Elementary solutions of the quantum planar two center problem

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Abstract

The quantum problem of an electron moving in a plane under the field created by two Coulombian centers admits simple analytical solutions for some particular inter-center distances. These elementary eigenfunctions, akin to those found by Demkov for the analogous three dimensional problem, are calculated using the framework of quasi-exact solvability of a pair of entangled ODE's descendants from the Heun equation. A different but interesting situation arises when the two centers have the same strength. In this case completely elementary solutions do not exist.

1 Introduction

The quantum spectral problem of a charged particle moving in the field created by two fixed Coulomb centers appears in a natural way in the study of diatomic molecular ions, in the Born-Oppenheimer approximation. Although the three-dimensional case has been profusely studied from different points of view: computational, see e.g. [1], analytical, see [2, 3], as far as we know the search for elementary solutions has been reduced to the work of Demkov [4] in the two-center problem in three dimensions.

In this letter, the existence of elementary solutions for the planar problem is studied. The underlying idea is similar to the Demkov approach [4] to the three-dimensional case, and thus we search for the eigenfunctions of the system that can be written essentially as polynomials. Unlike the three-dimensional problem, the planar system admits elementary solutions not only of hydrogenoid type, i.e., eigenfunctions with energy coinciding with the energy levels of an hydrogenoid atom, but also of a new type that we shall term as "quasi"-hydrogenoid. These new type of elementary solutions does not arise in the three dimensional problem and its existence is reminiscent of the different topologies subjacent to 2D and 3D two center problems.

The Schrödinger equation for the planar problem is separable in Euler elliptic coordinates. After the separation process the PDE wave equation reduces to two ODE's, namely a Razavy and a Whittaker-Hill equation, linked by the two invariants of the system. These equations are particular descendants of the Confluent Heun equation, and, thus, it is possible to obtain polynomial solutions when the parameters of the problem render the two ODE simultaneously quasi-exactly solvable [5]. The separability properties and the study of the general potentials that admit exact and quasi-exact solvability for a broad family of physical problems associated to the 3D two-center problem have been recently analyzed thoroughly in Reference [6].

When the two centers are of equal strength, contrary to expectations, the problem is more involved. The Whittaker-Hill equation descends to the Mathieu equation which is never quasi-exactly solvable. Thus, there are not completely elementary eigenfunctions in this situation, although interesting wave functions may be derived for certain intercenter distances determined from the Mathieu characteristic values.

2 The planar quantum problem posed by two Coulombian centers

The stationary Schrödinger equation governing the quantum dynamics of a charged particle moving in the potential of two fixed Coulombian centers (nuclei, ions, etc) in the plane reads:

$$\left(-\frac{1}{2}\Delta - \frac{Z_1}{r_1} - \frac{Z_2}{r_2}\right)\Psi = E\Psi\,, \tag{1}$$

where $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$, and atomic units are used: $\hbar = m_e = e = a_0 = 1$, a_0 being the Bohr radius. Z_1 and Z_2 are the atomic numbers of the two nuclei, and r_1 and r_2 are the distances from the electron to the nuclei:

$$r_1 = \sqrt{\left(x_1 - \frac{R}{2}\right)^2 + x_2^2}\,, \; r_2 = \sqrt{\left(x_1 + \frac{R}{2}\right)^2 + x_2^2}\,,$$

while R is the internuclear distance. Equation (1) admits separation of variables using Euler elliptic coordinates (ξ, η), $\xi = \frac{r_1 + r_2}{R} \in (1, +\infty)$ and $\eta = \frac{r_2 - r_1}{R} \in (-1, 1)$. Search for separated wave functions $\Psi(\xi, \eta) = F(\xi)G(\eta)$ converts equation (1) into two ODEs: one

$$(\xi^2 - 1)\frac{d^2 F(\xi)}{d\xi^2} + \xi\frac{dF(\xi)}{d\xi} + \left(\frac{ER^2}{2}\xi^2 + R(Z_1 + Z_2)\xi + \lambda\right)F(\xi) = 0 \tag{2}$$

