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# A Quasi-Analytical Study of the Nonrelativistic Two-Center Coulomb Problem

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**Abstract** The Schrödinger equation with a pertaining two-center mean field potential scheme is solved by the quasi-analytical ansatz methodology. The ground-state wave function and the corresponding energy of a nonrelativistic nucleon moving in the fields of two fixed Coulomb centers are reported and the behavior of the energy vs. engaged parameters is depicted via illustrative figures.

## 1 Introduction

In spite of being rather old, the two-center shell model (TCSM) [1–4], which considers a nucleon influenced by the fields of two nuclei, is still the focus of some sound studies [5–16]. Before proceeding any further, it should be noted that the application of the two-center model (TCM) is limited to a nuclear system and it successfully accounts for the observed phenomena in other branches of physics (see for example [6,9,10,17]). Papp [5] proposed an approximate method based on the separable expansion of the Coulomb-like potentials. Milek [6] investigated the quantum chaos in an axially symmetric TCSM. Bondarchuk and his colleagues [7] obtained the ground state wavefunction of a relativistic electron by the perturbation technique. The ground-state wave function and the corresponding energy of a relativistic electron in the field of two fixed Coulomb centers were reported by the LCAO method in [8]. Mecke et al. [9,10] proposed the equation of state for the two-center Lennard-Jones fluids. Using the expansion technique, the system was solved under the Woods-Saxon potential in refs. [11,12]. The model under realistic finite depth potentials was studied in Refs. [13,14]. A realistic TCM based on two spherical Woods-Saxon potentials was investigated by Diaz-Torres [15]. Gherghescu [16] worked on the splitting of a deformed parent nucleus into two ellipsoidal deformed fragments using this basis. Chen and his co-workers [17] discussed the effects of the cusp condition, the asymptotic condition, the electron-correlation and the configuration interaction on the energy levels. Gonzalez Leon [18] used the supersymmetry quantum mechanics after proper modifications to provide an analytical solution of the problem. The two-center MICZ Kepler system and the Zeeman effect in the charge-doyen system were studied by Bellucci and Ohanyan [19]. Diaz-Torres [20] proposed a new formalism based on the potential separable expansion to solve the problem with arbitrarily oriented deformed realistic potentials. Pachucki [21] calculated two-center two-electron integrals for exponential functions and for an arbitrary polynomial in electron-nucleus and electron-electron

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distances. Lau and Price to solve the three-dimensional helically reduced wave equation of two-center nature appearing in astrophysics [22] introduced a multidomain spectral-tau methodology. YuSheng et al. studied two-center correlated orbital approach and reported the electronic ground state energy for the $HeH^+$ [23].

In the present paper, we consider a nucleon in the field of two nuclei. After a brief introduction to the problem and the separation of variables via the ellipsoidal (or, prolate spheroidal) coordinates, we arrive at a second order differential equation. In solving the latter, we have to proceed on a numerical technique, which is, despite its reliability, cumbersome and rather vague in comparison to an analytic methodology that provides a deeper understanding and is more instructive for pedagogical purposes. To our best knowledge, the obtained differential equation cannot be solved via any of common analytical approaches such as the supersymmetry quantum mechanics (SUSYQM), Nikiforov–Uvarov (NU), point canonical transformation (PCT), Lie algebras, etc. In our work, after some innovative transformations, we propose physical ansatzs by which the problem can be solved in a quasi-analytical manner and thereby the ground-state wavefunction and the corresponding energy eigenvalue are calculated. Nevertheless, the approach is not restricted to the ground state and the higher ones can be simply obtained by the same token via the proposed ansatz.

## 2 Formulation of the Problem

The Schrödinger equation for the fixed two-center problem, i.e. one nucleon moving in the fields of two fixed nuclei with effective charges $Z_a$, $Z_b$ and internuclear separation distance $R$ is

$$-\frac{1}{2}\nabla^2\Psi_{n,m} - \left(\frac{Z_a}{r_a} + \frac{Z_b}{r_b} - \frac{Z_a Z_b}{R}\right)\Psi_{n,m} = E\Psi_{n,m}, \tag{1}$$

whose solution is normally written in the form

$$\Psi_{n,m}(\lambda,\mu) = \Lambda_{n,m}(\lambda)M_{n,m}(\mu)e^{im\varphi}. \tag{2}$$

In ellipsoidal (or prolate spheroidal) coordinates [17] (see Fig. 1)

