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K-harmonic Solution for Three Bound Unequal Particles*

H. T. COELHO, L. CONSONI
Departamento de física, Universidade Federal de Pernambuco, 50000 Recife, PE

and

M. VALLIÈRES
Department of Physics, McMaster University, Hamilton, Ontario, Canada

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The three bound unequal particles problem using K-harmonics is analysed concerning how the natur'e of interactions and asymmetries of the system will affect convergence of the solutions. Coulomb interaction which gives closed expressions for the matrix elements of thepotential inthe method is discussed.

O problema de três partículas distintas ligadas é analisado pelo método dos harmônicos K, tendo em vista como a natureza das interações e assimetrias do sistema afetarão a convergência das soluções. A interação Coulombiana, a qual dá expressões exatas do método, para os elementos de matrizes do potencial, é discutida.

1. INTRODUCTION

During the last decade much progress has been made in the study of the three-body problem in quantum mechanics. Faddeev's equations[1] and the hyperspherical harmonic approach[2,3] (also known as K-harmofics) allow one

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to handle the problem exactly. This in contrast to the older variational method which is very dependent on the choice of a trial wave function. Many three-body problems have been studied recently with these newer techniques[4] but most of them involve three particles with equal masses.

For bound systems the K-harmonic method treated according to Simonov[2,3] has proved to be very powerful and well accepted in the scientific community[5-7]. Some recent efforts[7] have even extended this method to scattering problems. Our aims in this paper are: 1) To extended thismethod, in a systematic way, to three-body systems of unequal particles. In particular, we consider Coulomb pairwise interaction since in this case, closed formulas can be obtained for most expressions in the formalism. (It is worth mentioning that Simonov[3] has previously suggested this for identical particle systems but did not carry out the calculation). 2) To analyse previous work on the three-body problem for unequal particles. For instance, Zickendraht[8] and Schoucri and Darling[9] have dealt with aspects of this problem using a more cumbersome formalism than the simple, elegant and currently well-accepted K-harmonic approach according to Simonov[2]. In this paper we also discuss the work in reference 9 which, in part, is incorrect.

Many physical systems can be considered as three bound unequal particle systems: $e^-e^+e^-$, $p\,e^+e^-$, Mg^{24} (as O^{16} + a + a) etc. For definiteness we analyse the system $e^-e^+e^-$ and discuss convergence of the solution. Comparison is made with previous methods. It is worth mentioning apaper by Amado, Coelho[10] wherein the unequal mass three body problem is analysed in one dimension using K-harmonic approach. That is done to conceptualize the hyperspherical method in three dimensions. In this paper we find possible to analyse its results on the basis of reference 10.

In sections 2 and 3 we introduce the method; in section 4 the Coulomb pairwise interaction is discussed in detail, and in section 5, we summarize our results. Appendices to clarify some of our mathematical manipulations are given at the end.

2. METHOD

The non-relativistic Schrödinger equation for three non-interacting particles of unequal masses m_1, m_2, m_3, may be written as

$$(-\sum_{i=1}^{3} \frac{\hbar^2}{2m_i} \nabla_i^2)\ \bar{\Psi} = \varepsilon\ \bar{\Psi}(\vec{r}_1, \vec{r}_2, \vec{r}_3) \tag{2.1}$$

If one introduces Jacobi coordinates* (see also the paper by Raynal in ref. 7)

$$\vec{\eta} = \frac{1}{a} (\vec{r}_1 - \vec{r}_2) \ ,$$

$$\vec{\xi} = \frac{1}{b} \left(\frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2} - \vec{r}_3\right), \tag{2.2}$$

$$\vec{R} = \frac{1}{\sqrt{mM}} \Sigma\, m_i\, \vec{r}_i \ ,$$

where

$$M = \sum_{i=1}^{3} m_i \ , \quad m = \frac{1}{M} \sum_{i<j} m_i\, m_j \ ,$$

$$a = \left[\frac{m(m_1 + m_2)}{m_1\, m_2}\right]^{1/2} ,$$

$$b = \left[\frac{m\, M}{m_3(m_1 + m_2)}\right]^{1/2} ,$$

eq. (2.1) may be rewritten, after taking out the CM motion, as

$$-\frac{\hbar^2}{2\,m} \left(\nabla^2_{\vec{\xi}} + \nabla^2_{\vec{\eta}}\right)\psi = E\psi. \tag{2.3}$$

The above expression is identical to the Schrödinger equation[2] for three non-interacting particles of equal masses m.