in the "radial" coordinate $\xi \in (1, \infty)$, the other

$$(1 - \eta^2)\frac{d^2 G(\eta)}{d\eta^2} - \eta\frac{dG(\eta)}{d\eta} - \left(\frac{ER^2}{2}\eta^2 + R(-Z_1 + Z_2)\eta + \lambda\right)G(\eta) = 0 \tag{3}$$

in the "angular" $\eta \in (-1, 1)$ coordinate. λ is the separation constant.

Equations (2) and (3) are no more than the algebraic form of Razavy and Whittaker-Hill equations respectively, see e.g. [7]. The wave functions of our problem are given by the product of solutions of (2) and (3) for identical values of the energy E and the separation constant λ.

The connection with the Confluent Heun equation

Both (2) and (3) are reduced to the Confluent Heun Equation (CHEq) [8, 9]:

$$\left(z^2 - 1\right)u''(z) + \left(\frac{\epsilon}{2}(z^2 - 1) + \gamma(z - 1) + \delta(z + 1)\right)u'(z) + \left(\frac{\alpha}{2}(z + 1) - q\right)u(z) = 0\,, \tag{4}$$

via the changes of variable:

$$F(\xi) = (\xi + 1)^{\frac{2\gamma - 1}{4}}(\xi - 1)^{\frac{2\delta - 1}{4}}e^{\frac{\epsilon\xi}{4}}u(\xi) \tag{5}$$

$$G(\eta) = (1 + \eta)^{\frac{2\gamma - 1}{4}}(1 - \eta)^{\frac{2\delta - 1}{4}}e^{\frac{\epsilon\eta}{4}}u(\eta) \tag{6}$$

that are compatible with the form of Razavy and Whittaker-Hill equations only in the four following cases: a) $\delta = \gamma = \frac{1}{2}$, b) $\delta = \gamma = \frac{3}{2}$, c) $\delta = \frac{1}{2}$, $\gamma = \frac{3}{2}$, and d) $\delta = \frac{3}{2}$, $\gamma = \frac{1}{2}$. The rest of CHEq constants are related to the physical parameters of equations (2) and (3) by the identities:

$$\epsilon^2 = -8ER^2$$

$$\lambda = \frac{\epsilon^2}{16} + \frac{\epsilon(\gamma - \delta)}{4} - \frac{(\gamma + \delta)(\gamma + \delta - 2)}{4} + \frac{2\alpha - 1}{4} - q$$

together with:

$$\frac{\alpha}{2} - \frac{\epsilon}{4}(\delta + \gamma) = R(Z_1 + Z_2)$$

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in the radial equation, and

$$\frac{\alpha}{2} - \frac{\epsilon}{4}(\delta + \gamma) = R(Z_2 - Z_1)$$

in the angular one.

If we interpret CHEq as an spectral problem $Du(z) = qu(z)$, it is not difficult to show, see [5], that the differential operator D can be written as a quadratic combination of the generators of the Lie algebra $sl(2, R)$ if and only if $\alpha = -n\epsilon$, being n a non-negative integer, and consequently CHEq represents a quasi-exactly solvable spectral problem [10, 11, 12, 13] for this special combination of parameters. In this situation it is possible to find an invariant module of polynomial solutions of (4) associated with each arbitrary value of n. The search for Frobenius solutions of the form:

$$u(z) = \sum_{k=0}^{\infty} \frac{(-1)^k \mathcal{P}_k(q)}{2^k k! (\gamma)_k} (z+1)^k, \tag{7}$$

where $(\gamma)_k = \gamma(\gamma+1)\ldots(\gamma+k-1)$ and $\mathcal{P}_0(q) = 1$, leads to the following three-term recurrence between the polynomials $\mathcal{P}_k(q)$ for $k \geq 1$:

$$\mathcal{P}_{k+1}(q) = (q - k(\delta + \gamma - \epsilon + k - 1)) \mathcal{P}_k(q) - k\epsilon(n - k + 1)(\gamma + k - 1)\mathcal{P}_{k-1}(q) \tag{8}$$