$$x = \frac{R}{2}\sqrt{(\lambda^2-1)(1-\mu^2)}\cos\varphi, \tag{3a}$$

$$y = \frac{R}{2}\sqrt{(\lambda^2-1)(1-\mu^2)}\sin\varphi, \tag{3b}$$

$$z = \frac{R}{2}\lambda\mu, \tag{3c}$$

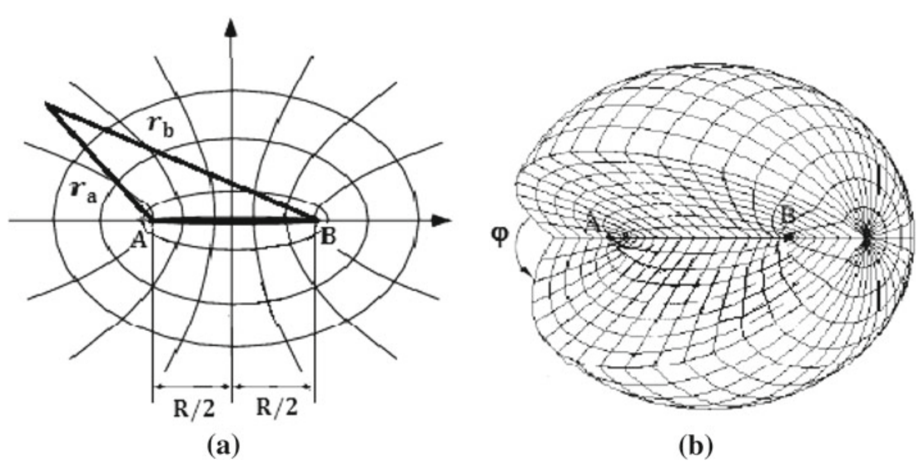


**Fig. 1** **a** Elliptical coordinates (λ, μ). **b** Prolate spheroidal coordinates (λ, μ, φ), (with λ = (ra + rb)/R and μ = (ra − rb)/R. The range of coordinates is 1 ≤ λ ≤ ∞, −1 ≤ μ ≤ 1 and 0 ≤ φ ≤ 2 π.)

and the Laplacian has the form

$$\nabla^2\Psi_{n,m}(\lambda,\mu,\varphi) = \frac{1}{h_\lambda h_\mu h_\varphi}\left[\frac{\partial}{\partial\lambda}\left(\frac{h_\mu h_\varphi}{h_\lambda}\frac{\partial}{\partial\lambda}\Psi_{n,m}(\lambda,\mu,\varphi)\right) + \frac{\partial}{\partial\mu}\left(\frac{h_\lambda h_\varphi}{h_\mu}\frac{\partial}{\partial\mu}\Psi_{n,m}(\lambda,\mu,\varphi)\right) + \frac{\partial}{\partial\varphi}\left(\frac{h_\lambda h_\mu}{h_\varphi}\frac{\partial}{\partial\varphi}\Psi_{n,m}(\lambda,\mu,\varphi)\right)\right], \tag{4a}$$

$$h_\lambda = \frac{R}{2}\frac{(\lambda^2-\mu^2)^{\frac{1}{2}}}{(\lambda^2-1)^{\frac{1}{2}}}\ ,\ h_\mu = \frac{R}{2}\frac{(\lambda^2-\mu^2)^{\frac{1}{2}}}{(1-\mu^2)^{\frac{1}{2}}}\ ,\ h_\varphi = \frac{R}{2}(\lambda^2-1)^{\frac{1}{2}}(1-\mu^2)^{\frac{1}{2}}. \tag{4b}$$

or [17]

$$\nabla^2\Psi_{n,m}(\lambda,\mu,\varphi) = \frac{4}{R^2(\lambda^2-\mu^2)}\left\{\frac{\partial}{\partial\lambda}\left[(\lambda^2-1)\frac{\partial}{\partial\lambda}\right] + \frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial}{\partial\mu}\right] + \frac{\lambda^2-\mu^2}{(\lambda^2-1)(1-\mu^2)}\frac{\partial^2}{\partial\varphi^2}\right\}\Psi_{n,m}(\lambda,\mu,\varphi), \tag{5}$$

which brings Eq. (1) into

$$-\frac{1}{2}\left[\frac{4}{R^2(\lambda^2-\mu^2)}\left\{\frac{\partial}{\partial\lambda}\left[(\lambda^2-1)\frac{\partial}{\partial\lambda}\right] + \frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial}{\partial\mu}\right] + \frac{(\lambda^2-\mu^2)m^2}{(\lambda^2-1)(1-\mu^2)}\right\}\Lambda_{n,m}(\lambda)M_{n,m}(\mu)\right] - \left(\frac{2z_a}{R(\lambda+\mu)} + \frac{2z_b}{R(\lambda-\mu)} - \frac{z_a z_b}{R}\right)\Lambda_{n,m}(\lambda)M_{n,m}(\mu) = E_{n,m}\Lambda_{n,m}(\lambda)M_{n,m}(\mu). \tag{6}$$

After a normal separation of variable, we arrive at

$$\frac{d}{d\lambda}\left\{(\lambda^2-1)\frac{d\Lambda_{n,m}(\lambda)}{d\lambda}\right\} + \left\{A + 2R_1\lambda - P^2\lambda^2 - \frac{m^2}{\lambda^2-1}\right\}\Lambda_{n,m}(\lambda) = 0,$$
$$R_1 = \frac{R(Z_a+Z_b)}{2},\quad \lambda \geq 1, \tag{7a}$$

$$\frac{d}{d\mu}\left\{(1-\mu^2)\frac{dM_{n,m}(\mu)}{d\mu}\right\} + \left\{-A + 2R_2\mu + P^2\mu^2 - \frac{m^2}{1-\mu^2}\right\}M_{n,m}(\mu) = 0,$$
$$R_2 = \frac{R(Z_b-Z_a)}{2},\quad |\mu| \leq 1, \tag{7b}$$

where

$$P^2 = \frac{1}{2}\left(-R^2E_{n,m} + RZ_aZ_b\right) \succ 0, \tag{8}$$

Before proceeding further, we write Eq. (7a) more neatly as

$$\Lambda''_{n,m}(\lambda) + \frac{2\lambda}{\lambda^2-1}\Lambda'_{n,m}(\lambda) + \left[\frac{A+2R_1\lambda}{\lambda^2-1} - \frac{P^2\lambda^2}{\lambda^2-1} - \frac{m^2}{(\lambda^2-1)^2}\right]\Lambda_{n,m}(\lambda) = 0, \tag{9}$$