In a classic paper, Simonov[2] proposed a method to solve eq.(2.3), now called the K-harmonics or hyperspherical harmonic approach. It consists in selecting the most important variables and then to expand the wave function $\psi(\vec{\xi},\vec{\eta})$ (or any other physical quantity of interest) in a complete set of functions, depending on all other variables, in the following way

$$\psi(\vec{\xi},\vec{\eta}) = \sum_{K\alpha} \chi_{K\alpha}(\rho)\, u_{K\alpha}(\hat{\xi},\hat{\eta},\theta) \; , \qquad (2.4)$$

where $\rho^2 = \xi^2 + \eta^2$ (the square of the length of the six-vector $(\vec{\xi},\vec{\eta})$), and $\theta (0 \leq \theta \leq \pi/2)$ by $\eta = \rho\cos\theta$ and $\xi = \rho\sin\theta$. A complete orthonormal set of angular functions $u_{K\alpha}$ has been derived by Simonov[2,7]. They are the angular part of the homogeneous polynomial $P_{K\alpha}$ of degree K which satisfy the Laplace equation and a stands for all other necessary quantum numbers.

For the important case of total angular momentum $L=0$ the angular functions have a simplified dependence on the angles, depending only on ϕ and θ where ϕ is defined by $\cos\phi = \hat{\eta}\cdot\hat{\xi}$. Furthermore, only one extra quantum number, v, besides K, is necessary to specify the states. As we will see, the $L=0$ case will give closed expressions for the matrix elements of some important pairwise interactions.

If we substitute the expansion (2.4) into the Schrödinger equations, we find that the radial functions $\chi_{K\nu}(\rho)$ should satisfy a system of coupled differential equations[11]. In the case where an interaction is considered between the particles, these equations involve an effective radial potential defined as the matrix elements of the physical potential in the angular hyperspherical functions.

The angular functions $u_{K\nu}$ are given[2,3] by

$$u_{K\nu} \to \begin{cases} u_{K\nu}^{(c)} = \left[\dfrac{K+2}{\pi^3(1+\delta_{\nu 0})}\right]^{1/2} \cos(\lambda\nu)\, A^{\nu} \times P^{(\nu,0)}_{\frac{1}{4}K-\frac{1}{2}\nu}(1-2A^2) \\ u_{K\nu}^{(s)} = \left[\dfrac{K+2}{\pi^3}\right]^{1/2} \sin(\lambda\nu)\, A^{\nu} \times P^{(\nu,0)}_{\frac{1}{4}K-\frac{1}{2}\nu}(1-2A^2), \end{cases} \tag{2.5}$$

where $\nu = K/2, K/2-2, \ldots \geq 0$ and the relations

$$\begin{aligned} \cos 2\theta &= A\cos\lambda, \\ \sin 2\theta \cos\phi &= A \sin\lambda, \end{aligned} \tag{2.5'}$$

for $0 \leq A \leq 1$ and $0 \leq \lambda \leq 2$ were used.

The angular functions $u_{K\nu}^{(c)}$ $(\nu \geq 0)$ and $u_{K\nu}^{(s)}$ $(\nu > 0)$ form a complete orthonormal set which satisfy the relation[2]

$$\int u_{K'\nu'}^{(j')*}\, u_{K\nu}^{(j)}\, d\Omega_6 = \delta_{j'j}\,\delta_{K'K}\,\delta_{\nu'\nu}, \tag{2.6}$$

where $d\Omega_6 = \pi^2 A\, dA\, d\lambda$. We should notice that $\psi(\vec{\xi},\vec{\eta})$ is now written as

$$\psi(\vec{\xi},\vec{\eta}) = \sum_{K\nu}\left[\chi_{K\nu}^{(c)}(\rho)\, u_{K\nu}^{(c)} + \chi_{K\nu}^{(s)}(\rho)\, u_{K\nu}^{(s)}\right] \tag{2.7}$$

We will call the $u_{K\nu}^{(c)}$'s the *cosine states* and the $u_{K\nu}^{(s)}$'s *the sine states*. Under particle permutations, $u_{K\nu}^{(c)}$'s with ν a multiple of three are *symmetric* functions[2], while $u_{K\nu}^{(s)}$'s with these values of ν are *antisymmetric* functions[2].