Thus, given a concrete value of n, and fixing q as one of the $n+1$ roots of $\mathcal{P}_{n+1}(q)$, q_j, $j = 1, \ldots, n+1$, solutions (7) truncate to polynomials of degree n,

$$u_{n,j}(z) = \sum_{k=0}^{n} \frac{(-1)^k \mathcal{P}_k(q_j)}{2^k k! (\gamma)_k} (z+1)^k \tag{9}$$

and consequently a $n+1$ dimensional module of polynomial eigenfunctions of (4) can be determined algebraically.

3   Elementary solutions of Razavy equation

Translating the QES condition of (4) to the Razavy equation (2): $\alpha = -n^r \epsilon$, $n^r \in \mathbb{N}$, a quantization condition in the expression of ϵ appears

$$\frac{\alpha}{2} - \frac{\epsilon}{4}(\gamma + \delta) = R(Z_1 + Z_2) \Longrightarrow \epsilon = -\frac{4R(Z_1 + Z_2)}{(2n^r + \gamma + \delta)} \tag{10}$$

and consequently, in the energy eigenvalues:

$$E = -\frac{\epsilon^2}{8R^2} \Longrightarrow E_{n^r} = -\frac{2(Z_1 + Z_2)^2}{(2n^r + \gamma + \delta)^2} \tag{11}$$

Meanwhile, the separation constant is characterized by n^r but also by $j = 1, \ldots, n^r + 1$, because the explicit dependence in the q_j parameter:

$$\lambda_{n^r,j} = \frac{R^2(Z_1 + Z_2)^2}{(2n^r + \gamma + \delta)^2} + \frac{(2n^r - \gamma + \delta)R(Z_1 + Z_2)}{(2n^r + \gamma + \delta)} - \frac{(\gamma + \delta)(\gamma + \delta - 2)}{4} - \frac{1}{4} - q_j \tag{12}$$

As it was mentioned above, the compatibility between Razavy and CHEq is only possible in four concrete choices of constants δ and γ. Thus we find the following expressions for energies, separation constants and eigenfunctions:
Type a. $\delta = \gamma = \frac{1}{2}$.

$$E_{n^r} = -\frac{2(Z_1 + Z_2)^2}{(2n^r + 1)^2}, \quad \lambda_{n^r,j} = -\frac{R^2 E_{n^r}}{2} + \frac{2n^r R(Z_1 + Z_2)}{2n^r + 1} - q_j$$

$$F_{n^r,j}(\xi) = e^{-\frac{R(Z_1 + Z_2)}{2n^r + 1}\xi} u_{n^r,j}(\xi)$$

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Type b. $\delta = \gamma = \frac{3}{2}$.

$$E_{n^r} = -\frac{2(Z_1 + Z_2)^2}{(2n^r + 3)^2} \ , \quad \lambda_{n^r,j} = -\frac{R^2 E_{n^r}}{2} + \frac{2n^r R(Z_1 + Z_2)}{2n^r + 3} - q_j - 1$$

$$F_{n^r,j}(\xi) = \sqrt{\xi^2 - 1}\, e^{-\frac{R(Z_1+Z_2)}{2n^r+3}\xi} u_{n^r,j}(\xi)$$

In these two cases a) and b) the energies are the corresponding to planar hydrogenlike atoms with nuclear charge $Z_1 + Z_2$.