and introduce a change of variable of the form

$$\Lambda_{n,m}(\lambda) = \frac{\phi_{n,m}(\lambda)}{\sqrt{\lambda^2-1}}, \tag{10}$$

to obtain

$$\frac{d^2\phi_{n,m}(\lambda)}{d\lambda^2} + \left\{-\frac{1}{\lambda^2-1} + \frac{\lambda^2}{(\lambda^2-1)^2} + \frac{A+2R_1\lambda}{\lambda^2-1} - \frac{P^2\lambda^2}{\lambda^2-1} - \frac{m^2}{(\lambda^2-1)^2}\right\}\phi_{n,m}(\lambda) = 0. \tag{11}$$

By decomposition of fractions we have

$$\frac{d^2\phi_{n,m}(\lambda)}{d\lambda^2} + \left\{\frac{1/4 + (2R_1-A)/2 - m^2/4 + P^2/2}{\lambda+1} + \frac{-1/4 + (A+2R_1)/2 + m^2/4 - P^2/2}{\lambda-1} + \frac{1/4 - m^2/4}{(\lambda+1)^2} + \frac{1/4 - m^2/4}{(\lambda-1)^2} - P^2\right\}\phi_{n,m}(\lambda) = 0, \tag{12}$$

Let us now return to Eq. (7b), i.e.

$$M''_{n,m}(\mu) - \frac{2\mu}{1-\mu^2} M'_{n,m}(\mu) + \left[\frac{-A+2R_2\mu}{1-\mu^2} + \frac{P^2\mu^2}{1-\mu^2} - \frac{m^2}{(1-\mu^2)^2}\right] M_{n,m}(\mu) = 0, \tag{13a}$$

where

$$M_{n,m}(\mu) = \frac{\psi_{n,m}(\mu)}{\sqrt{1-\mu^2}}, \tag{13b}$$

Decomposition of fractions brings the latter into the form

$$\frac{d^2\psi_{n,m}(\mu)}{d\mu^2} + \left\{\frac{1/4 + (-A-2R_2)/2 + P^2/2 - m^2/4}{1+\mu} + \frac{1/4 + (-A+2R_2)/2 + P^2/2 - m^2/4}{1-\mu} \right.$$
$$\left. + \frac{1/4 - m^2/4}{(1+\mu)^2} + \frac{1/4 - m^2/4}{(1-\mu)^2} - P^2 \right\} \psi_{n,m}(\mu) = 0 \tag{14}$$

which again cannot be solved by an exact analytical method.

## 3 Ansatz Solution

### 3.1 The Ansatz Solution for $\phi_{n,m}(\lambda)$

Eq. (12) fails to admit exact analytical solutions. Therefore, we follow the ansatz approach with the starting square

$$\phi_{n,m}(\lambda) = h_n(\lambda)\exp(y_m(\lambda)), \tag{15}$$

where

$$h_n(\lambda) = \begin{cases} 1, & if\ n = 0, \\ \prod_{i=1}^{n} (\lambda - \alpha_i^n), & \text{if } n \geq 1, \end{cases} \tag{16}$$

and

$$y_m(\lambda) = \alpha Ln(\lambda - 1) + \beta Ln(\lambda + 1) + \delta\lambda, \tag{17}$$

By substitution of $h_n(\lambda)$ and $y_m(\lambda)$ into Eq. (15), we find

$$\phi''_{n,m}(\lambda) = \left[y''_m(\lambda) + {y'_m}^2(\lambda) + \frac{h''_n(\lambda) + 2y'_m(\lambda)h'_n(\lambda)}{h_n(\lambda)}\right]\phi_{n,m}(\lambda), \tag{18}$$

Here, we consider the case $n = 0$. From Eqs. (16)– (18) we find

$$\phi''_{0,m}(\lambda) + \left[\frac{\alpha\beta - 2\beta\delta}{\lambda+1} + \frac{-\alpha\beta - 2\alpha\delta}{\lambda-1} + \frac{\beta-\beta^2}{(\lambda+1)^2} + \frac{\alpha-\alpha^2}{(\lambda-1)^2} - \delta^2\right]\phi_{0,m}(\lambda) = 0, \tag{19}$$

By comparing the corresponding powers of Eqs. (12) and (19), we have

$$\alpha\beta - 2\beta\delta = \frac{1}{4} + (2R_1 - A)/2 - m^2/4 + P^2/2, \tag{20a}$$
$$-\alpha\beta - 2\alpha\delta = -1/4 + (A + 2R_1)/2 + m^2/4 - P^2/2, \tag{20b}$$
$$\beta - \beta^2 = 1/4 - m^2/4, \tag{20c}$$
$$\alpha - \alpha^2 = 1/4 - m^2/4, \tag{20d}$$
$$-P^2 = -\delta^2, \tag{20e}$$

