Analysis of Completeness of Angular Equation Solutions in the Hyperspherical Method

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An analysis is made of the completeness of the solutions of the angular equation of the hyper-spherical method used in three body problems. In this method the relative distances between two particles and the third one are given by $r_1 = R \sin \alpha$, , $r_2 = R \cos \alpha$. Some relations obtained from this completeness between the non-adiabatic couplings of the radial equations are investigated. It is shown that for large R the contribution of states with positive eigenvalues is not negligible. This could explain ome discrepancies found using this method with either first or second order radial equations for atomic helium and electron-hydrogen systems.

Introduction

Hyperspherical coordinates have been used in Atomic Physics to obtain bound state solutions for three body systems[1−8] such a He and H$^-$. They have also been used for partial wave solutions and phase shifts of e-H scattering[2,8−11].

The hyperspherical coordinates consist of the angular variables for the two electrons and (α, R), related to the radial coordinates by:

$$r_1 = R \sin \alpha \quad , \quad r_2 = R \cos \alpha$$

where the new angular variable α is in the interval $(0, \pi/2)$.

The two electron wave function for a state with total angular momentum L and z-component M is expressed in the form:

$$\Psi^{KLM} = \sum_{u,l_1,l_2} (R^{5/2}\sin \alpha \cos \alpha)^{-1} F_\mu^{KL}(R) u_{\mu l_1 l_2}^L(R, \alpha) Y_{l_1 l_2}^{LM}(\Omega_1, \Omega_2) \tag{1.1}$$

where $Y_{l_1 l_2}^{LM}$, which represents an angular state in which the two electrons have angular momentum l_1 and l_2 respectively, is given by:

$$Y_{l_1 l_2}^{LM}(\Omega_1, \Omega_2) = \sum_{m_1,m_2} \langle l_1, m_1, l_2, m_2 | L, M \rangle Y_{l_1}^{m_1}(\Omega_1) Y_{l_2}^{m_2}(\Omega_2). \tag{1.2}$$

$$F_\mu^{KL}(R) u_{\mu l_1 l_2}^L(R, \alpha) Y_{l_1 l_2}^{LM}(\Omega_1, \Omega_2) \tag{1.1}$$

The index K is an energy quantum number that is discrete for a two electron bound state or continuous if one electron is free.

A generalization of the Bohr-Openheimer method is used to solve the Schrodinger equation by separation of variables. First one solves an equation for the angular

variable α which has R as a parameter. The eigenvalues labelled by the index μ, will be functions of R which represent interaction potentials in the radial equations. Both the angular and radial equations form actually infinite sets of coupled equations. For a numerical solution a cutoff l_{max} has to be introduced for l_1, l_2 in the angular equations as well as a limit on the number of potential curves used in the radial equations. The radial equations are second order differential equations which depend on the potential functions as a diagonal interaction and also on non-diagonal, non-adiabatic couplings, $P_{\mu\nu}(R)$ and $Q_{\mu\nu}(R)$ [1−4].

Assuming completeness of the solutions of the angular equations the second order radial equations can be replaced by a set of first order equations in which the $Q_{\mu\nu}$ couplings are eliminated.[12] Recent numerical calculations for the e-H system, using the second order radial equations with up to 6 potential curves, for both the $L = 0$, $L = 1$ binding energy[1−8] as well as for the low energy $L = 0$, phase shifts,[2,8−11] give very good agreement with calculations using variational methods.[13−16] On the other hand the first order radial equations without the $Q_{\mu\nu}$'s have also been used[8,9,17,18] giving results in disagreement with those obtained with the second order equations.

In this paper the completeness of the angular equations is discussed in connection with relations between the non-adiabatic couplings $Q_{\mu\nu}(R)$ and $P_{\mu\nu}(R)$. It is shown that for large R the contribution to these relations of eigenstates of the angular equations with positive eigenvalues $W_\mu(R) = 2U_\mu(R)R^2$, is not negligible.

