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The calculation of the ground state energy of the positronium negative ion Ps^-

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Abstract With the introduction of an effective hamiltonian, a regular perturbation method is developed systematically for the calculation of the ground state energy of the positronium negative ion. Results upto the second order is very encouraging

Keywords Positronium negative ion Ps⁻, ground state energy, perturbation approach

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The positronium negative ion (Ps^-), the system composed of two electrons and a positron, has been reinvestigated theoretically. The calculation of the binding energy of the system has a long history that can be traced back to the early work of Wheeler [1]. Subsequently many authors [2, 3] with varying degrees of sophistication have reported reasonably good estimate of the ground state energy. Despite these moderate to superior calculations, the interest in this system remains unabated perhaps because of challenging quest for even simpler and more transparent method. It is in this spirit that we present here a simple intuitive method which is a combination of an effective soluble hamiltonian and Rayleigh-Schrodinger perturbation theory (RSPT). The essence of the method, which leads to a good estimate of the GS energy, lies in a suitable partitioning of the exact hamiltonian into a soluble one with a complete basis set and a perturbation.

The hamiltonian of the positronium negative ion is given by

$$\tilde{H} = -\frac{1}{2m_e}\nabla^2_{r_1'} - \frac{1}{2m_e}\nabla^2_{r_2'} - \frac{1}{2m_p}\nabla^2_{R} - \frac{e}{|r_1' - R|} - \frac{e}{|r_2' - R|} \quad |r_1' - r_2'| \tag{1}$$

where r_1', r_2' and R denote the position vectors of the electrons 1, 2 and positron respectively. m_e and m_p are the masses of the electron and the positron respectively.

In reduced atomic unit (where energy is scaled by $\frac{e}{a_0}(\mu / m_e)$ and length by $a_0(m_e/\mu)$).

The hamiltonian is reduced to

$$H = -\frac{1}{2}\left(\nabla_{r_1}^2 + \nabla_{r_2}^2\right) - \left(\frac{1}{r_1} + \frac{1}{r_2}\right) - \frac{1}{1+\rho}\nabla_{r_1}.\nabla_{r_2} + \frac{1}{r_{12}} \tag{2}$$

where the reduced mass $\mu = \dfrac{m_p m_e}{m_p + m_e}$, $\rho = m_p / m_e$ and $\boldsymbol{r}_1, \boldsymbol{r}_2$ are the vectors from the positive particles in units of $(m_e / \mu)a_0$. We essentially rearrange the hamiltonian in the following way,

$$H = \left(-\frac{1}{2}\nabla_{r_1}^2 - \frac{Z}{r_1}\right) + \left(-\frac{1}{2}\nabla_{r_2}^2 - \frac{Z}{r_2}\right)$$

$$-(1-z)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) - \frac{1}{1+\rho}\nabla_{r_1}.\nabla_{r_2} + \frac{1}{r_{12}}, \tag{3}$$

where Z is the effective charge of the positive particle.

For reasons to be apparent presently we introduce the following simple scaling

$$\rho_1 = Z r_1 \quad \text{and} \quad \rho_2 = Z r_2 \tag{4}$$

with the results that

$$\bar{H} = H_0 + H_I, \tag{5}$$

where

$$H_0 = -\frac{1}{2}\left(\nabla_{\rho_1}^2 + \nabla_{\rho_2}^2\right) - \left(\frac{1}{\rho_1} + \frac{1}{\rho_2}\right) \tag{6}$$

and

$$H_I = \frac{1}{Z}(Z-1)\left(\frac{1}{\rho_1} + \frac{1}{\rho_2}\right) + \frac{1}{\rho_{12}} - \frac{1}{1+\rho}\nabla_{\rho_1}.\nabla_{\rho_2} \tag{7}$$

In this form, H_0 is exactly solvable with a basis

$$\psi_{ij}(\rho_1, \rho_2) = \begin{cases} \frac{1}{\sqrt{2}}\left[\phi_i(\rho_1)\phi_j(\rho_2) + \phi_j(\rho_1)\phi_i(\rho_2)\right], & i \neq j \\ \phi_i(\rho_1)\phi_j(\rho_2), & i = j \end{cases} \tag{8}$$

ϕ's being the Coulomb functions. In the discrete and the continuum state these are respectively given by

$$\phi_n = \phi_{nlm}(\rho) = -N_{nl}\,\rho^l\, L_{n+l}^{2l+1}(2\gamma_n \rho) Y_{lm}(\rho), \quad \boldsymbol{n} = (n, l, m) \tag{9}$$

$$N_{nl} = \frac{\epsilon}{n^2}(2/n)^l \left[\frac{(n-l-1)!}{(n+l)!}\right]^{3}$$

$$\gamma_n = 1/n .$$

$L_{n+1}^{2l+1}(2\gamma_n \rho)$ is the Laguere polynomial [4] and $Y_{lm}(\rho)$ is the spherical harmonic and

$$\phi_k(\rho) = N_k \exp(i\boldsymbol{k}.\rho)\ {}_1F_1(i/k, 1, ik\rho - i\boldsymbol{k}.\rho). \tag{10}$$

where $N_k = \dfrac{1}{(2\pi)^{3/2}} \exp\left(\dfrac{\pi}{2k}\right) |\Gamma(1-ik)$

and ${}_1F_1(i/k, 1, ik\rho - i\boldsymbol{k}.\rho)$ is the confluent hypergeometric function [5].

