GROUND STATE ENERGY OF THREE-BODY COULOMB SYSTEMS THROUGH HYPERSPHERICAL HARMONICS

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ABSTRACT - The ions $e^-e^+e^-$, H^- and the Helium atom are studied within the hyperspherical formalism. The results obtained are compared with the experimental results and with other techniques. We also show the convergence trend of the method in this case, comparable to known ones.

We have studied the ground state energy of several three body systems wherein the potential is a Coulomb one. We present our results for the ions $e^-e^+e^-$, H^- and for the He atom. In the last two cases, the calculations were made with real and infinite nuclear masses.

Our procedure consists* of solving the Schrödinger equation turned into an algebraic linear system. This is achieved using the generalized harmonic oscillator basis (Erens et al 1970, Vallières et al 1976) for the solution of the equation written in terms of hyperspherical harmonics (Zickendraht 1965, Simonov 1966). That is, if the Schrödinger equation is written as:

$$\left[-\frac{\hbar^2}{2}\sum_{i=1}^{3}\frac{1}{m_i}\nabla^2_{\vec{x}_i} + V(\vec{x}_1, \vec{x}_2, \vec{x}_3) - E\right]\Phi(\vec{x}_1, \vec{x}_2, \vec{x}_3) = 0 \quad (1)$$

with m_i being the mass of the i-th particle, E the total energy of the system, and V any potential, we may pass to the hyperspherical basis by choosing

$$\begin{aligned} \xi_1 &= \rho \sin \zeta_1 \\ \xi_2 &= \rho \cos \zeta_1 \end{aligned} \quad (2)$$

and

$$\rho^2 = \vec{\xi}_1^{\,2} + \vec{\xi}_2^{\,2} \tag{3}$$

with:

$$\vec{\xi}_\alpha = (\mu_\alpha)^{1/2}\left[\left(\sum_{\beta=1}^{\alpha} m_\beta \vec{x}_\beta\right)\left(\sum_{\beta=1}^{\alpha} m_\beta\right)^{-1} - \vec{x}_{\alpha+1}\right] \tag{4}$$

$$\mu_\alpha = m_\alpha \left(\sum_{\beta=1}^{\alpha} m_\beta\right)\left(\sum_{\beta=1}^{\alpha+1} m_\beta\right)^{-1} \qquad \alpha=1,2$$

Then, the Schrödinger equation reads:

$$\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) + \frac{\nabla_\Omega^2}{\rho}\right]\Psi(\rho;\Omega) + \frac{2\varepsilon}{\hbar^2}\Psi(\rho;\Omega) = \tag{5}$$

$$= \frac{2}{\hbar} V\, \Psi(\rho;\Omega)$$

The solution of this equation can be written in terms of the hyperspherical harmonics, eigenfunctions of ∇_Ω^2 (Granzow 1963)

$$\nabla_\Omega^2\, U_{k\{\ell_i\, m_i\}}(\Omega) = -k(k+4)U_{k\{\ell_i\, m_i\}}(\Omega) \tag{6}$$

whose form is

$$U_{k\{\ell_i\ m_i\}}(\Omega) = \prod_{\alpha=1}^{2} Y_{\ell_\alpha\ m_\alpha}(\Theta_\alpha,\phi_\alpha)\ \gamma^1_{k\{\ell_i\ m_i\}}(\zeta_1) \tag{7}$$

with the $Y_{\ell_\alpha m_\alpha}$ eigenfunctions of

$$\Delta_\alpha = \frac{1}{\sin\Theta_\alpha}\frac{\partial}{\partial\Theta_\alpha}\left(\sin\Theta_\alpha \frac{\partial}{\partial\Theta_\alpha}\right) + \frac{1}{\sin^2\Theta_\alpha}\frac{\partial^2}{\partial\phi_\alpha^2} \tag{8}$$

and $\{\Theta_1,\ \Theta_2,\ \phi_1,\ \phi_2,\ \zeta_1\}$ is the set Ω . The function γ is given by

$$\gamma^1_{k\{\ell_i\ m_i\}}(\zeta_1) = (\cos\zeta_1)^{\ell_2}\ {}_2F_1\ (a,b,c,\cos^2\zeta_1) \tag{9}$$