The radial system of differential equations is given as the following[1]:

$$\left[\frac{1}{\rho^5}\frac{d}{d\rho}\left(\rho^5 \frac{d}{d\rho}\right) - \frac{K(K+4)}{\rho^2} \ldots (@I)\right] \chi_{K\nu}^{(i)}(\rho) \tag{2.8}$$

$$+ \sum_{K'\nu'j'=c,s} V^{(jj')}_{K\nu,K'\nu'}(\rho)\, \chi^{(j')}_{K'\nu'}(\rho) = 0,$$

where

$$V^{(jj')}_{K\nu,K'\nu'}(\rho) = -\left(\frac{2m}{\hbar^2}\right) < u^{(j)}_{K\nu} \mid V_{123}(\vec{\xi},\vec{\eta}) \mid u^{(j')}_{K'\nu'} >_{\Omega_6}$$

and

$$k^2 = \left(\frac{2m}{\hbar^2}\right) |E|, \qquad (2.9)$$

E being the energy of the bound state.

The operator or function V_{123} is the interaction potential among the three particles. It's very important to emphasize that if V_{123} is chosen to be a local potential, the K-harmonic method keeps that nature of the interaction. Technically the problern is clearly quite similar to the three -body problem of equal masses[2,3]. Two fundamental differences are worth mentioning: particie symmetry ir now broken and $V_{123}(\vec{\xi},\vec{\eta})$ will depend on the rnasses m_1, m_2, m_3.

3. PROPERTIES OF THE MATRIX ELEMENTS $V^{(j,j')}_{K\nu,K'\nu'}$

The explicit form of eq. *(2.9)* is for the *cosine states*

$$V^{(c,c)}_{K\nu,K'\nu'}(\rho) \equiv V^{(c)}_{K\nu,K'\nu'}(\rho) \equiv -\left(\frac{2m}{\hbar^2}\right) \frac{1}{2\pi} \times$$

$$\times \left[\frac{(K+2)\quad(K+2)}{(1+\delta_{\nu 0})\quad(1+\delta_{\nu' 0})}\right]^{1/2} 0 \left[\cos(\ell\lambda) + \cos(\ell'\lambda')\right], \qquad (3.1)$$

$$\nu',\nu \geq 0 ,$$

and for the *sine states*

$$V^{(s,s)}_{K\nu,K'\nu'}(\rho) \equiv V^{(s)}_{K\nu,K'\nu'}(\rho) = -\left(\frac{2m}{\hbar^2}\right)\frac{1}{2\pi} \times$$

$$\times \left[(K+2)(K'+2)\right]^{1/2} O\left[-\cos(\ell\lambda) + \cos(\ell'\lambda)\right] ,$$

$$\nu', \quad \nu > 0 \tag{3.2}$$

and for the *Mixed States*

$$V^{(c,s)}_{K\nu,K'\nu'}(\rho) = V^{(M)}_{K\nu,K'\nu'}(\rho) = -\left(\frac{2m}{\hbar^2}\right)\frac{1}{2\pi} \times$$

$$\times \left[\frac{(K+2)(K'+2)}{(1+\delta_{\nu 0})}\right]^{1/2} O\left[\sin(\ell\lambda) \pm \sin(\ell'\lambda)\right] , \quad \begin{Bmatrix} \nu' \geq \nu \\ \nu' < \nu \end{Bmatrix}$$

$$\nu' > 0 , \quad \nu \geq 0 \tag{3.3}$$

where the operator O is defined as

$$O \equiv \left[\int_0^1 dA\, A\, A^{\nu}\, P^{(\nu,0)}_{\frac{1}{4}K-\frac{1}{2}\nu}(1-2A^2)\, A^{\nu'}\, P^{(\nu',0)}_{\frac{1}{4}K'-\frac{1}{2}\nu'}(1-2A^2) \times\right.$$

$$\left.\times \int_0^{2\pi} d\lambda\, V_{123}(\vec{\xi},\vec{\eta})\right]$$

and $\ell = \nu + \nu'$ and $\ell' = |\nu' - \nu|$, and the following relations have been used

$$\cos(\nu\lambda)\cos(\nu'\lambda) = \frac{1}{2}\left[\cos(\ell\lambda) + \cos(\ell'\lambda)\right],$$

$$\sin(\nu\lambda)\sin(\nu'\lambda) = \frac{1}{2}\left[-\cos(\ell\lambda) + \cos(\ell'\lambda)\right],$$

$$\cos(\nu\lambda)\sin(\nu'\lambda) = \frac{1}{2}\left[\sin(\ell\lambda) \pm \sin(\ell'\lambda)\right], \quad \begin{matrix} \nu' \geq \nu \\ \nu' < \nu \end{matrix}$$