In deriving the first order radial equations from truncated second order equations the sum of states used to eliminate the $Q_{\mu\nu}$'s extends only over a finite set of channel functions which for large R does not include an infinite set of states with positive $W_\mu(R)$. This could explain the discrepancies found in the results of the two formalisms.

In section II we give a brief review of the hyperspherical method. Throughout this paper we use atomic units $(m_e c^2 \alpha^2 = 1)$ In section III we consider some consequences of the completeness of the angular equations in connection with relations obtained from it, between the non-adiabatic couplings $Q_{\mu\nu}$ and $P_{\mu\nu}$ of the radial equations.

II. The angular and radial equations[1−4]

The angular equations for α are:

$$\left[\frac{\partial^2}{\partial \alpha^2} - \frac{l_1(l_1+1)}{\sin^2\alpha} - \frac{l_2(l_2+1)}{\cos^2\alpha} + 2R\left(\frac{Z}{\sin\alpha} + \frac{Z}{\cos\alpha} \right) + W_\mu^L(R) \right] u_{\mu l_1 l_2}^L - 2R \sum_{l_1', l_2'} C_{l_1 l_2 l_1' l_2'}^L(\alpha) u_{\mu l_1' l_2'}^L = 0 \qquad (2.1)$$

where

$$C_{l_1 l_2 l_1' l_2'}^L(\alpha) = \frac{1}{\cos\alpha} \sum_J (\tan\alpha)^J C_{l_1 l_2 l_1' l_2'}^{LJ} \qquad (2.2)$$

and the coefficients $C_{l_1 l_2 l_1' l_2'}^{LJ}$ are defined in terms of 3-J and 6-J symbols (Ref. [1]). The physical solutions in a state of total spin S of the electron pair must satisfy the Pauli principle:

$$u_{\mu l_1 l_2}^L \left(R, \frac{\pi}{2} - \alpha \right) = (-1)^{L+S+l_1+l_2} u_{\mu l_2 l_1}^L(R, \alpha) \qquad (2.3)$$

Hence they are obtained by imposing the boundary conditions at $\alpha = \pi/4$:

$$u_{\mu l_1 l_2}^L \left(R, \frac{\pi}{4} \right) = (-1)^{L+S+l_1+l_2} u_{\mu l_2 l_1}^L \left(R, \frac{\pi}{4} \right) \qquad (2.4)$$

$$\frac{d}{d\alpha} u_{\mu l_1 l_2}^L(R,,\alpha) \big|_{\alpha=\pi/4} = -(-1)^{L+S+l_1+l_2} \frac{d}{d\alpha} u_{\mu l_2 l_1}^L(R,\alpha) \big|_{\alpha=\pi/4} \qquad (2.5)$$

We shall consider the $u^L_{\mu l_1 l_2}$'s as components of a vector u^L_μ, with the pair $l_1 l_2$ as the component indices. From now on the superscript L will be omitted.

Invariance under parity implies that for any solution of given parity the components $u_{\mu l_1 l_2}$, are non-zero only if $(l_1 + l_2)$ is either even or odd according to the parity.

The solutions are normalized by:

$$\langle u_\mu | u_\nu \rangle = \sum_{l_1 l_2} \int^{\pi/2} u^L_{\mu l_1 l_2}(R, \alpha) u^L_{\nu l_1 l_2}(R, \alpha) d\alpha = \delta_{\mu\nu}$$

$$(2.6)$$

The radial equations are:

$$\left(\frac{\partial^2}{\partial R^2} + \frac{1}{4R^2} - 2U_\mu(R) + 2E \right) F_\mu(R) + \sum_\nu \left(2P_{\mu\nu}(R)\frac{\partial}{\partial R} + Q_{\mu\nu}(R) \right) F_\nu(R) = 0 \qquad (2.7)$$

where the potential function $U_\mu(R)$ is related to $W_\mu(R)$ by $2R^2 U_\mu(R) = W_\mu(R)$, and the non-adiabatic couplings are given by:

$$P_{\mu\nu}(R) = \langle u_\mu \frac{\partial}{\partial R} u_\nu \rangle \qquad (2.8)$$

$$Q_{\mu\nu}(R) = \langle u_\mu \frac{\partial^2}{\partial R^2} u_\nu \rangle \qquad (2.9)$$

The $Q_{\mu\nu}$'s can also be calculated by:

$$Q_{\mu\nu} = \dot{P}_{\mu\nu} - \langle \dot{u}_\mu | \dot{u}_\nu \rangle \qquad (2.10)$$

where a dot represents derivative with respect to R.