$$a = \frac{1}{2}\ (k_1 - k_0 - \ell_2)$$

$$b = \frac{1}{2}\ (k_1 + k_0 + \ell_2 + 4)$$

$$c = \ell_2 + \frac{3}{2}$$

$$k_0 = \ell_1,\ k_1 = 2n + k_0 + \ell_2\ ,\ n=0,1,2,\ldots$$

$$k_1 = K = 2n + \ell_1 + \ell_2\ ,\ n=0,1,2,\ldots$$

In terms of these functions the wave function is expanded as

$$\Psi\ (\rho;\Omega) = \sum_{k'\alpha'} \chi_{k'\alpha'}(\rho)\ U_{k'\alpha'}(\Omega) \tag{10}$$

The coefficientes $\chi_{k'\alpha'}(\rho)$ are called partial waves. On substituting these quantities the original equation becomes a system of coupled differential linear equations

$$\left\{\frac{1}{\rho^5}\frac{d}{d\rho}\left(\rho^5\frac{d}{d\rho}\right) - \frac{K\ (K+4)}{\rho^2} + \frac{2\varepsilon}{\hbar^2}\right\}\chi_{K\alpha}(\rho) =$$

$$= \frac{2}{\hbar^2}\sum_{K'\alpha'} V_{K\alpha,K'\alpha'}\ (\rho)\ \chi_{k'\alpha'}\ (\rho) \tag{11}$$

$$V_{K\alpha,\ K'\alpha'}\ (\rho) = \int d\ \Omega\ U_{K\alpha}\ (\Omega)\ V\ U_{K'\alpha'}\ (\Omega) \tag{12}$$

When the interaction for the three body system is provided by a harmonic oscillator potential, as is well known these equations can be solved exactly (Fabre de la Ripelle 1969). The solutions $\phi_{n\alpha}(\rho)$ are the generalized harmonic oscillator functions and form a complete set, in terms of which we can expand the partial waves $\chi_{K\alpha}(\rho)$.

$$\phi_{nK}(\rho) = \left[\frac{2n!}{\Gamma(K+n+3)}\right]^{1/2} \xi^K\ e^{-\xi^2/2}\ {}_1F_1(-n,\ K+3;\ \xi^2) \tag{13}$$

$$\varepsilon_{nK} = (2n + K + 3)\sqrt{3}\,\hbar\,\omega$$

$$\xi = \alpha\rho\,,\ \alpha^2 = \frac{\sqrt{3}}{2}\,\frac{\omega}{\hbar}$$

$$_1F_1\,(a,b;z) = 1 + \frac{a}{b}\,\frac{z}{1!} + \frac{a(a+1)}{b(b+1)}\,\frac{z^2}{2!} + \ldots$$

The expansion takes the form:

$$\chi_{K\nu}(\rho) = \sum_n a_{nK\nu}\phi_{nK}(\alpha\rho) \qquad (14)$$

In this way we arrive at the algebraic linear system

$$\sum_{n'} a_{nK\nu} < \phi_{nK}\,|T|\,\phi_{n'K}> + \sum_{n'K'} a_{n'K'\nu'} < \phi_{nK}|V_{K\nu,\,K'\nu'}|\phi_{n'K'}> =$$

$$= -\,\chi^2\,a_{nK\nu} \qquad (15)$$

where

$$T = \frac{1}{\rho^5}\,\frac{d}{d\rho}\left(\rho^5\,\frac{d}{d\rho}\right) - \frac{K(K+4)}{\rho^2}$$

is the kinetic energy operator and $\chi^2 = 2|\varepsilon|$.

The numerical solution is worked out using current computer codes. The matrix elements corresponding to the kinetic energy T are well known (Erens et al 1970) and for the potential we have calculated the matrix elements using the program SCHOONSCHIP developed by M. Veltman (Veltman

1967, Strubbe 1974), able to perform calculations analytically. Closed expressions can also be found (Coelho et al 1978).

The calculations have been performed with values of K varying from 0 to 12, and the results are exhibited in tables 1 to 4 . In these tables, the parameter N refers to the maximum value of the index n in the expression. The parameter α is not used as a fitting quantity, but is kept fixed and is only changed from case to case. In table 5 we show the contribution of the various partial waves $\chi_{K\nu}(\rho)$ to the norm of the wave function $\Psi(\rho;\Omega)$.