Eqs. (20c), (20d) and (20e) give

$$\alpha = \beta = \frac{1+m}{2}, \tag{21a}$$

$$\delta = -\sqrt{\frac{1}{2}(-R^2 E_{0,m} + R Z_a Z_b)}, \tag{21b}$$

From Eqs. (17), (20a) and (20b), we simply have

$$y_m(\lambda) = \left(\frac{1+m}{2}\right) Ln(\lambda - 1) + \left(\frac{1+m}{2}\right) Ln(\lambda + 1) - \lambda\sqrt{\frac{1}{2}(-R^2 E_{0,m} + R Z_a Z_b)}, \tag{22a}$$

$$\phi_{0,m}(\lambda) = (\lambda^2 - 1)^{\left(\frac{1+m}{2}\right)} \ \exp\left(-\lambda\sqrt{\frac{1}{2}(-R^2 E_{0,m} + R Z_a Z_b)}\right) \tag{22b}$$

and

$$\Lambda_{0,m}(\lambda) = N_{\lambda,0,m}(\lambda^2 - 1)^{\frac{m}{2}} \ \exp\left(-\lambda\sqrt{\frac{1}{2}(-R^2 E_{0,m} + R Z_a Z_b)}\right). \tag{23}$$

### 3.2 The Ansatz Solution $\psi_{n,m}(\mu)$

In this case, we introduce the ansatz

$$\psi_{n,m}(\mu) = h_n(\mu) \exp(y_m(\mu)), \tag{24}$$

where

$$h_n(\mu) = \begin{cases} 1, & \text{if } n = 0, \\ \prod_{i=1}^{n} (\mu - \tilde{\alpha}_i^n), & \text{if } n \geq 1, \end{cases} \tag{25}$$

and

$$y_m(\mu) = \tilde{\alpha} Ln(1 - \mu) + \tilde{\beta} Ln(1 + \mu) + \tilde{\delta}\mu, \tag{26}$$

Substitution of the proposed ansatz gives

$$\psi''_{n,m}(\mu) = \left[y''_m(\mu) + y'^{\,2}_m(\mu) + \frac{h''_n(\mu) + 2y'_m(\mu)h'_n(\mu)}{h_n(\mu)}\right] \psi_{n,m}(\mu), \tag{27}$$

For $n = 0$ we have

$$\psi''_{0,m}(\mu) + \left[\frac{-2\tilde{\beta}\tilde{\delta} + \tilde{\alpha}\tilde{\beta}}{1+\mu} + \frac{2\tilde{\alpha}\tilde{\delta} + \tilde{\alpha}\tilde{\beta}}{1-\mu} + \frac{\tilde{\beta} - \tilde{\beta}^2}{(1+\mu)^2} + \frac{\tilde{\alpha} - \tilde{\alpha}^2}{(1-\mu)^2} - \tilde{\delta}^2\right] \psi_{0,m}(\mu) = 0, \tag{28}$$

By comparing Eqs. (14) and (28), we find

$$\tilde{\alpha}\tilde{\beta} - 2\tilde{\beta}\tilde{\delta} = 1/4 + (-A - 2R_2)/2 + P^2/2 - m^2/4, \tag{29a}$$

$$\tilde{\alpha}\tilde{\beta} + 2\tilde{\alpha}\tilde{\delta} = 1/4 + (-A + 2R_2)/2 + P^2/2 - m^2/4, \tag{29b}$$

$$\tilde{\beta} - \tilde{\beta}^2 = 1/4 - m^2/4, \tag{29c}$$

$$\tilde{\alpha} - \tilde{\alpha}^2 = 1/4 - m^2/4, \tag{29d}$$

$$\tilde{\delta}^2 = P^2. \tag{29e}$$

From Eqs. (29c), (29d) and (29e) we obtain

$$\tilde{\alpha} = \tilde{\beta} = \frac{1+m}{2}, \tag{30a}$$

$$\tilde{\delta} = -\sqrt{\frac{1}{2}(-R^2 E_{0,m} + RZ_a Z_b)}. \tag{30b}$$

Then, we have

$$y_m(\mu) = \left(\frac{1+m}{2}\right) Ln(1-\mu) + \left(\frac{1+m}{2}\right) Ln(1+\mu) + \left(-\sqrt{\frac{1}{2}(-R^2 E_{0,m} + RZ_a Z_b)}\right)\mu, \tag{31a}$$

$$\psi_{0,m}(\mu) = (1-\mu^2)^{\left(\frac{1+m}{2}\right)} \exp\left(-\mu\sqrt{\frac{1}{2}(-R^2 E_{0,m} + RZ_a Z_b)}\right) \tag{31b}$$

From Eqs. (13b) and (31b), we have

$$M_{0,m}(\mu) = N_{\mu,0,m}(1-\mu^2)^{\frac{m}{2}} \exp\left(-\mu\sqrt{\frac{1}{2}(-R^2 E_{0,m} + RZ_a Z_b)}\right), \tag{32}$$

By solving Eqs. (20a)–(20e) and (29a)–(29e) and by considering the lowest amount of energy as the ground state energy, we obtain the energy eigenvalue as

$$E_{0,m} = -\frac{1}{2}\left\{\frac{RZ_a^2 - 2RZ_a Z_b + RZ_b^2 - 2Z_a Z_b - 4Z_a Z_b m - 2Z_a Z_b m^2}{R(1+m)^2}\right\}. \tag{33}$$

By combining Eqs. (23) and (32), the ground state wave-function is written as

$$\Psi_{0,m}(\lambda,\mu,\varphi) = N_{0,m}\Lambda_{0,m}(\lambda)M_{0,m}(\mu)e^{im\varphi}, \tag{34a}$$

$$\begin{aligned}\Psi_{0,m}(\lambda,\mu,\varphi) = N_{0,m}(\lambda^2-1)^{\left(\frac{m}{2}\right)}(1-\mu^2)^{\left(\frac{m}{2}\right)} \exp\Bigg(&-\lambda\sqrt{\frac{1}{2}(-R^2 E_{0,m} + RZ_a Z_b)} \\ &-\mu\sqrt{\frac{1}{2}(-R^2 E_{0,m} + RZ_a Z_b)}\Bigg)e^{im\varphi}.\end{aligned} \tag{34b}$$

To ensue capability of the approach, we include the first excited state solution in the next subsection.