An obvious property of eq. (2.9) is that $V^{(c,s)}_{K\nu,K'\nu'}(\rho) = V^{(s,c)}_{K'\nu',K\nu}(\rho)$. If we restrict ourselves to pairwise inter'actions only, V_{123} may be written as

$$V_{123}(\vec{\xi},\vec{\eta}) = V_{12}(a\eta) + V_{13}(|b\vec{\xi} + c\vec{\eta}|) + V_{23}(|b\vec{\xi} - d\vec{\eta}|), \tag{3.4}$$

where

$$c = \frac{m_2 a}{m_1 + m_2} \quad \text{and} \quad d = a - c .$$

The potential V_{123} can always be expressed as a function of ρ, A and X. In order to do that we first define

$$x = (\eta^2 - \xi^2)/\rho^2 \text{ and } y = 2\vec{\xi}\cdot\vec{\eta}/\rho^2. \tag{3.5}$$

It is straightforward to show that

$$|\alpha\vec{\xi} + \beta\vec{\eta}| = \rho\left(\frac{\alpha^2 + \beta^2}{2}\right)^{1/2}\left[1 - \left(\frac{\alpha^2 - \beta^2}{\alpha^2 + \beta^2}\right)x + \left(\frac{2\alpha\beta}{\alpha^2 + \beta^2}\right)y\right]^{1/2} . \tag{3.5'}$$

It is possible and convenient to express the coefficients of x and y as a cosine and a sine respectively of a common angle. Using eqs.(2.5') and (3.5) we finally obtain

$$a\eta = \rho\,\frac{a}{\sqrt{2}}\,(1 + A\cos\lambda)^{1/2} ,$$

$$|b\vec{\xi} + c\vec{\eta}| = \rho\left(\frac{b^2 + c^2}{2}\right)^{1/2}\left[1 - A\cos(\lambda + \delta)\right]^{1/2} ,$$

$$|b\vec{\xi} - d\vec{\eta}| = \rho\left(\frac{b^2 + d^2}{2}\right)^{1/2}\left[1 - A\cos(\lambda + \delta')\right]^{1/2} ,$$

where

$$\sin\delta = \frac{2bc}{b^2 + c^2} \quad \text{and} \quad \cos\delta = \frac{b^2 - c^2}{b^2 + c^2} ,$$
$$\sin\delta' = -\frac{2bd}{b^2 + d^2} \quad \text{and} \quad \cos\delta' = \frac{b^2 - d^2}{b^2 + d^2} \tag{3.6}$$

Suppose that the two-body potential $V_{ij}(r_{ij})$ can for small $r_{ij} \equiv r$ be expanded in the following way

$$V_{ij}(r) = \ldots + \frac{a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + \ldots = \sum_{t=-\infty}^{+\infty} a_t r^t. \quad (3.7)$$

All potentials in physics somehow have such expansion. For instance, the term a_{-1} corresponds to a Coulomb potential and Yukawa type potentials, etc. That means that basically in the end we may be looking at a standard integral of the type

$$J_n(p,\tau) = \int_0^{2\pi} d\lambda \frac{\begin{Bmatrix} \sin(n\lambda) \\ \cos(n\lambda) \end{Bmatrix}}{(1 - A\cos(\lambda+\tau))^p} = \begin{Bmatrix} -\sin(n\tau) \\ \cos(n\tau) \end{Bmatrix} \hat{J}_n(p), \quad (3.8)$$

where

$$\hat{J}_n(p) = \int_0^{2\pi} dh \frac{\cos(nh)}{(1 - A\cos\lambda)^p} , \quad (3.8')$$

where n = R, R' and p is any positive or negative real number which appear in eqs. (3.1), (3.2) and (3.3), if the integration over h is carried out first. We should also notice that r = 6, δ' and $p = t/2$. Depending onthe value of p, $J_n(p,\tau)$ may converge or not, and conrequently $V^{(j,j')}_{K\nu,K'\nu'}(\rho)$ exists or not in the K-harmonic approach. So this is a fundamental point. For instance, eq. (3.1) for K = K' = 0, may be written as

$$V^{(C,C)}_{00,00}(\rho) = -\left(\frac{2m}{\hbar^2}\right)\frac{1}{\pi}\int_0^1 dA\, A \int_0^{2\pi} d\lambda \sum_{i<j} V_{ij}$$

where looking only at the contribution coming from V_{12}, one can obtain

$$-\left(\frac{2}{\hbar^2}\right)\frac{16}{\pi}\int_0^1 dz\, z^2 \sqrt{1-z^2}\, V_{12}(a\rho z),$$

where $z = \cos\theta$. Let $V_{12}(a\rho z) \propto 1/z^{2p}$ which implies that the above integral only converges[1]* if $p \leq 1$. If this is the situation for the $K = K' = 0$

case, one can conclude that in eq (3.8) only $p \lesssim 1$ can be corisidered. As a result, a pairwise interaction, like the 6–12 potential, sometimes used in Molecular physics[13], can not be handled in the K-harmonic approach.'

