Quasi-exact solutions for two interacting electrons in two-dimensional anisotropic dots

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Abstract
We present an analysis of the two-dimensional Schrödinger equation for two electrons interacting via Coulombic force and confined in an anisotropic harmonic potential. The separable case of $\omega_y : \omega_x = 2$ is studied particularly carefully. The closed-form expressions for bound-state energies and the corresponding eigenfunctions are found at some particular values of ω_x. For highly accurate determination of energy levels at other values of ω_x, we apply an efficient scheme based on the Fröbenius expansion.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The Hookean system composed of N interacting particles trapped in an external harmonic potential

$$V(\mathbf{r}) = \frac{m_*}{2}\left[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right] \tag{1}$$

has been considered first as a model of the nucleus in the early days of nuclear physics [1]. In the case where the two particles interact via central forces, the Hookean system enjoys a particularly nice feature that the centre-of-mass motion may be separated out. Because of its relatively easy tractability, the system has nowadays become a standard tool for testing the quality of many-body approximation methods in studying correlations between electrons. Recently, the Hookean system attracted renowned interest, since the progress in semiconductor technology has allowed the formation of quantum dots (QDs), which are the systems of few electrons confined on the scale of hundreds of nanometres in an approximately harmonic

potential [2]. For the simplest QD, consisting of two electrons ($N = 2$), the Hamiltonian can be written as

$$H = \sum_{i=1}^{2} \left[\frac{\mathbf{p}_i^2}{2m_*} + V(\mathbf{r}_i) \right] + \frac{e^2}{\varepsilon_*|\mathbf{r}_2 - \mathbf{r}_1|}, \tag{2}$$

where m_* is the effective electron mass and ε_* the effective dielectric constant. Introducing centre of mass and relative coordinates

$$\mathbf{R} = \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) = (X, Y, Z), \qquad \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 = (x, y, z), \tag{3}$$

the above Hamiltonian is separated into $H = H^{\mathbf{R}} + H^{\mathbf{r}}$, where the centre of mass Hamiltonian

$$H^{\mathbf{R}} = \frac{\mathbf{P}^2}{4m_*} + m_*\left(\omega_x^2 X^2 + \omega_y^2 Y^2 + \omega_z^2 Z^2\right) \tag{4}$$

is exactly solvable. The problem is thus reduced to the Schrödinger equation for the relative motion

$$H^{\mathbf{r}}\psi = \varepsilon^{\mathbf{r}}\psi, \tag{5}$$

described by the Hamiltonian

$$H^{\mathbf{r}} = -\hbar^2\nabla^2/m_* + \frac{m_*}{4}\left[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right] + \frac{e^2}{\varepsilon_* r}, \tag{6}$$

where $r = |\mathbf{r}|$. By a transformation $\hat{x} = x/a_*$, $\hat{y} = y/a_*$, the relative motion equation is rescaled to the form

$$\left[-\frac{\partial^2}{\partial \hat{x}^2} - \frac{\partial^2}{\partial \hat{y}^2} - \frac{\partial^2}{\partial \hat{z}^2} + \hat{\omega}_x^2\hat{x}^2 + \hat{\omega}_y^2\hat{y}^2 + \hat{\omega}_z^2\hat{z}^2 + \frac{1}{\sqrt{\hat{x}^2 + \hat{y}^2 + \hat{z}^2}} \right]\psi = \hat{\varepsilon}^{\mathbf{r}}\psi \tag{7}$$

where $\varepsilon^{\mathbf{r}} = R^*\hat{\varepsilon}^{\mathbf{r}}$, $\omega_{x,y,z}/2 = \hat{\omega}_{x,y,z}(\hbar/m_* a_*^2)$ with the effective Bohr radius $a_* = \hbar^2\varepsilon_*/m_* e^2$ and the effective Rydberg constant $R^* = m_* e^4/\hbar^2\varepsilon_*^2$. In the following, we skip the hats over the spatial coordinates x, y, z, frequencies $\omega_{x,y,z}$ and relative energy $\varepsilon^{\mathbf{r}}$.

In the case of some particular relation between the frequencies ω_x, ω_y and ω_z, the problem of the relative motion becomes easier to solve, and at some specific values of frequencies it even appears quasi-solvable, i.e., one of the states of the spectrum can be analytically determined. The most studied example, important for describing QDs in a constant magnetic field, is the case the two of confinement frequencies are equal, e.g. $\omega_x = \omega_y = \omega$. For such an axially symmetric system there are three cases where the problem of the relative motion (7) is integrable: (1) $\omega_z = \omega$, being separable in spherical coordinates, (2) $\omega_z : \omega = 2$, being separable in parabolic coordinates, and (3) $\omega_z : \omega = 1/2$, which is one of few examples of integrable problems that is generally not separable [3]. The quasi-solvability of the case (1) has been known for a long time [4, 5], and recently it has been demonstrated [6] that, also in the two other cases, one of the bound-state solutions (not necessarily the ground state) can be obtained in a closed form at some particular values of ω.