### 3.3 The Excited States

For $n = 1$, according to Eq. (16), we choose

$$h_1(\lambda) = (\lambda - \alpha_1^{(1)}) \tag{35}$$

and $y_m(\lambda)$ from Eqs. (16)–(18), we find

$$\phi''_{1,m}(\lambda) + \left[\frac{\alpha\beta - 2\beta\delta}{\lambda+1} + \frac{-\alpha\beta - 2\alpha\delta}{\lambda-1} + \frac{\beta-\beta^2}{(\lambda+1)^2} + \frac{\alpha-\alpha^2}{(\lambda-1)^2} - \delta^2 + \frac{-\frac{2\alpha}{\lambda-1} - \frac{2\beta}{\lambda+1} - 2\delta}{\lambda - \alpha_1^{(1)}}\right]\phi_{1,m}(\lambda) = 0, \tag{36}$$

By comparing the above equation and Eq. (7), we find

$$\begin{aligned}&\frac{1/4 + (2R_1 - A)/2 - m^2/4 + P^2/2}{\lambda+1} + \frac{-1/4 + (A+2R_1)/2 + m^2/4 - P^2/2}{\lambda-1} + \frac{1/4 - m^2/4}{(\lambda+1)^2} \\ &+ \frac{1/4 - m^2/4}{(\lambda-1)^2} - P^2 = \frac{\alpha\beta - 2\beta\delta}{\lambda+1} + \frac{-\alpha\beta - 2\alpha\delta}{\lambda-1} + \frac{\beta-\beta^2}{(\lambda+1)^2} + \frac{\alpha-\alpha^2}{(\lambda-1)^2} - \delta^2 + \frac{-\frac{2\alpha}{\lambda-1} - \frac{2\beta}{\lambda+1} - 2\delta}{\lambda - \alpha_1^{(1)}}\end{aligned} \tag{37}$$

By equating the corresponding powers on both sides, we have

$$\begin{aligned}
&-\frac{(2R_1-A)}{2}-\frac{P^2}{2}-\frac{\alpha_1^{(1)}}{4}-\frac{(2R_1-A)\alpha_1^{(1)}}{2}+\frac{m^2\alpha_1^{(1)}}{4}-\frac{P^2\alpha_1^{(1)}}{2}\\
&\quad=-\beta^2-\alpha\beta+2\beta\delta-\alpha\alpha_1^{(1)}\beta+2\beta\delta\alpha_1^{(1)}-\beta,\\
&\frac{(2R_1+A)}{2}-\frac{P^2}{2}+\frac{\alpha_1^{(1)}}{4}-\frac{(2R_1+A)\alpha_1^{(1)}}{2}-\frac{m^2\alpha_1^{(1)}}{4}+\frac{P^2\alpha_1^{(1)}}{2}\\
&\quad=-\alpha^2-\alpha\beta-2\alpha\delta+\alpha\alpha_1^{(1)}\beta+2\alpha\delta\alpha_1^{(1)}-\alpha,\\
&-\frac{1}{4}+\frac{m^2}{4}-\frac{\alpha_1^{(1)}}{4}+\frac{m^2\alpha_1^{(1)}}{4}=-\beta+\beta^2-\beta\alpha_1^{(1)}+\beta^2\alpha_1^{(1)},\\
&\frac{1}{4}-\frac{m^2}{4}-\frac{\alpha_1^{(1)}}{4}+\frac{m^2\alpha_1^{(1)}}{4}=\alpha-\alpha^2-\alpha\alpha_1^{(1)}+\alpha^2\alpha_1^{(1)},\\
&2R_1+P^2\alpha_1^{(1)}=\delta^2\alpha_1^{(1)}-2\alpha\delta-2\beta\delta-2\delta,\\
&-P^2=-\delta^2.
\end{aligned} \tag{38}$$

By solving the above equations one can find $A, \alpha, \beta, \delta, \alpha_1^{(1)}$ and $P$, and thereby the energy of the system. We can repeat the same process for higher states by choosing $h_n(\lambda)=(\lambda-\alpha_1^{(n)})\cdots(\lambda-\alpha_n^{(n)})=\prod_{i=1}^{n}(\lambda-\alpha_i^{(n)})$. Let us now return to Eq. (7b) for the first node. A decomposition of fractions gives

$$\begin{aligned}
&\frac{d^2\psi_{1,m}(\mu)}{d\mu^2}+\left\{\frac{1/4+(-A-2R_2)/2+P^2/2-m^2/4}{1+\mu}+\frac{1/4+(-A+2R_2)/2+P^2/2-m^2/4}{1-\mu}\right.\\
&\quad\left.+\frac{1/4-m^2/4}{(1+\mu)^2}+\frac{1/4-m^2/4}{(1-\mu)^2}-P^2\right\}\psi_{1,m}(\mu)=0,
\end{aligned} \tag{39}$$

