Schrödinger type equation results for these light electrons, which in principle can be solved, if one keeps  $\vec{R}$  fixed, obtaining an effective energy as a parametric function of  $\vec{R}$ . That effective energy is used in another Schrödinger equation which results the energy of the system. In the HH method we do not need to consider the two heavy centers fixed and the problem can be treated exactly. The rate of convergence for the HH expansion method can profitably be enhanced by including correlation function in the many-body wave function<sup>17</sup>. Haftel and Mandelzweig<sup>17</sup> could get a high degree of precision for a reasonable number of partial waves by this method. The AA comes in exactly at the point to reduce the number of coupled differential

TABLE 2

Comparison of the uncoupled and extreme adiabatic approximations with exact calculations (energies in MeV) for chosen potentials and various numbers (N) of coupled differential equations for  $^3\text{He}$ .

Potential	N	UAA	EAA	Exact
Baker	1	9.2048	9.2058	9.2077
	2	9.5982	9.6654	9.6150
	4	9.7409	9.8451	9.7661
	6	9.7532	9.8627	9.7795
	8	9.7544	9.8646	9.7808
	10	9.7546	9.8649	9.7811
	12	9.7547	9.8650	9.7812
Volkov	1	7.7076	7.7076	7.708
	2	8.0348	8.1888	8.079
	4	8.3227	8.5237	8.376
	6	8.3876	8.5967	8.443
	8	8.4013	8.6136	8.4575
	10	8.4065	8.6204	8.4630
	12	8.4082	8.6227	8.4648
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	6.4923
	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

TABLE 3

Comparison of UAA and EAA with exact solution (Energies in atomic units). N stands for the number of coupled equations.

N	$1s\sigma_g$			$2s\sigma_g$		
	UAA	EAA	Exact	UAA	EAA	Exact
2	-0.99607	-0.99704	-1.08368	-0.26368	-0.26379	-0.35845
4	-1.00324	-1.00452	-1.09997	-0.26515	-0.26547	-0.36051
6	-1.00397	-1.00530	-1.10184	-0.26532	-0.26566	-0.36078
8	-1.00414	-1.00548	-1.10230	-0.26536	-0.26570	-0.36082

equation, in a way mathematically well founded (as discussed in section 2), while in the BO approximation that is done in an ad hoc form, justified basically by the mass ratio argument. We know that BO approximation works fine for molecular systems, exactly because the mass ratio involved is adequate, but still without a rigorous mathematical background. In this way AA is more fundamental and can be as efficient as BO approximation. We are at present doing a separate calculation using AA and BO approximation in order to investigate their range of applicability in Atomic and Nuclear scales.

#### 4. CONCLUSIONS

From the foregoing discussions, we conclude that the adiabatic approximation is a convenient and practical calculational scheme for systems involving large degrees of freedom and eventually leading to a large number of coupled equations, where an exact numerical calculation is prohibitively time consuming. The AA appears to be reliable for systems interacting via short range interactions, for which a plausible justification has been provided. This is evident from the results of application to the nuclear problem (triton binding energy). However for the molecular problem investigated (a simplified  $H_2^+$  model) the AA does not fare so well. By the arguments shown in section 3, the factorization of  $v_{\alpha\alpha'}$  similar to eq. (11) is impossible.

We calculated the parameter values of  $\mu$  (given by eq. (12')) to be about  $\mu \lesssim 1/6$ ,  $\lesssim 1/5$  and  $\sim 1/3$  for Figs. 1a, 1b and 2, respectively. Between the S3 and S4 potentials,  $\mu$  is smaller for the S4 than for S3. In fact UAA is better for S4 than for S3, in agreement with what we expect from the definition of  $\mu$ . For Fig. 2 ( $H_2^+$  ion),  $\mu \sim 1/3$  much larger than the value of  $\mu$  in the previous cases. As a result in the case of Fig. 2, UAA does not fare well and this then is in agreement with the criterion for  $\mu$ . But in this case it seems that we are contradicting our previous work (first paper of reference 13). In that work we only investigated a limited class of potentials, each one of them describing the *same* physical system ( $^3H$ ) and so there was no great deal of variation of the parameter  $\mu$ . As a result the applicability of the approximation appeared then to be independent of  $\mu$ .

Of course, one has to be rather cautious, since in eq. (12), the coupling terms depend not only on  $[\omega_{\lambda'}(r) - \omega_{\lambda}(r)]^{-1}$ , but this multiplied by quantities involving derivatives of  $v_{\alpha\alpha'}(r)$ . Hence if the coupling potentials  $v_{\alpha\alpha'}(r)$  are so rapidly varying that its derivatives are large enough, one can upset the largeness of  $[\omega_{\lambda'}(r) - \omega_{\lambda}(r)]$ , then the parameter  $\mu$  may be not by itself a good criterion of validity of the UAA.

#### REFERENCES

1. L.I. Schiff, Quantum Mechanics, 3<sup>rd</sup> ed., McGraw Hill, Chapter 12.
2. Yu. A. Simonov, in Proceedings of the International Symposium on the Present Status and Novel Developments in the Nuclear Many-body Problems, Rome, 1972, edited by F. Calogero and C. Ciofi degli Atti (Editrice Compositori, Bologna, 1973), p. 527.
3. J.L. Ballot and M. Fabre de la Ripelle, Ann. Phys. (N.Y.) 127 (1980) 62.