Type c. $\delta = \frac{1}{2}$, $\gamma = \frac{3}{2}$.

$$E_{n^r} = -\frac{2(Z_1 + Z_2)^2}{(2n^r + 2)^2} \ , \quad \lambda_{n^r,j} = -\frac{R^2 E_{n^r}}{2} + \frac{(2n^r - 1)R(Z_1 + Z_2)}{2n^r + 2} - q_j - \frac{1}{4}$$

$$F_{n^r,j}(\xi) = \sqrt{\xi + 1}\, e^{-\frac{R(Z_1+Z_2)}{2n^r+2}\xi} u_{n^r,j}(\xi)$$

Type d. $\delta = \frac{3}{2}$, $\gamma = \frac{1}{2}$.

$$E_{n^r} = -\frac{2(Z_1 + Z_2)^2}{(2n^r + 2)^2} \ , \quad \lambda_{n^r,j} = -\frac{R^2 E_{n^r}}{2} + \frac{(2n^r + 1)R(Z_1 + Z_2)}{2n^r + 2} - q_j - \frac{1}{4}$$

$$F_{n^r,j}(\xi) = \sqrt{\xi - 1}\, e^{-\frac{R(Z_1+Z_2)}{2n^r+2}\xi} u_{n^r,j}(\xi)$$

In the cases c) and d) the energies do not correspond to the planar hydrogenoid atoms, because the even character of the denominator, $2n^r + 2$, recall that the spectrum of the planar hydrogen problem[7] is: $E = \frac{-2}{(2n+1)^2}$. Nevertheless, there exist interesting elementary solutions of Types c) and d) which are reminiscent of the lemniscatic orbits of the classical problem and we shall refer to as "quasi"hydrogenoid.

4 Elementary solutions of Whittaker-Hill equation

An equivalent analysis can be performed for the angular equation (3) simply changing the relative sign of the charge Z_1 and the range of variation for the angular coordinate. Thus, the condition: $\alpha = -n^a \epsilon$, $n^a \in \mathbb{N}$, leads to the following structure of solutions:

Type a. $\delta = \gamma = \frac{1}{2}$.

$$E_{n^a} = -\frac{2(-Z_1 + Z_2)^2}{(2n^a + 1)^2} \ , \quad \lambda_{n^a,j} = -\frac{R^2 E_{n^a}}{2} + \frac{2n^a R(-Z_1 + Z_2)}{2n^a + 1} - q_j$$

$$G_{n^a,j}(\eta) = e^{-\frac{R(-Z_1+Z_2)}{2n^a+1}\eta} u_{n^a,j}(\eta)$$

Type b. $\delta = \gamma = \frac{3}{2}$.

$$E_{n^a} = -\frac{2(-Z_1 + Z_2)^2}{(2n^a + 3)^2} \ , \quad \lambda_{n^a,j} = -\frac{R^2 E_{n^a}}{2} + \frac{2n^r R(-Z_1 + Z_2)}{2n^a + 3} - q_j - 1$$

$$G_{n^a,j}(\eta) = \sqrt{1 - \eta^2}\, e^{-\frac{R(-Z_1+Z_2)}{2n^a+3}\eta} u_{n^a,j}(\eta)$$

Type c. $\delta = \frac{1}{2}$, $\gamma = \frac{3}{2}$.

$$E_{n^a} = -\frac{2(-Z_1 + Z_2)^2}{(2n^a + 2)^2} \ , \quad \lambda_{n^a,j} = -\frac{R^2 E_{n^a}}{2} + \frac{(2n^a - 1)R(-Z_1 + Z_2)}{2n^a + 2} - q_j - \frac{1}{4}$$

$$G_{n^a,j}(\eta) = \sqrt{1 + \eta}\, e^{-\frac{R(-Z_1+Z_2)}{2n^r+2}\eta} u_{n^a,j}(\eta)$$

Type d. $\delta = \frac{3}{2}$, $\gamma = \frac{1}{2}$.