Now let's return to the evaluation of expression (3.8). It's possible to show (see appendix) that for $p \lesssim 1$

$$J_n(p,\tau) = \left\{\begin{matrix} -\sin(n\tau) \\ \cos(n\tau) \end{matrix}\right\} \frac{2\pi A^n}{2^n} \times$$

$$\times \frac{(p+n-1)!}{n!\,(p-1)!} F\left(\frac{1}{2}(p+n), \frac{1}{2}(p+n+1); n+1; A^2\right), \qquad (3.9)$$

where F is the Gauss hypergeometric function.

If $J_n(p,\tau)$ is known, we are basically left with integrals in A in order to have the effective potential

$$V^{(j,j')}_{K\nu,K'\nu'}(\rho) .$$

Only for very few cases of two-body potentials we can obtain

$$V^{j,j'}_{K\nu,K'\nu'}(\rho)$$

in closed form.

4. APPLICATION TO COULOMB INTERACTION

For some special forms of the pairwise interaction, the matrix elements, $V^{(j,j')}_{K\nu,K'\nu'}(\rho)$, can be obtained in closed form. This is the case, for instance, for the harmonic oscillator[11,21], inverse square[22], Gaussian[3] and square well[3].

A case of pratical interest is the Coulomb-Kepler pairwise interaction. We can see by the use of eqs. (3.1) - (3.6), that it is convenient to set

$$V^{(c)}_{K\nu,K'\nu'} = C^{\nu\nu'}_{KK'}/\rho \ , \quad V^{(s)}_{K\nu'K'\nu'} = S^{\nu\nu'}_{KK'}/\rho$$

and

$$V^{(M)}_{K\nu,K'\nu'} = M^{\nu\nu'}_{KK'}/\rho \ ,$$

where

$$C^{\nu\nu'}_{KK'} = -\left(\frac{2m}{\hbar^2}\right)\frac{1}{2\pi}\left[\frac{(K+2)\quad(K'+2)}{(1+\delta_{\nu 0})(1+\delta_{\nu' 0})}\right]^{1/2} \times \Big[Z'_{12}\ ((-)^{\ell} J^{\nu\nu'}_{KK'}(\ell) + (-)^{\ell'} J^{\nu\nu'}_{KK'}(\ell')) + Z'_{13}(J^{\nu\nu'}_{KK'}(\ell) \times \cos(\ell\delta) + J^{\nu\nu'}_{KK'}(\ell')\ \cos(\ell'\delta)) + Z'_{23}(J^{\nu\nu'}_{KK'}(\ell) \times \cos(\ell\delta') + J^{\nu\nu'}_{KK'}(\ell')\ \cos(\ell'\delta'))\Big] \ , \tag{4.6}$$

$$S^{\nu\nu'}_{KK'} = -\left(\frac{2m}{\hbar^2}\right)\frac{1}{2\pi}\Big[(K+2)\quad(K'+2)\Big]^{1/2}\ \Big[Z'_{12}(-)^{\ell+1} \times J^{\nu\nu'}_{KK'}(\ell) + (-)^{\ell'} J^{\nu\nu'}_{KK'}(\ell')) + Z'_{13}(-J^{\nu\nu'}_{KK'}(\ell) \times \cos\ (\ell\delta) + J^{\nu\nu'}_{KK'}(\ell')\ \cos(\ell'\delta)) + Z'_{23}\ (-J^{\nu\nu'}_{KK'}(\ell) \times \cos(\ell\delta') + J^{\nu\nu'}_{KK'}(\ell')\ \cos(\ell'\delta'))\Big] \ , \tag{4.7}$$

$$M^{\nu\nu'}_{KK'} = +\left(\frac{2m}{\hbar^2}\right)\frac{1}{2\pi}\left[\frac{(K+2)\quad(K'+2)}{(1+\delta_{\nu 0})}\right]^{1/2}$$

$$\times \Big[Z'_{13}\ (J^{\nu\nu'}_{KK'}(\ell)\ \sin(\ell\delta) \pm J^{\nu\nu'}_{KK'}(\ell')\ \sin(\ell'\delta))$$

$$+ Z'_{23} \left(J^{\nu\nu'}_{KK'}(\ell) \sin(\ell\delta') \pm J^{\nu\nu'}_{KK'}(\ell') \sin(\ell'\delta')\right)\Big], \left\{ \begin{matrix} \nu' \geq \nu \\ \nu' < \nu \end{matrix} \right\},$$