We now estimate the ground state (GS) of H with H_I as perturbation. The unperturbed energy E_0 is given by

$$E^{(0)} = \langle \psi_{gg} | H_0 | \psi_{gg} \rangle = -1 \tag{11}$$

with $\psi_{gg}(\rho_1, \rho_2) = \varphi_g(\rho_1)\varphi_g(\rho_2)$ and (12)

$$\varphi_g(\rho) = \pi^{-1/2} \exp(-\rho). \tag{13}$$

where the perturbation H_I has untill now an unknown parameter Z which has to be determined.

We fix this parameter by the prescription that the first order perturbation correction to the GS energy.

$$E^{(1)} = \langle \psi_{gg}(\rho_1, \rho_2) | H_0 | \psi_{gg}(\rho_1, \rho_2) \rangle \qquad \text{to be zero.}$$

Thus, we get

$$\frac{1}{Z}(2Z - 11/8) = 0, \qquad Z = 11/16. \tag{14}$$

The next order correction $E^{(2)}$ is given by

$$E^{(2)} = \sum_{ij \neq gg}{}' \frac{\langle \psi_{gg}(\rho_1, \rho_2) | H_{Int} | \psi_{ij}(\rho_1, \rho_2) \rangle}{E_{ij} - E_{gg}}$$

where as usual prime in the summation indicates that the intermediate state $\psi_{ij}(\rho_1, \rho_2) = \psi_{gg}(\rho_1, \rho_2)$ is excluded and

$$H_0\ \psi_{ij}(\rho_1, \rho_2) = E_{ij}\ \psi_{ij}(\rho_1, \rho_2).$$

In the evaluation of $E^{(2)}$ we essentially split it into three terms

$$E^{(2)} = E^{(2)}_{nn'} + E^{(2)}_{nk} + E^{(2)}_{kk'},$$

where

$$E^{(2)}_{nn'} = -\sum' \frac{|<\psi_{gg}(\rho_1,\rho_2)|H_{Int}|\psi_{nn'}(\rho_1,\rho_2)>|}{E_{..} - E_{..}}$$

$$E^{(2)}_{nk} = -\sum_{k,n\neq g}' \int \frac{|<\psi_{gg}(\rho_1,\rho_2)|H_{Int}|\psi_{nk}(\rho_1,\rho_2)>|}{E_{kn} - E_{g.}} \cdot dk,$$

$$E^{(2)}_{kk'} = -\int\int \frac{|\psi_{gg}(\rho_1,\rho_2)|H_{Int}|\psi_{kk'}(\rho_1,\rho_2)|}{E_{kk'} - E_{gg}} \cdot dk\, dk'.$$

To simplify the calculation of these three terms, we have gainfully employed the contour integral representation of the Laguerre polynomial [6] and the confluent hypergeometric function [7]. It turns out that the matrix elements in $E^{(2)}_{nn'}$ are obtained in closed analytic form while those in $E^{(2)}_{nk}$ and $E^{(2)}_{kk'}$ are reduced to one dimensional integral which are evaluated numerically. The discrete summation has been performed only upto $n = 5$ and the second order perturbative correction turns out to be

$$E^{(2)} = -0.0398/z^2.$$

Therefore, the ground state energy of the positronium negative ion upto second order RSPT is given by

$$E = (E_0 + E^{(1)} + E^{(2)})Z^2 = -(11/16)^2 - 0.0398 = -0.5123.$$

The result is quite encouraging. Further contribution from the other bound states are likely to increase the result. The most accurate ground state energy of Ps^- in the literature is that of Frolov and Yeremin [8] who used a 700 terms exponential variational expansion wave function. They obtained $E = -0.52401404656 \pm 1\times 10^{-12}$. Bhatia and Drachman [3] obtained $E = -0.5240101300$ Ryd by the use of 220 term hylleraas – type wave function with two non-linear parameters. Ho [9] reported $E = -0.52401014041$ Ryd with 946 terms hylleraas type wave functions. Though the qualities of the wave functions used by them are very accurate, the calculations they performed are very complicated. We have carried out a simple calculation for the GS energy of the positronium negative ion. Our success due to the dominant contribution from 2nd order perturbation term is a very interesting feature of our method. Higher order corrections are likely to improve the result. With the expected improvement of the result in our method, further investigation of the corrections due to the other bound states is under progress.

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