$$E_{n^a} = -\frac{2(-Z_1 + Z_2)^2}{(2n^a + 2)^2} \ , \quad \lambda_{n^a,j} = -\frac{R^2 E_{n^a}}{2} + \frac{(2n^a + 1)R(-Z_1 + Z_2)}{2n^a + 2} - q_j - \frac{1}{4}$$

$$G_{n^a,j}(\eta) = \sqrt{1 - \eta}\, e^{-\frac{R(-Z_1+Z_2)}{2n^a+2}\eta} u_{n^a,j}(\eta)$$
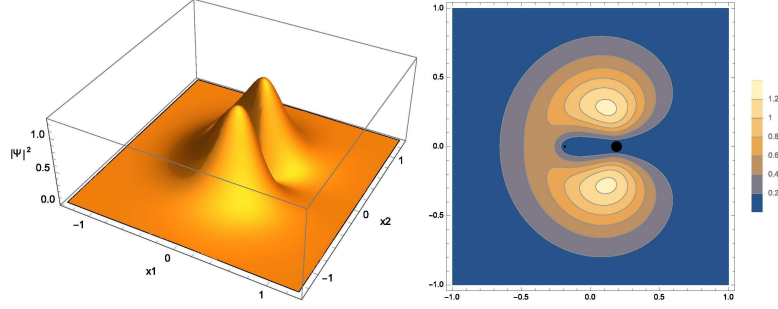
Figure 1: Graphical representation of the probability density $\rho(x_1, x_2) = |\Psi|^2$ for the normalized eigenfunction (14), and several level curves of $\rho(x_1, x_2)$.

5 Elementary solutions of the Schrödinger equation

The simultaneous existence of elementary solutions in both radial and angular equations, for fixed values of Z_1 and Z_2, is obviously possible only if the parameters E and λ determined in the resolution process are the same for both equations.

Thus, there exist elementary solutions of the Schrödinger equation only for those values of $n_1 \in \mathbb{N}$ and $n_2 \in \mathbb{N}$ that solve the diophantine equation:

$$\frac{(Z_1 + Z_2)^2}{n_1^2} = \frac{(-Z_1 + Z_2)^2}{n_2^2}, \tag{13}$$

where n_1 can be equal to $2n^r + 1$, $2n^r + 3$ or $2n^r + 2$, whereas n_2 is: $2n^a + 1$, $2n^a + 3$ or $2n^a + 2$. Moreover, the value of the separation constant λ in (2) and (3) must be the same and because of the dependence of λ on R, the equality will only be satisfied for certain values of the internuclear distance.

As illustrative examples, we present several elementary solutions for two pairs of charges: $Z_1 = 5$, $Z_2 = 1$, and $Z_1 = 2$, $Z_2 = 1$.

Charges $Z_1 = 5$, $Z_2 = 1$. The elementary eigenfunction of minimum energy corresponds to the $n_1 = 3$ and $n_2 = 2$ solution of (13): $E = -8$. This solution appears considering Type b) in Razavy equation with $n^r = 0$ and Type d) in Whittaker-Hill equation with $n^a = 0$. The compatible value of λ is $-\frac{7}{16}$ that is obtained for $R = \frac{3}{8}$. Thus, we have the eigenfunction:

$$\Psi(\xi, \eta) = \sqrt{\xi^2 - 1}\sqrt{1 - \eta}e^{-\frac{3}{4}(\xi - \eta)} \tag{14}$$

The next energy level where elementary solutions are found is $E = -2$. These solutions are obtained for $n_1 = 6$ and $n_2 = 4$ in (13), in four different combination of Types c) and d):

- Type d) in both equations. The values of the constants are: $\lambda = -\frac{583}{256}$ and $R = \frac{3}{16}$ and the wave function reads:

$$\Psi(\xi, \eta) = \sqrt{\xi - 1}\sqrt{1 - \eta}\left(\eta + \frac{1}{3}\right)\left(\xi^2 - 10\xi - 7\right)e^{-\frac{3}{16}(\xi - \eta)} \tag{15}$$