(4.8)

and

$$Z'_{12} = Z_{12}\, e^2 \sqrt{2/a}, \quad Z'_{23} = Z_{23}\, e^2 \sqrt{2/(b^2+d^2)}, \quad Z'_{13} = Z_{13}\, e^2 \sqrt{2/(b^2+c^2)},$$

$$J^{\nu\nu'}_{KK'}(n) = \int_0^1 \hat{J}_n\left(\tfrac{1}{2}\right) A^{\nu} P^{(\nu,0)}_{\frac{1}{4}K-\frac{1}{2}\nu}(\;)A^{\nu'} P^{(\nu',0)}_{\frac{1}{4}K'-\frac{1}{2}\nu'}(1-2A^2)\, A\, dA, \qquad (4.9)$$

where n = L, ℓ' and $\hat{J}_n\left(\frac{1}{2}\right)$ is defined by eq. (3.8').

A convenient expression for the Jacobi polynomial $P^{(\nu,0)}_{\frac{1}{4}K-\frac{1}{2}\nu}(1-2A^2)$ is given by[14]

$$P^{(\nu,0)}_{\frac{1}{4}K-\frac{1}{2}}(1-2A^2) = \sum_{s=0}^{\frac{1}{4}K-\frac{1}{2}\nu} \frac{\Gamma(1+\frac{1}{4}K+\frac{1}{2}\nu+s)\,(-)^s}{s!\,(\frac{1}{4}K-\frac{1}{2}\nu-s)!\,\Gamma(1+\nu+s)} A^{2s}$$

which can be used in eq. (4.9):

$$J^{\nu\nu'}_{KK'}(n) = \frac{1}{2} \sum_{s=0}^{\frac{1}{4}K-\frac{1}{2}\nu} \frac{(1+\frac{1}{4}K+\frac{1}{2}\nu+s)\,(-)^s}{s!\,(\frac{1}{4}K-\frac{1}{2}\nu-s)!\,\Gamma(1+\nu+s)}$$

$$\times \sum_{s'=0}^{\frac{1}{4}K'-\frac{1}{2}\nu'} \frac{(1+\frac{1}{4}K'+\frac{1}{2}\nu'+s')\,(-)^{s'}}{s'!\,(\frac{1}{4}K'-\frac{1}{2}\nu'-s')!\,\Gamma(1+\nu'+s')} I_n(s+s')$$

(4.10)

where n = L, ℓ' and

$$I_n(s+s') = \frac{2\pi}{2^{3n}} \times \frac{(2n)!}{(n!)^2} \int_0^1 z^{(\ell+n)/2} \; F_{1/2}(n,z) \times z^{s+s'} \, dz \, , \qquad (4.11)$$

and $z = A^2$,

$$F_{1/2}(n,z) = F\left(\tfrac{1}{4}(2n+1), \tfrac{1}{4}(2n+3);\ 1+n\ ;\ z\right).$$

A recurrence relation (see appendix B) can be used to calculate $I_n(s+s')$:

$$I_n(s+s') = \frac{16\sqrt{2}}{(2n+1)(2n+3) + 4(\ell+n+2(s+s')+2)(\ell-n+2(s+s'))}$$

$$+ \frac{4(\ell+n+2(s+s'))(\ell-n+2(s+s'))}{(2n+1)(2n+3)+4(\ell+n+2(s+s')+2)(\ell-n+2(s+s'))} I_n(s+s'-1)$$

(4.12)

where for $n = \ell$

$$I_\ell(0) = \frac{16\sqrt{2}}{(2\ell+1)(2\ell+3)} \, , \qquad (4.13)$$

and for $n = \ell'$

$$I_{\ell'}(0) = \frac{4\pi\ (2\ell')!}{2^{3\ell'}\ (\ell'!)^2} \times \frac{1}{(\ell+\ell'+2)}$$

$$\times\ {}_3F_2\left(\frac{2\ell'+1}{4}, \frac{2\ell'+3}{4}, \frac{\ell+\ell'+2}{2};\ \ell'+1, \frac{\ell+\ell'+4}{2};\ 1\right) \qquad (4.14)$$

The knowledge of $C^{\nu\nu'}_{KK'}$, $S^{\nu\nu'}_{KK'}$ and $M^{\nu\nu'}_{KK'}$ allows us to write eq. (2.8) as

$$\left[\frac{1}{\rho^5}\frac{d}{d\rho}\left(\rho^5\frac{d}{d\rho}\right) - \frac{K(K+4)}{\rho^2} - k^2\right]\chi^{(c)}_{K\nu}(\rho)$$

$$+\frac{1}{\rho}\sum_{K'\nu'}\left[C^{\nu\nu'}_{KK'}\chi^{(c)}_{K'\nu'} + M^{\nu\nu'}_{KK'}\chi^{(s)}_{K'\nu'}(\rho)\right] = 0 \qquad (4.15)$$

which can be solved numerically[11,15] easily. Similar equation can also be written for sine χ states.