By inserting $h_1(\mu)=(\mu-\tilde{\alpha}_1^{(1)})$, Eqs. (25)–(27) give

$$\psi''_{1,m}(\mu)+\left[\frac{-2\tilde{\beta}\tilde{\delta}+\tilde{\alpha}\tilde{\beta}}{1+\mu}+\frac{2\tilde{\alpha}\tilde{\delta}+\tilde{\alpha}\tilde{\beta}}{1-\mu}+\frac{\tilde{\beta}-\tilde{\beta}^2}{(1+\mu)^2}+\frac{\tilde{\alpha}-\tilde{\alpha}^2}{(1-\mu)^2}-\tilde{\delta}^2+\frac{\frac{2\tilde{\alpha}}{1-\mu}-\frac{2\tilde{\beta}}{1+\mu}-2\tilde{\delta}}{\mu-\tilde{\alpha}_1^{(1)}}\right]\psi_{1,m}(\mu)=0, \tag{40}$$

or

$$\begin{aligned}
&\frac{1/4+(-A-2R_2)/2+P^2/2-m^2/4}{1+\mu}+\frac{1/4+(-A+2R_2)/2+P^2/2-m^2/4}{1-\mu}+\frac{1/4-m^2/4}{(1+\mu)^2}\\
&\quad+\frac{1/4-m^2/4}{(1-\mu)^2}-P^2=\frac{-2\tilde{\beta}\tilde{\delta}+\tilde{\alpha}\tilde{\beta}}{1+\mu}+\frac{2\tilde{\alpha}\tilde{\delta}+\tilde{\alpha}\tilde{\beta}}{1-\mu}+\frac{\tilde{\beta}-\tilde{\beta}^2}{(1+\mu)^2}+\frac{\tilde{\alpha}-\tilde{\alpha}^2}{(1-\mu)^2}-\tilde{\delta}^2+\frac{\frac{2\tilde{\alpha}}{1-\mu}-\frac{2\tilde{\beta}}{1+\mu}-2\tilde{\delta}}{\mu-\tilde{\alpha}_1^{(1)}},
\end{aligned} \tag{41}$$

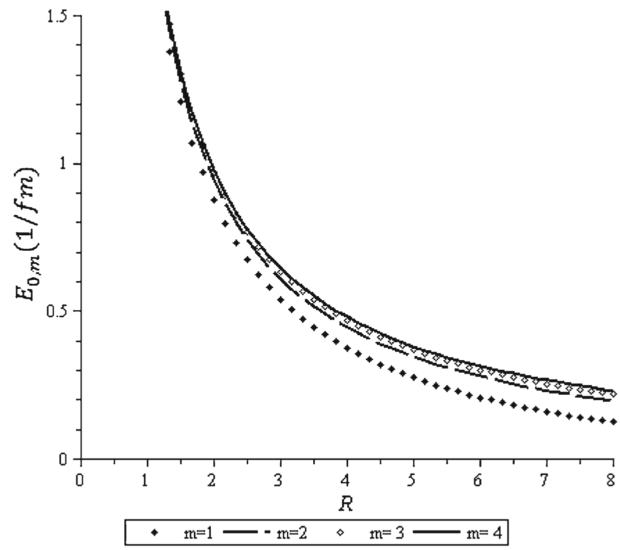


**Fig. 2** Energy vs. $R$ for $Z_a = 2$, $Z_b = 1$

by comparing the corresponding powers, we find

$$\begin{aligned}
&\frac{(A+2R_2)}{2}-\frac{P^2}{2}-\frac{\tilde{\alpha}_1^{(1)}}{4}+\frac{(A+2R_2)\tilde{\alpha}_1^{(1)}}{2}-\frac{P^2\tilde{\alpha}_1^{(1)}}{2}+\frac{m^2\tilde{\alpha}_1^{(1)}}{4}\\
&\quad=-\tilde{\beta}^2+2\tilde{\beta}\tilde{\delta}-\tilde{\alpha}\tilde{\beta}+2\tilde{\beta}\tilde{\delta}\tilde{\alpha}_1^{(1)}-\tilde{\alpha}\tilde{\beta}\tilde{\alpha}_1^{(1)}-\tilde{\beta},\\
&\frac{(-A+2R_2)}{2}+\frac{P^2}{2}-\frac{\tilde{\alpha}_1^{(1)}}{4}+\frac{(A-2R_2)\tilde{\alpha}_1^{(1)}}{2}-\frac{P^2\tilde{\alpha}_1^{(1)}}{2}+\frac{m^2\tilde{\alpha}_1^{(1)}}{4}\\
&\quad=\tilde{\alpha}^2+2\tilde{\alpha}\tilde{\delta}+\tilde{\alpha}\tilde{\beta}-2\tilde{\alpha}\tilde{\delta}\tilde{\alpha}_1^{(1)}-\tilde{\alpha}\tilde{\beta}\tilde{\alpha}_1^{(1)}+\tilde{\alpha},\\
&-\frac{1}{4}+\frac{m^2}{4}-\frac{\tilde{\alpha}_1^{(1)}}{4}+\frac{m^2\tilde{\alpha}_1^{(1)}}{4}=-\tilde{\beta}+\tilde{\beta}^2-\tilde{\beta}\tilde{\alpha}_1^{(1)}+\tilde{\beta}^2\tilde{\alpha}_1^{(1)},\\
&\frac{1}{4}-\frac{m^2}{4}-\frac{\tilde{\alpha}_1^{(1)}}{4}+\frac{m^2\tilde{\alpha}_1^{(1)}}{4}=\tilde{\alpha}-\tilde{\alpha}^2-\tilde{\alpha}\tilde{\alpha}_1^{(1)}+\tilde{\alpha}^2\tilde{\alpha}_1^{(1)},\\
&-2R_2+P^2\tilde{\alpha}_1^{(1)}=\tilde{\delta}^2\tilde{\alpha}_1^{(1)}-2\tilde{\beta}\tilde{\delta}-2\tilde{\alpha}\tilde{\delta}-2\tilde{\delta},\\
&-P^2=-\tilde{\delta}^2.
\end{aligned}\tag{42}$$