By insertion of a complete set of functions in the second term, and assuming completeness of the angular equations one obtains:

$$Q_{\mu\nu} = \dot{P}_{\mu\nu} - \sum_\lambda P_{\mu\lambda} P_{\nu\lambda} \qquad (2.11)$$

Using this relation one can replace the set of second order radial equations by the following et of first order equations:[12]

$$\frac{dF_\mu}{dR} + \sum_\nu P_{\mu\nu} F_\nu = G_\mu \ , \qquad (2.12)$$

$$\frac{dG_\mu}{dR} + \sum_\nu P_{\mu\nu} G_\nu = - \left(\frac{1}{4R^2} - 2U_\mu(R) + 2E \right) F_\mu \qquad (2.13)$$

where the $Q_{\mu\nu}$'s have been eliminated.

At $R = 0$ the equations decouple and the solutions are given in terms of Jacobi polynomials[19] $P^{l_1+1/2, l_2+1/2}(\cos 2\alpha)$, where j is an integer. The eigenvalues are $W_\mu(0) = m^2$, $(m = 2j + l_1 + l_2 + 2)$. We take the index μ to correspond to eigenstates of $W_\mu(R)$ in increasingly order so that $\mu = 1$ corresponds to the lowest potential curve. At $R = 0$ the eigenstates $W_\mu(0)$ are degenerate for $m > L+2$ but the degeneracy is removed for $R > 0$ by the interaction terms proportional to R.

At asymptotic large R, Macek[1] has proposed that the functions $u_{\mu l_1 l_2}(\alpha)$ for $\alpha < \frac{\pi}{4}$ are given in leading order in R^{-1} by the Coulomb one electron wave functions of a variable $\rho = R\alpha$, for bound states in the nucleus of charge Z corresponding to a state with angular momentum l_1 and energy $U_\mu = -\frac{Z^2}{2n_\mu^2}$, $(n_\mu > l_1)$. For $n_\mu > 1$ the Coulomb wave functions are degenerate. The degeneracy of the wave functions u_μ is removed when $\frac{1}{R^2}$ corrections are taken into account. The leading non-vanishing components u_μ will be given by

$$u_{\mu l_1 l_2} = a_{\mu l_1 l_2} \sqrt{\frac{R}{2}} \rho \Psi^{l_1}_{n_\mu}(\rho) \qquad (2.14)$$

where $\Psi^{l_1}_{n_\mu}(\rho)$ is a Coulomb wave function with energy U_μ as given above and angular momentum $l_1 < n_\mu$. The coefficients $a_{\mu l_1 l_2}$ are the solutions of the eigenvalue equations obtained using $\frac{1}{R^2}$ energy corrections and degenerate perturbation theory.[3]

Macek's assumption is well born out by numerical computations.

III. Investigation of completeness of the angular equations

The angular equations (2.1) with $R \neq 0$, due to the electron-electron interaction, form an infinite set.

When this interaction is neglected, the equations decouple as the angular momenta $l_1 l_2$ become constants of the motion. For a given pair of values of $l_1 l_2$, taking both values $S = 0, 1$ of the total spin the completeness of solutions of the angular equations follows from a general theorem[20] which applies when $l_1 \neq 0$ and $l_2 \neq 0$. If $l_1 = 0$ or $l_2 = 0$, one needs boundary conditions $u_{\mu l_1 l_2}(\alpha) = 0$ at the boundaries $\alpha = \left(0, \frac{\pi}{2}\right)$. At $R = 0$ the equations always decouple and the solution (with these boundary conditions), are given in terms of Jacobi polynomials $P^{l_1+1/2, +l_2+1/2}(x)$, $x = \cos 2\alpha$, which form a complete orthogonal set in the interval (-1,1), with measure $(1-x)^{2l_1+1}(1+x)^{2l_2+1}dx$. For $R > 0$, we shall assume that the solutions of the infinite system of equations (with the same boundary conditions) also form a complete set in the interval $\alpha = \left(0, \frac{\pi}{2}\right)$.