The change of variable $\chi^{(j)}_{K\nu}(\rho) = \rho^{-5/2}\,\phi^{(j)}_{K\nu}(\rho)$ can further simplify the system as follows

$$\left[\frac{d}{d\rho^2} - \frac{\Lambda(\Lambda+1)}{\rho^2} - k^2\right]\phi^{(c)}_{K\nu}(\rho) + \frac{1}{\rho}\sum_{K'\nu'}\left[C^{\nu\nu'}_{KK'}\phi^{(c)}_{K'\nu'}(\rho)\right.$$

$$\left. + M^{\nu\nu'}_{KK'}\phi^{(s)}_{K'\nu'}(\rho)\right] = 0\,, \qquad (4.16)$$

where $\Lambda = K + 3/2$ and these equations have the usual form known in the two-body problem.

The symmetry of a particular system will impose conditionson the allowed values of $C^{\nu\nu'}_{KK'}$, $S^{\nu\nu'}_{KK'}$ and $M^{\nu\nu'}_{KK'}$.

5. CONCLUSIONS

In this paper we have dealt with the use of the K-harmonic method[2] for bound unequal particle systems in a systematic way. We have shown that the applicability of the method depends essentially on the kind of pair-wise interaction involved among the three particles. For insfance, if the nature of ttie interaction is local it will remain local throughout the method (as it is seen by eqs. 2-8, 2-9). A constraint is also imposed on the allowed forms of the potentials, mainly the condition that $p \leq 1$ in eq. (3-8). Coelho et al.[15] have also showed that for three body equal particle systems, the nature of the interaction affects very much the convergence of the solutions.

Another important aim of this work is to show how the symmetry among the particles manifests itself in the geometry and how very asymmetric situations cause problem for the method. The asymmetries should get into the problem through the evaluation of the matrix elements contained in $V_{123}(\vec{\xi},\vec{\eta})$ (see eqs. 2-9 and 3-4). In order to illustrate the method we have considered a kind of pairwise interactions: Coulomb force. This kind of interaction appears in a great variety of problems in physics and we have shown that relatively simple closed expressions can be obtained for the matrix elements of the potential which appear in eq. (2-8). In this point we should mention a paper by Schoucri and Darling[9] which tried to describe the ground state of the He atom using an approach quite similar to this one but much more complicated. The results obtained by Schoucri and Darling are not correct since, as it could be seen easily, eqs. (A10) and (A11) in reference 9, derived by them, are true only for $n=\ell$. The case $n=\ell'$ was completely ignored.

A recent paper by Chowdhury *et al.*[19] considers the system $e^-e^+e^-$ where only Coulomb interaction acts between the particles. The masses of the three particles are equal. The interest is in the ground state with zero total orbital angular momentum ($L=0$). The total wave function (including spin) shouid be antisymmetric with respect to exchange of the two electrons. The corresponding spin functions for the electrons is the singlet functions, which implies that only symmetric states (cosine states) are allowed for the space part of the wavefunction under interchange of the two electrons. This paper does not solve the problem in general but only for particular values of K. Their table 1 contains some numerical values for the coefficients $C^{\nu\nu'}_{KK'}$ (eq.4-6) and it is easy to show that the formalism derived by Schoucri and Darling[9] is unable to reproduce all these coefficients. Chowdhury *et al.*[19] claim that with K only varying up to $K=2$ ($K=0,2$), convergence is achieved. We find hard to trust their numerical results for two main reasons: 1) even for very well behaved potentials, like Gaussian types[15,7], convergence is only achieved for $K \gtrsim 4$. And that is not supposed to be expected for a more singular potential, like the Coulomb case; 2) by making K=O in eq. (4.16), we can obtain[20] an exact solution for the ground state, energy B_0 and wave function $\chi_0(\rho)$, namely

$$B_0 = \frac{512}{225\pi^2} = 0.2306 \text{ amu} ,$$
$$\chi_0(\rho) = N e^{-k\rho} \tag{5.1}$$

It is hard to believe that by adding one more partial wave (K=2) one already gets convergence. It is too bad that Chowdhury[19] did not give their value for K=0.