Having found $A, \tilde{\alpha}, \tilde{\beta}, \tilde{\delta}, \tilde{\alpha}_1^{(1)}$ and $P$ from the above equations, the energy of the system can be obtained from Eq. (8). We can repeat the story for higher states by substituting $h_n(\mu) = (\mu - \tilde{\alpha}_1^{(n)}) \cdots (\mu - \tilde{\alpha}_n^{(n)}) = \prod_{i=1}^{n} (\mu - \tilde{\alpha}_i^{(n)})$. We have included some numerical results and illustrative figures to provide a better view to the results. In particular, Fig. 2 depicts the energy behavior vs. the internuclear separation distance $R$ for different values $m$. We see that the energy decreases with increasing $R$. In Figs. 3–4 is plotted energy variation vs. $m$ and $Z_b$. The eigenfunction is plotted in Fig. 5 for the individual parts, and the overall wavefunction. In Fig. 2, $E_{0,m}$ is plotted vs. $R$ for some values $m$. It reveals that as $R$ increases the energy decreases and tends to a constants value. Figure 3 represents the variation of ground state energy vs. m for different values of R. We see that the saturation occurs for $m = 4$. Figure 4 depicts the energy behavior vs. $Z_b$ for different values of $Z_a$ and it well shows that how the energy increases to a limit and then decreases for increasing $Z_b$. In Fig. 5 we can see the wavefunctions for $n = 0$ in the interval $1 \le \lambda \le \infty$, $-1 \le \mu \le 1$. The left and right figures in the upper panel of Fig. 5 respectively represent $\Lambda_{0,5}(\lambda)$ vs. $\lambda$ and $M_{0,5}(\mu)$ vs. $\mu$. There, the lower panel depicts the total wavefunction $\Psi_{0,5}(\lambda, \mu)$.

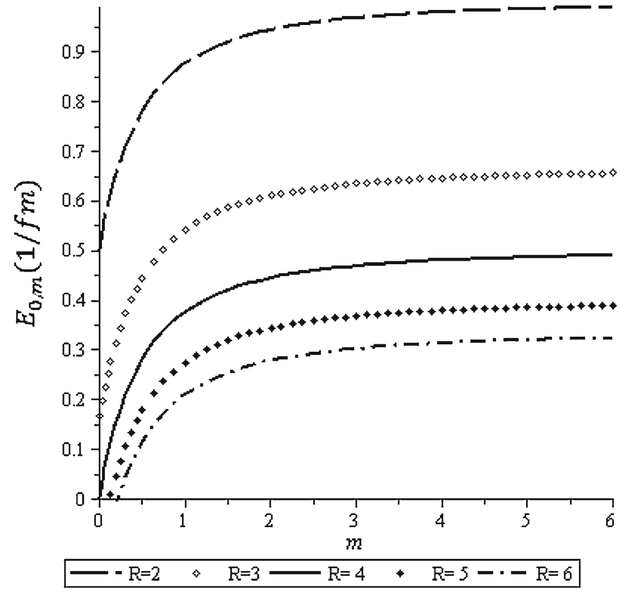


**Fig. 3** Energy vs. $m$ for $Z_a = 2$, $Z_b = 1$

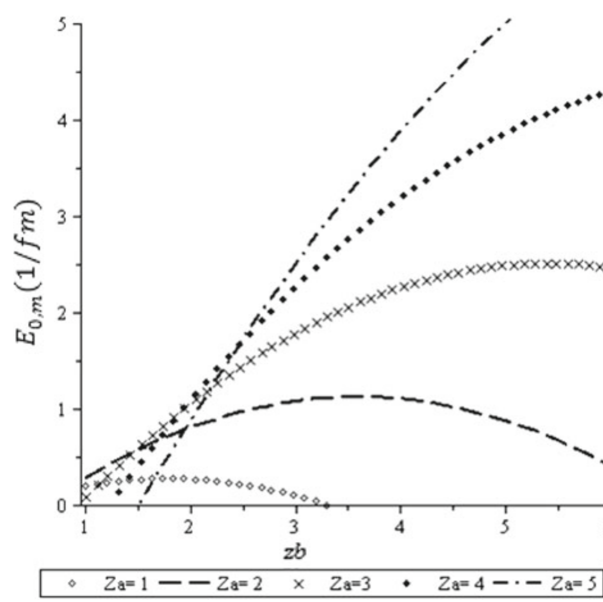


**Fig. 4** Energy vs. $Z_b$ for $R = 5fm, m = 1fm^{-1}$

## 4 Conclusion

Bearing in mind the wide application of the two-center problem in various branches of physics including nuclear and solid state physics, we considered the problem under Coulomb interactions. By proposing an elegant ansatz and several transformations, we obtained the ground state eigenfunction of the system as well as the corresponding energy eigenvalue. The higher states can be directly obtained via the introduced ansatz function. Our results, after proper fits and modifications done, can be used in nuclear and molecular physics, and to be more precise, in the study of equilibrium separation between the nuclei, decay properties of bound state wavefunction, different cross sections, nuclear fusion rates, interference patterns, charge transfer, excitation, ionization and electron-positron pair production that accompany slow collisions of heavy ions, systematic analysis of the quantum electrodynamics (QED) corrections to the energy levels of heavy quasi-molecules, static multipole polarizabilities of the interacting atoms, description of the interacting nuclei as well as that of