We shall investigate this completeness in connection with relations obtained from it, between the $Q_{\mu\nu}$'s and the $P_{\mu\nu}$'s.

First we consider the relation (2.11) espressing $Q_{\mu\nu}$'s in terms of $P_{\mu\nu}$'s. We have calculated, for a range of values of R, the values of Q_{11} as given by this relation and compared with the values obtained from (2.9) or (2.10). The angular equations for the case $L = 1, S = 1$, were calculated using a cutoff $l_{max} = 7$ for l_1 and l_2. The set of 15 solutions with the lowest potential curves were used in the sum of $P_{1\lambda}^2$ in (2.11). The results are given in Table I. One can see that for small values of R the results are in good agreement but they become increasingly different as R increases. This shows that for large R the contribution of solutions corresponding to higher potential curves becomes non-negligible.

One can also obtain additional relations between the $P_{\mu\nu}$'s and $Q_{\mu\nu}$'s involving derivatives of the eigenvalues $W_\mu(R)$.

Let us introduce a matrix $H = H_0 + RH_1$, where H_0 is diagonal with matrix element $l_1 l_2$ given by:

$$H_0 = \frac{d^2}{d\alpha^2} - \frac{l_1(l_1 + 1)}{\sin^2(\alpha)} - \frac{l_2(l_2 + 1)}{\cos^2 \alpha} \qquad (3.1)$$

and RH_1 corresponds to $(-2R^2)$ times the Coulomb interaction potential which has a non-diagonal piece due to the electron-electron interaction. Its R dependence has been made explicit.

Table I. This table gives the values of Q_{11} as a function of R calculated from the definition (2.9) or (2.10) as compared with the expression given by Eq. (2.11) obtained using completeness. The maximum value of λ taken in the sum was $\lambda = 15$, corresponding to the lowest 15 potential curves.

R	$Q_{1,1}$	$-\sum_{n=2}^{15} P_{1,n}^2$
0.02	-5.2339302E-003	-5.2244385E-003
2.02	-1.5405433E-002	-1.5377055E-002
4.02	-3.6085809E-002	-3.5821157E-002
8.02	-1.2543067E-002	-1.1368447E-002
12.02	-5.2493846E-003	-4.3807186E-003
18.02	-2.3191034E-003	-1.5383282E-003
24.05	-1.2990827E-003	-7.6045943E-004
30.05	-8.3152465E-004	-4.5427866E-004
38.05	-5.1839665E-004	-2.7093976E-004

The α-equation can then be written in vector form as $Hu_\mu = -W_\mu(R)u_\mu$. Taking first and second derivatives of this equation with respect to R one obtains:

$$H\dot{u}_\mu + H_1 u_\mu = -\dot{W}_\mu u_\mu - W_\mu \dot{u}_\mu \qquad (3.2)$$

$$H\ddot{u}_\mu + 2H_1\dot{u}_\mu = -\ddot{W}_\mu u_\mu - 2\dot{W}_\mu \dot{u}_\mu - W_\mu \ddot{u}_\mu \qquad (3.3)$$

Multiplying these equations by u_ν and integrating in α one obtains[4]:

$$(W_\mu - W_\nu)P_{\nu\mu} + \langle u_\nu|H_1|u_\mu\rangle = -\dot{W}_\mu\delta_{\mu\nu} \qquad (3.4)$$

$$(W_\mu - W_\nu)Q_{\nu\mu} + 2\langle u_\nu|H_1|\dot{u}_\mu\rangle = -\dot{W}_\mu\delta_{\mu\nu} - 2\dot{W}_\mu P_{\nu\mu} \qquad (3.5)$$