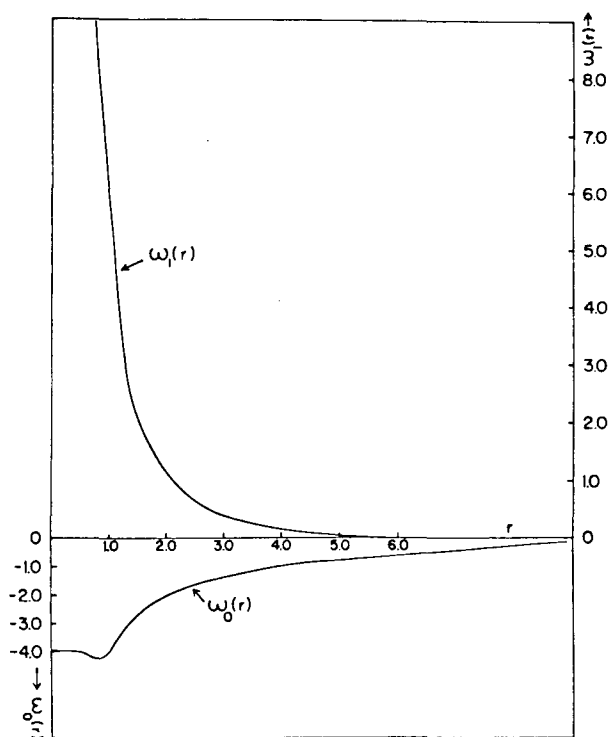


Fig. 2 - Plot of the lowest ( $\omega_0$ ) and first excited ( $\omega_1$ ) "eigenpotentials" (in atomic units) against  $r$  (in Bohr) for the fixed center  $H_2^+$  ion. ( $N = 8$ ).

It is also worth noting that the Born-Oppenheimer approximation is somewhat similar in spirit to the AA, however a direct correlation between the two schemes cannot be established. While the former method has its basis in the physics of the problem and is expected to be reliable when two of the particles are much heavier than the third, the latter method appears to have a more mathematical foundation than a physical basis. Thus the AA is just a mathematical technique for a system of coupled differential equations, insensitive to the physics of the problem, provided that the interaction terms  $M_{\alpha\alpha'}$  of eq. (5) can, at least, approximately be factorized in the manner of eq. (11). The AA can be a very convenient tool in nuclear, atomic or molecular problems involving any number of particles, whenever the criterion of eq. (11) is approximately satisfied. In particular while BO approximation is not expected to be so good for nuclear problems, the AA works well.

4. M. Fabre de la Ripelle, Few-body Systems 1 (1986) 181.
5. E.W. Schmid and H. Ziegelmann, The Quantum Mechanical Three-body Problem, in Vieweg Tracts in Pure and Applied Physics (Vieweg, Braunschweig, 1974); F.S. Levin, Proceedings of the Ninth International Conference on the Few-body Problem, ed. by F.S. Levin [North Holland, Amsterdam, 1981].
6. O.A. Yakubowski, Yad. Fiz. 5 (1967) 1312 [Sov. J. Nucl. Phys. 5 (1967) 937].
7. H.T. Coelho, W. Glöckle, A. Delfino, Phys. Rev. C22 (1980) 1796.
8. M. Born, R. Oppenheimer, Ann. Physik 84 (1927) 457.

9. J. Macek, *J. Phys. B* 1 (1968) 831.
10. C.D. Lin, *Phys. Rev. A* 10 (1974) 1986.
11. A.C. Fonseca, P.E. Shanley, *Ann. Phys. (N.Y.)* 117 (1979) 258; A.C. Fonseca, M.T. Pena, preprint on Faddeev-Born-Oppenheimer equations for Molecular three-body systems: I – application to  $H_2^+$ .
12. H.T. Coelho, A. Delfino Jr., N. Majlis, *Physics* 122B (1983) 74; H.T. Coelho, L. Consoni, M. Vallières, *Rev. Bras. de Física* 8 (1978) 734.
13. T.K. Das, H.T. Coelho, M. Fabre de la Ripelle, *Phys. Rev. C* 26 (1982) 2281; J.O. Ballot, M. Fabre de la Ripelle, J.S. Levinger, *Phys. Rev. C* 26 (1982) 2301; T.K. Das, H.T. Coelho, *Proc. Nucl. Phys. and Solid State Phys. Symposium, Mysore (India) (December 1985)*.
14. T.K. Das, H.T. Coelho, M. Fabre de la Ripelle, *Phys. Rev. C* 26 (1982) 2288.
15. G. Erens, J.L. Visschers, R. van Wageningen, *Ann. Phys. (N.Y.)* 67 (1971) 461.
16. B.R. Johnson, *J. Chem. Phys.* 69 (1978) 4678.
17. M.I. Haftel, V.B. Mandelzweig, *Ann. Phys. (N.Y.)* 150 (1983) 48.

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