- Type d) in Razavy equation and Type c) in Whittaker-Hill equation. $\lambda = -2.25$, $R = 0.43$

$$\Psi(\xi, \eta) = \sqrt{\xi - 1}\sqrt{1 + \eta}(\eta - 0.71)\left(\xi^2 - 3.89\xi - 3.54\right)e^{-0.43(\xi - \eta)}$$

- Type c) and d) respectively. $\lambda = -3.11$, $R = 1.64$

$$\Psi(\xi, \eta) = \sqrt{\xi + 1}\sqrt{1 - \eta}(\eta - 0.58)\left(\xi^2 - 0.63\xi - 0.88\right)e^{-1.64(\xi - \eta)}$$
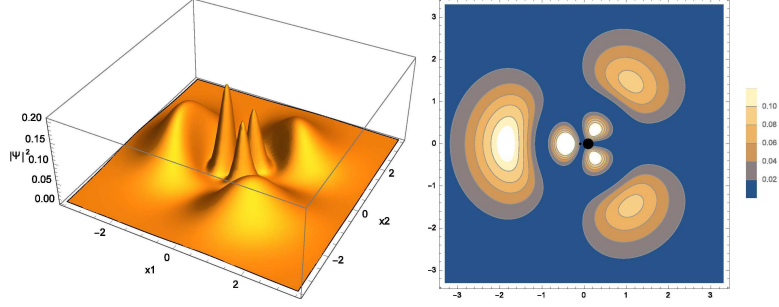
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Figure 2: Graphical representation of $\rho(x_1, x_2)$ for the normalized eigenfunction (15) and several level curves of $\rho(x_1, x_2)$.

- Type c) and d) again. $\lambda = -0.59$, $R = 0.29$

$$\Psi(\xi, \eta) = \sqrt{\xi + 1}\sqrt{1 - \eta}(\eta + 3.20)\left(\xi^2 - 10.06\xi + 16.82\right)e^{-0.29(\xi-\eta)}$$

Charges $Z_1 = 2$, $Z_2 = 1$. In this case we present the three elementary eigenfunctions that appears for: $E = -\frac{1}{2}$. The corresponding solution of (13) is $n_1 = 6$ and $n_2 = 2$.

- $\lambda = \frac{1}{36}(59 - 4\sqrt{19})$, $R = \frac{2}{3}(1 + \sqrt{19})$

$$\Psi(\xi, \eta) = \sqrt{\xi - 1}\sqrt{1 - \eta}\,e^{-\frac{1}{3}\left(1+\sqrt{19}\right)(\xi-\eta)}\left(\xi^2 + \frac{1}{2}\left(3 - \sqrt{19}\right)\xi + \frac{1}{4}\left(3 - 2\sqrt{19}\right)\right)$$

- $\lambda = -\frac{31}{64}$, $R = \frac{3}{4}$

$$\Psi(\xi, \eta) = \sqrt{\xi + 1}\sqrt{1 - \eta}(\xi^2 - 8\xi + 11)e^{-\frac{3}{8}(\xi-\eta)}$$

- $\lambda = \frac{1}{36}(59 + 4\sqrt{19})$, $R = \frac{2}{3}(-1 + \sqrt{19})$

$$\Psi(\xi, \eta) = \sqrt{\xi + 1}\sqrt{1 + \eta}\,e^{-\frac{1}{3}(-1+\sqrt{19})(\xi-\eta)}\left(\xi^2 - \frac{1}{2}\left(3 + \sqrt{19}\right)\xi + \frac{1}{4}\left(3 + 2\sqrt{19}\right)\right)$$

In order to facilitate the presentation we have written some of the numbers rounded to three significative digits, although all these elementary eigenfunctions have been obtained using exact analytic expressions. There exists also elementary solutions containing polynomials of higher orders, that have to be calculated using numerical approximations because the determination of the roots of $\mathcal{P}_{n+1}(q)$ in (8) with $n \geq 5$ is involved.