TABLE 1: ENERGY EIGENVALUES FOR $e^-e^+e^-$. (α=0.5)

K \ N	10	15
0	-0.115281	-0.115281
2	-0.203794	-0.202314
4	-0.220021	-0.214318
6	-0.234499	-0.235417
8	-0.240796	-0.241886
10	-0.244796	-0.245849
12	-0.248105	

TABLE 2: ENERGY EIGENVALUES FOR H^- WITH REAL PROTON MASS. (α=0.7)

K \ N	10	15
0	-0.385068	-0.385068
2	-0.411513	-0.410829
4	-0.472267	-0.455140
6	-0.472607	-0.474052
8	-0.491866	-0.493991
10	-0.491933	-0.494065

TABLE 3: ENERGY EIGENVALUES FOR H^- WITH INFINITE PROTON MASS. (α=0.7).

K \ N	10	15
0	-0.385401	-0.385401
2	-0.411767	-0.411083
4	-0.478575	-0.457676
6	-0.478983	-0.480452
8	-0.498683	-0.500818
10	-0.506111	-0.510129

TABLE 4: ENERGY EIGENVALUES FOR He WITH INFINITE NUCLEAR MASS. (α=1.8).

K \ N	10	15
0	-2.500017	-2.500017
2	-2.525135	-2.523696
4	-2.773994	-2.700426
6	-2.774572	-2.782179
8	-2.832803	-2.844403
10	-2.836355	-2.846499

TABLE 5: PERCENTUAL CONTRIBUTION FROM THE PARTIAL WAVES $\chi_{K\nu}$ TO THE NORM OF THE WAVE FUNCTION Ψ .

K	ν	$e^-e^+e^-$	H^-	He
0	0	70,16	83,66	94,43
2	1	19,83	1,43	0,42
4	2	1,03	7,77	3,39
4	0	4,64	3,00	1,30
6	3	2,24	0,01	10^{-4}
6	1	0,77	0,01	10^{-3}
8	4	0,27	2,35	0,18
8	2	0,16	0,57	0,18
8	0	0,36	0,28	0,08
10	5	0,05	10^{-3}	10^{-3}
10	3	0,25	10^{-3}	10^{-4}
10	1	0,04	0,91	10^{-3}
12	6	0,09	—	—
12	4	0,03	—	—
12	2	0,02	—	—
12	0	0,05	—	—

As it may be observed, the values obtained are not in agreement for the ion $e^-e^+e^-$ with those calculated by Chowdhury et al. (1975). They claim that convergence is attained with k=4 and their value is -0.259 a.u. This result is quite unexpected because as it is known (Ballot et al, 1973) even for a Gaussian potential convergence is obtained for K>>4.

On the other hand, we have performed an extra - polation based on the following formula

$$a\ E\ (K) + b\ K^{-\gamma} + c = 0. \tag{16}$$

which was inspired by the works of Schneider (1972) and Bruinsma and van Wageningen (1973). The parameter γ is a general feature of the potential and within the accuracy required we used $\gamma=1$. With a simple least square fit we obtain the results for $E(\infty)$ presented on table 6, for the ions $e^-e^+e^-$, H^- (with real proton mass) and for the Helium atom, where they are compared with other theoretical values.

TABLE 6: GROUND-STATE ENERGIES OBTAINED WITH VARIOUS THEORETICAL TECHNIQUES.

$e^- e^+ e^-$	H^-	He
-0.2689[a]	-0.5257[a]	-2.9631[a]
-0.25142[b]	-0.52815[b]	-2.8837[b]
-0.259[c]	-0.52775[e]	-2.85649[f]
-0.262[d]		-2.90372[g]

[a]Present study, [b]Colegrave and King (1977), [c]Chowdhury et al. (1975), [d]Ferrante and Geracitano (1970), [e]Pekeris (1962), [f]Choudhury and Pitchers (1977), [g]Pekeris et al. (1971)

In a forthcoming publication we shall give more details concerning this work and we shall also present results concerning the ion H_2^+, which shows a pattern very much alike the ones exhibited here. Moreover, the limit of the proton mass going to infinity is not simple in this case.

Shortly, it seems that the method of hyperspherical harmonics converges slowly to the correct values. Nonetheless, the method shows a trend which allows to get quite approximate results for the quantities to be calculated.

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