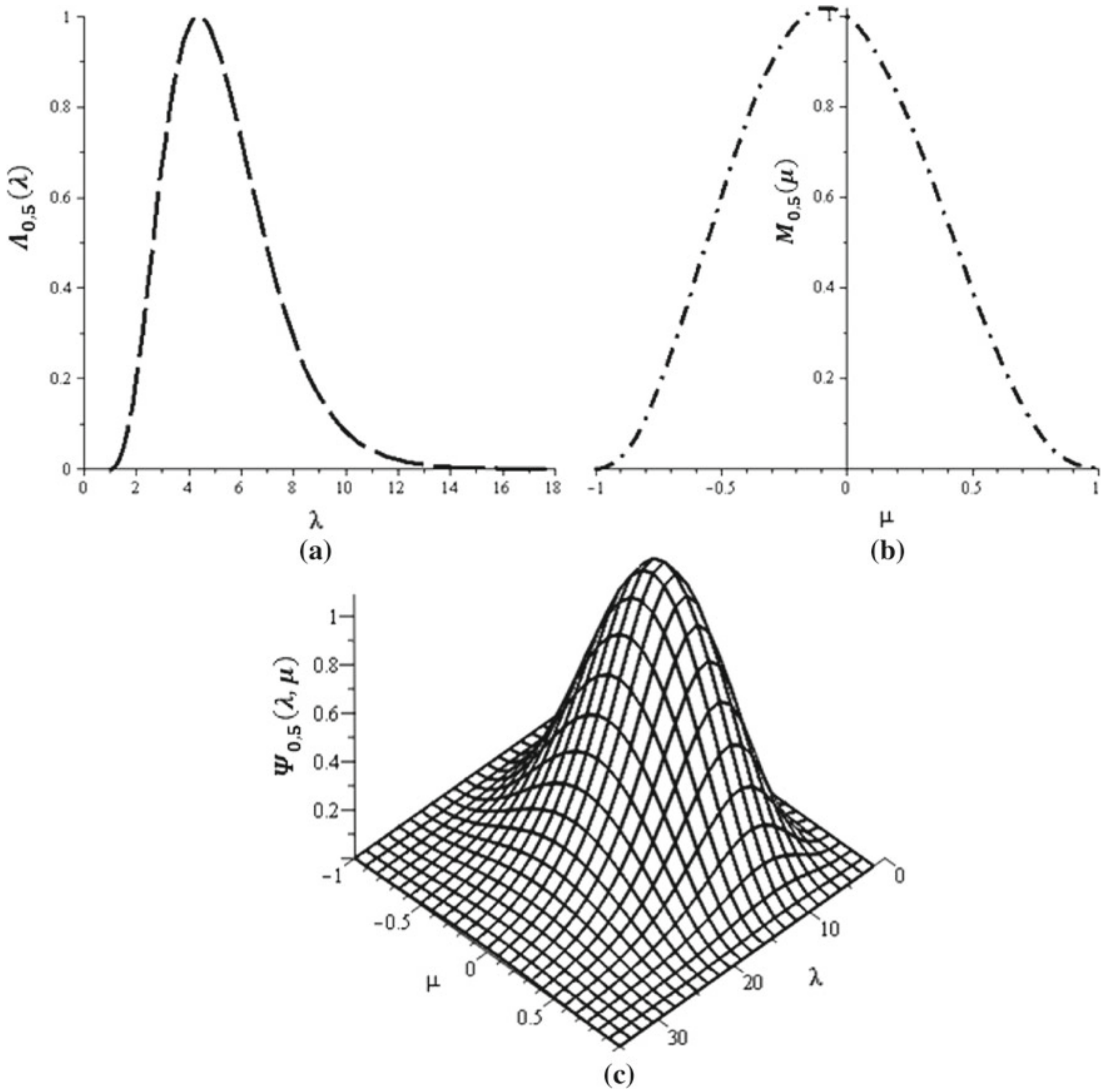


**Fig. 5** **a** $\Lambda_{0,5}(\lambda)$ vs. $\lambda$ for $Z_a = 2$, $Z_b = 1$, $R = 5fm$. **b** $M_{0,5}(\mu)$ vs. $\mu$ for $Z_a = 2$, $Z_b = 1$, $R = 5fm$. **c** Ground state wavefunction, $\Psi_{0,5}(\lambda, \mu)$ vs. $\lambda$ and $\mu$ for $Z_a = 2$, $Z_b = 1$, $R = 5fm$

the two-body channels, form factors, Slater orbitals, ejected electrons in the double ionization, spectroscopy of diatomic molecules, dinuclear configurations, quasi-molecular resonance states, etc.

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