6 Two-equal centers

It is very interesting to analyze the symmetric case, i.e., when $Z_1 = Z_2 = Z$. The radial equation (2) is still a Razavy equation, but the angular one (3) reduces to the algebraic version of Mathieu equation:

$$(1 - \eta^2)\frac{d^2G(\eta)}{d\eta^2} - \eta\frac{dG(\eta)}{d\eta} - \left(\frac{ER^2}{2}\eta^2 + \lambda\right)G(\eta) = 0 \tag{16}$$

The standard form of Mathieu equation [15, 16] is obtained by the change of variable: $\eta = \cos\nu$, where ν varies in the interval $\nu \in [-\pi, \pi]$ in such a way that the $x_2 > 0$ half-plane is described in the range $\nu \in (0, \pi)$ whereas $\nu \in (-\pi, 0)$ corresponds to the $x_2 < 0$ half-plane, i.e., the original change of coordinates:

$$x_1 = \frac{R}{2}\xi\eta \quad , \qquad x_2 = \pm\frac{R}{2}\sqrt{\xi^2 - 1}\sqrt{1 - \eta^2}$$
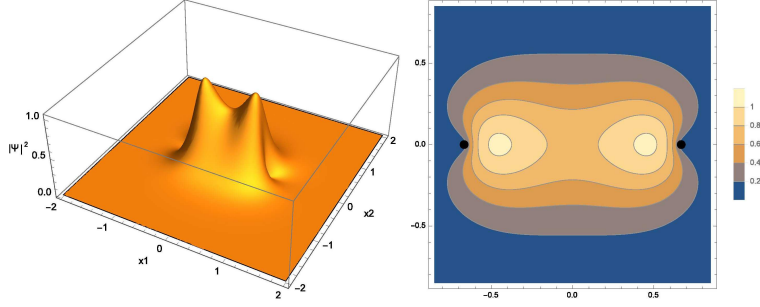
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Figure 3: Graphical representation of $\rho(x_1, x_2)$ for (20) and several level curves of $\rho(x_1, x_2)$.

is redefined in a one-to-one version:

$$x_1 = \frac{R}{2}\xi \cos \nu \quad , \qquad x_2 = \frac{R}{2}\sqrt{\xi^2 - 1}\sin \nu$$

Thus, equation (16) reduces to standard form:

$$\frac{d^2 G(\nu)}{d\nu^2} + (a - 2q \cos 2\nu)\, G(\nu) = 0 \tag{17}$$

where $a = -\lambda - \frac{ER^2}{8}$ and $q = \frac{ER^2}{8}$.

Mathieu equation (17) does not admit polynomial solutions [16], this fact can be easily checked because the quasi-exact solvability condition for CHEq is not compatible with the form of Mathieu equation (16). Complete elementary solutions, products of two polynomials, for the planar two center problem in the symmetric case do not exist.

Nevertheless, it is possible to consider elementary solutions only for Razavy equation and to determine the solutions of Mathieu equation corresponding to the values of E_{n^r} and $\lambda_{n^r,j}$, (11,12). Each elementary Razavy solution is associated with a Mathieu equation (17) with the parameters:

$$a_{n^r,j} = -\lambda_{n^r,j} - \frac{E_{n^r}R^2}{4} \;, \quad q_{n^r} = \frac{E_{n^r}R^2}{8}$$

There exist solutions of Mathieu equation (17) with different periodicity or quasi-periodicity properties, and they are applicable to a physical problem depending on its special characteristics, see for instance [14]. In the two-center problem, the physically admissible eigenfunctions of the Schrödinger equation must be univalued and thus it is necessary to consider only the 2π-periodic solutions of (17), the proper Mathieu functions: $Ce_n(q, z)$ and $Se_n(q, z)$ [15, 16, 17]. The Mathieu cosine $Ce_n(q, z)$, $n = 0, 1, \ldots$, and sine $Se_n(q, z)$, $n = 1, 2, \ldots$, are solutions of (17) only if the parameter a takes the Mathieu characteristic values $a_n(q)$ and $b_n(q)$ respectively.