Eq. 3.4 is known as the Hellman-Feynman theorem. This equation allows one to compute $P_{\mu\nu}$ without using derivatives of the wave function, while the second equation will give $Q_{\mu\nu}$ in terms of the wave function and its first derivative. In addition for $\nu = \mu$ these equations give:

$$\dot{W}_\mu = -\langle u_\mu|H_1|u_\mu\rangle \qquad (3.6)$$

$$\ddot{W}_\mu = -2\langle u_\mu|H_1|\dot{u}_\mu\rangle \qquad (3.7)$$

If one assumes completeness of the solutions of the angular equations and introduce the complete set into Eq. 3.7 one obtains:

$$\ddot{W}_\mu = -2 \sum_\lambda (W_\mu - W_\lambda) P_{\mu\lambda} P_{\lambda\mu} \qquad (3.8)$$

or using Eq. 2.11

$$\frac{1}{2} \frac{\ddot{W}_\mu}{W_\mu} + Q_{\mu\mu} = - \sum_\lambda \frac{W_\lambda}{W_\mu} P_{\mu\lambda}^2 \qquad (3.9)$$

As $R \to \infty$, according to Macek's conjecture, the eigenvalues of the set of solutions of the angular equations approach the set of binding energies $2U_\mu = -\frac{Z^2}{n_\mu^2}$ of the Coulomb bound states. Then, since $W_\mu = 2U_\mu R^2$, Eq.(3.9) would give:

$$1 + (R^2 Q_{\mu\mu} = - \sum \frac{n_\mu^2}{n_\lambda^2} (R P_{\mu\lambda})^2 \qquad (3.10)$$

For large R, the coefficients in the asymptotic expansions of the $P_{\mu\nu}$'s and $Q_{\mu\nu}$'s can be calculated either by fitting numerical results or by using Coulomb wave functions with subsequent corrections in inverse powers of R. The leading terms in these expansions are $\frac{p_{\mu\nu}^{(1)}}{R}$ for $P_{\mu\nu}$ and $\frac{q_{\mu\nu}^{(2)}}{R^2}$ for $Q_{\mu,\nu}$. They can be obtained by using the asymptotic wave functions a function of the variable ρ and the following espression[1]

$$\frac{\partial}{\partial R} u_\mu = \frac{1}{R} \left(\frac{1}{2} + \rho \frac{\partial}{\partial \rho} \right) u_\mu(\rho) \ . \qquad (3.11)$$

If $n_\mu = n_\nu$ it has been shown[4] that $p_{\mu\nu}^{(1)} = 0$ and the leading term becomes of order R^{-3}. For $\mu = 1, q_{11}^{(2)}$ calculated numerically by taking the value of $R^2 Q_{11}$ at $R = 40$ agrees very well with the theoretical value which is $q_{11}^{(2)} = -.75$. This result is independent of the values of L, S and parity. Taking this result into Eq. 3.10, the left hand side becomes positive whereas the right hand side is always negative. Therefore the use of completeness of the solutions of the angular equations seems to lead to a contradiction.

This paradox however can be resolved by remarking that Eq.(3.10) is obtained by interchanging the order of taking the limit $R \to \infty$ with the summation of an infinite series. This interchange would be allowed if the convergence of the solutions of the equations to bound state Coulomb wave functions as $R \to \infty$ were uniform, that is, if given an ϵ one could find an $R(\epsilon)$ such that

for $R > R(\epsilon)$, $| < u_\mu(R)|u_{C\mu} > -1| < \epsilon$ for all solutions $u_\mu(R)$ whose limiting values are $u_{C\mu}$. One can indeed find that the convergence is not uniform. For any finite value of R, as large as one wants, there is always an infinite discrete set of solutions whose eigenvalues are positive. The separation between the energy levels $2U_\mu(R)$ would approach zero as $R \to \infty$. The corresponding wave functions will, to order $O(R^{-2})$, be given by Coulomb wave functions with the corresponding *positive* eigenvalues. For any finite R it is the contribution from this infinite set of positive eigenvalue solutions that give a non-negligible contribution to the sum over states in the relations (2.11) and (3.9). Indeed taking (3.9) for $\mu = 1$, for large R, $W_\mu \to -R^2$, and the left hand side becomes very dose to $(1 - .75) = .25$. It is then clear that, in order for the right hand side to become positive, the states with positive energy have to overcome the contribution from the negative energy bound states.