Another work by Amado and Coelho[10] has also studied three body unequal particle systems using K-harmonics but in one dimension. In one dimension, three particles have two internal coordinates, therefore the K-harmonic method is easy to conceptualize. The problem of dealing with asymnetric systems is carefully analysed on the basis of convergence of the solutions and consequently the convenience or not of using K-harmonic approach. It is found a great similarity with the corresponding three dimensional case.

The conventional way to obtain the radial functions is to solve numerically the system of coupled differential equations. In an earlier work[11], we showed that an easier alternative to this procedure is to further expand the radial functions in a complete set of basis functions, to allow the use of standard matrix diagonalization techniques. This has the advantage, among others, to take autmatically into account the boundary conditions and to allow the simultaneous solution for both ground and excited states (the later is particularly important for $Mg^{24} \to O^{16} + \alpha + \alpha$ in the ground and ffrst few excited 0^+ states).

We are right-now applying this technique to many physical systems like e^+e^-, H_2^+, He atom, etc., in one and three dimensions, for any value of K. Results will appear in a future publication.

Appendix A: Evaluation of $J_n(p,\tau)$

From eq. (3.8) we can analyse the integral

$$\hat{J}_n(p) = \int_0^{2\pi} \frac{\cos(n\lambda)d\lambda}{(1 - A\cos\lambda)^p}$$

Notice that

$$(1 - A\cos\lambda)^{-p} = \sum_{q=0}^{\infty} \frac{p(p+1)\dots(p+q-1)}{q!} A^q \cos^q\lambda, \quad A < 1, \tag{A.1}$$

and

$$\int_0^{2\pi} e^{in\lambda}\cos^q\lambda d\lambda = \frac{\pi}{2^{q-1}} \times \frac{q!}{u!(q-\mu)!} \tag{A.2}$$

where $\mu = 1/2\ (q-n)$ is a non negative integer, and zero otherwise.

Hence

$$\hat{J}_n(p) = \sum_{q=0}^{\infty} \frac{\pi\ (p)_q\ A^q}{2^{q-1}\ \mu!\ (q-\mu)!}\ \delta_{q,n+2}, \quad \mu \gtrsim 0. \tag{A.3}$$

Eq. (A.3) can also be written as

$$\hat{J}_n(p) = A^n \sum_{\mu=0}^{\infty} C_\mu A^{2\mu}, \tag{A.4}$$

where

$$C_\mu = \frac{\pi}{2^{n+2\mu-1}} \times \frac{(p+n+2\mu-1)!}{(p-1)!\ \mu!\ (n+\mu)!}$$

Since

$$\frac{C_{\mu+1}}{C_\mu} = \frac{\left[\frac{1}{2}(p+n+1)+\mu\right]\left[\frac{1}{2}(p+n)+\mu\right]}{(\mu+1)(n+\mu+1)}$$

and

$$C_0 = \frac{\pi}{2^{n-1}} \times \frac{(p+n-1)!}{(p-1)!\,n!} \quad ,$$

we have

$$\hat{J}_n(p) = \frac{2\pi A^n}{2^n} \times \frac{(p+n-1)!}{n!\,(p-1)!} \times F\left(\frac{1}{2}(p+n), \frac{1}{2}(p+n+1); n+1; A^2\right) \equiv$$

$$\equiv \frac{2\pi A^n}{2^n} \times \frac{(p+n-1)!}{n!\,(p-1)!} F_p(n,A^2) . \qquad \text{(A.5)}$$

APPENDIX B: DERIVATION OF EQUATION (4.12)

In order to derive eq. (4.12), we should integrate by parts eq.(4.11) and make use of the differential equation for the hypergeometric function

$$z(1-z)\,F'' + \left[(1+n) - (2+n)z\right]F' = \frac{1}{16}(2n+1)(2n+3)\,F(n,z) . \qquad \text{(B.1)}$$

The following relations are useful for the upper limit of the integrals (Refs.12, 16-18):

$$z^{n+1}(1-z)F'(z) \to \frac{2^{3n}\,(n!)^2}{\pi\,(2n)!} \times \frac{1}{\sqrt{2}} \quad \text{as} \quad z \to 1 \qquad \text{(B.2)}$$

$$F(n,z) \to \frac{\Gamma(n+1)}{\Gamma(\frac{2n+1}{4})\,\Gamma(\frac{2n+3}{4})} \log\left(\frac{1}{1-z}\right) \quad \text{as} \quad z \to 1, \qquad \text{(B.3)}$$

and

$$(1-z)\log(1-z) \to 0 \quad \text{as} \quad z \to 1 . \qquad \text{(B.4)}$$

Reference (16) gives all the basic properties required in order to obtain $I_n(s + s')$.

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