An elementary Razavy solution determined by E_{n^r} and $\lambda_{n^r,j}$ is compatible only with values of R such that the Mathieu parameter $a_{n^r,j}$ coincides with a characteristic value of the Mathieu cosine or sine functions, i.e.

$$-\lambda_{n^r,j} - \frac{E_{n^r}R^2}{4} = a_n\left(\frac{E_{n^r}R^2}{8}\right) \tag{18}$$

for some $n = 0, 1, 2, \ldots$, or:

$$-\lambda_{n^r,j} - \frac{E_{n^r}R^2}{4} = b_n\left(\frac{E_{n^r}R^2}{8}\right) \tag{19}$$

for some $n = 1, 2, \ldots$.

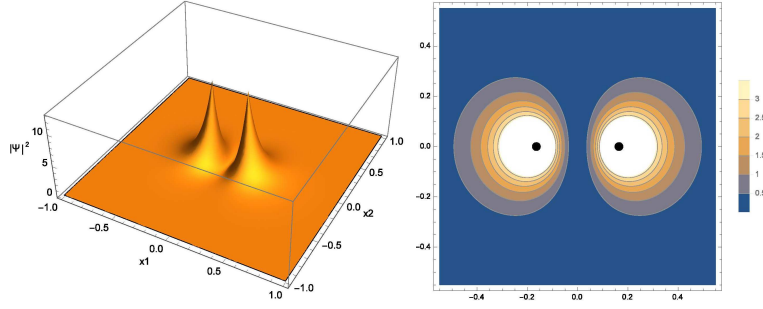As examples, several eigenfunctions of this type are presented:

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Figure 4: Graphical representation of $\rho(x_1, x_2)$ for (21) and several level curves of $\rho(x_1, x_2)$.

Charges $Z_1 = Z_2 = 3$. We illustrate the process with the simplest example: Choosing the energy $E = -8$, obtained for $n^r = 1$ in the Type a) of Razavy equation, there are two allowable values for the separation constant: $\lambda_{1,1}$ and λ_{12}.

The associated Mathieu equations have parameters: $a_{1,1}$ and $a_{1,2}$ respectively, and $q_1 = -R^2$. There exists only one possibility for R that leads $a_{1,1}$ and/or $a_{1,2}$ to be a characteristic value of the Mathieu equation: if $R = 1.33$, then $a_{1,2} = b_1(q_1) = 2.30$, $\lambda_{1,2} = 1.27$. For these values, the trascendent equation (19) is satisfied. Thus the eigenfunction is:

$$\Psi(\xi, \nu) = e^{-2.67\xi}(\xi + 0.91)Se_1(-1.78, \nu) \tag{20}$$

Other examples are:

- $E = -18$, $\lambda = -0.26$, $R = 0.33$, $a_1(q_0) = 0.75$.

$$\Psi(\xi, \nu) = e^{-0.99\xi}\sqrt{\xi + 1}Ce_0(-0.24, \nu) \tag{21}$$

- $E = -\frac{9}{2}$, $\lambda = -3.13$, $R = 0.87$, $b_2(q_1) = 3.98$.

$$\Psi(\xi, \nu) = e^{-1.30\xi}\sqrt{\xi + 1}(\xi + 0.49)Se_2(-0.43, \nu)$$

- $E = -\frac{72}{25}$, $\lambda = 6.41$, $R = 4.49$, $a_2(q_2) = 8.11$.

$$\Psi(\xi, \nu) = e^{-5.39\xi}\left(\xi^2 + 1.73\xi + 0.74\right)Ce_2(-7.26, \nu)$$

For aesthetic reasons, the characteristic values and the other quantities involved in (20,21) and rest of equations, are presented using only three significative digits, although obviously an arbitrary precision can be obtained.

It is possible to find a plethora of solutions of this mixed type with specific values of R physically meaningful in the atomic/molecular range.

Acknowledgments

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