These results also hold when the electron-electron interaction is neglected and the angular equations decouple.

The correctness of this analysis was tested for Q_{11}, in Eq.(2.1) for an arbitrarily large R.

For large R, and $\nu = 1$, $(n_\nu = 1)$, Eqs. (2.8,10) and (3.11) give:

$$p_{\mu1}^{(1)} = \frac{2}{R} \int u_{\mu,0L}(\rho) \left(\frac{1}{2} + \rho \frac{\partial}{\partial \rho} \right) u_{1,0L}(\rho) d\rho \quad (3.12)$$

$$q_{11}^{(2)} = -\frac{2}{R} \int \left[\left(\frac{1}{2} + \rho \frac{\partial}{\partial \rho} \right) u_{1,0L}(\rho) \right]^2 d\rho \qquad (3.13)$$

We have calculated $p_{\mu1}^{(1)}$ analytically using Eq.(2.14) for the asymptotic wave functions u_μ. For states with a given n_μ the result is:

$$p_{\mu1}^{(1)} = a_{\mu,0L} \cdot 8\sqrt{n_\mu} \left(\frac{n_\mu}{n_\mu^2 - 1} \right)^2 \left(\frac{n_\mu - 1}{n_\mu + 1} \right)^{n_\mu} \quad (3.14)$$

Since for states with the same n_μ, $\Sigma_\mu a_{\mu,0L}^2 = 1$, it will not be necessary to determine the coefficients $a_{\mu,0L}$ in order to obtain the sum of the squares $S_1 = \Sigma_\mu (p_{\mu1}^{(1)})^2$. We have done this sum numerically for states with n_μ, up to $n_\mu = 10^6$. The result was $S_1 = .423753113$.

On the other hand we calculated what should be a $p_{\eta 1}^{(1)}$, if in Eq.(3.12) $u_{\eta,0L}(\rho)$ is replaced by $\sqrt{\frac{R}{2}}\Psi_\eta^0(\rho)$ where $\Psi_\eta^0(\rho)$ is a free Coulomb wave function corresponding to a state of angular momentum $l = 0$

and positive energy $2U_\eta = \frac{1}{\eta^2}$. We used for the free Coulomb wave function an integral representation given in Ref.[19], pg.539, Eq.(14.3.3). The result was:

$$p_{\eta 1}^{(1)} = \left(\frac{4\eta^3}{(1+\eta^2)^2} \left(\frac{2\pi\eta}{1-\exp(-2\pi\eta)} \right)^{1/2} \exp\left(-2\eta\tan^{-1}\left(\frac{1}{\eta}\right)\right) \right) \tag{3.15}$$

With the normalization used in Ref.[19] the sum of the squares of $p_{\eta 1}^{(1)}$ for the free states will be given by

$$S_2 = \int_0^\infty (p_{\eta 1}^{(1)})^2 \frac{2}{\pi} \frac{d\eta}{\eta^2} \ . \tag{3.16}$$

This integral was calculated numerically giving $S_2 = 0.326246887$. Adding this to the sum of $(p_{\mu,1}^{(1)})^2$ for the bound states one obtains, within the nine digit precision of the numerical calculation, the exact value of $-q_{11}^{(2)} = .75$.

We conclude from this analysis that at large R the contribution from eigenstates of the angular equations with positive eigenvalues $W_\mu(R)$ to the relations between the $P_{\mu\nu}$'s and $Q_{\mu\nu}$'s obtained from completeness become increasingly important and cannot be neglected. This could explain some differences between results obtained, especially for phase shifts, when using a set of truncated first order equations as compared to those using second order equations.

Acknowledgements

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