Another example, which is important in studying two-dimensional (2D) QDs, is that where one of the frequencies is much larger than the other two, e.g. $\omega_z \to \infty$. The 2D approximation is usually justified in practice, since QDs are realized by lateral confinement of electron gas at the boundaries of semiconductor nanostructures. The above problem is integrable in two cases: that of $\omega_x = \omega_y$, and that of $\omega_y : \omega_x = 2$ (which is equivalent to the case of $\omega_y : \omega_x = 1/2$, under the exchange of ω_x and ω_y). In the first case, the harmonic potential has circular symmetry and the problem of the relative motion becomes separable in polar coordinates. This case was much studied in the literature [7–9] and the closed-form solutions for particular frequencies have been derived [10]. The influence of the anisotropy aspect ratio ω_x/ω_y on

the QDs properties has been recently studied in [11, 12], where the separability of the case of $\omega_y : \omega_x = 2$ in parabolic coordinates has been pointed out. Here we shall study this integrable case in detail. The main result of our paper is the demonstration that for particular values of ω_x the exact solutions can be found in a closed form. Although the property of quasi-solvability appears only at particular confinement frequencies, it is very appealing, as the knowledge of exact bound-state energies and the corresponding eigenfunctions in a closed form can be used for extracting information about the model and for testing the performance of approximation methods. Therefore, we discuss the quasi-solvable cases in detail, providing the values of confinement frequencies ω_x as well as the corresponding energy eigenvalues and the closed-form solutions for wavefunctions. For determining the energy spectrum at arbitrary values of ω_x, we develop a numerical scheme based on the Fröbenius method (FM), which was successfully used for calculating bound state energies of one-dimensional [13–15] and spherically symmetric potentials [16, 17]. The comparison of the bound-state solutions determined within the FM with the exact ones allows us to demonstrate how good is the performance of the numerical approximation scheme.

The outline of our work is as follows. In section 2, we give a brief discussion of the spectrum in the 2D case of motion (8), paying a particular attention to the integrable case of $\omega_y : \omega_x = 2$. In section 3, the quasi-solvable cases are derived. In section 4 the calculation within the FM are described and a comparison with exact results is given. The paper ends with concluding remarks in section 5.

2. Theoretical study

In the case of laterally confined QD, the relative motion equation (7) takes the form

$$\left[-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \omega_x^2 x^2 + \omega_y^2 y^2 + \frac{1}{\rho} \right] \psi(\mathbf{r}) = \varepsilon^{\mathbf{r}} \psi(\mathbf{r}), \tag{8}$$

where $\rho = \sqrt{x^2 + y^2}$. The singlet (s) and triplet (t) spin states of the two-electron system correspond to symmetric and antisymmetric spatial wavefunctions, respectively. As the centre-of-mass coordinate remains the same upon the interchange of electrons, the symmetry requirement reduces to the symmetry of the relative wavefunction under inversion $\mathbf{r} \to -\mathbf{r}$. Because of the invariance of equation (8) to reflections about the x- and y-axes, the (x, y)-parity of spatial wavefunctions is well defined. The parity $(+, +)$ or $(-, -)$ corresponds to spin singlet eigenfunctions, and the parity $(+, -)$ or $(-, +)$ to the spin triplet ones.

The simplest case of circular symmetry has been much studied in the literature [7–9]. Here we discuss the other integrable case, $\omega_y : \omega_x = 2$. Introducing two-dimensional parabolic coordinates through

$$x = \eta_1 \eta_2, \qquad y = \tfrac{1}{2}\left(\eta_1^2 - \eta_2^2 \right), \qquad \eta_2 \geqslant 0 \tag{9}$$

the Schrödinger equation is transformed into the form

$$H^{\mathbf{r}}(\eta_1, \eta_2) \psi(\eta_1, \eta_2) = \varepsilon^{\mathbf{r}} \psi(\eta_1, \eta_2) \tag{10}$$

with the Hamiltonian given by

$$H^{\mathbf{r}}(\eta_1, \eta_2) = \frac{1}{\eta_1^2 + \eta_2^2} \left[-\frac{\partial^2}{\partial \eta_1^2} - \frac{\partial^2}{\partial \eta_2^2} + \frac{1}{4}\omega_y^2 \left(\eta_1^6 + \eta_2^6 \right) - \frac{1}{4}\eta_1^2 \eta_2^2 \left(\eta_1^2 + \eta_2^2 \right) \left(\omega_y^2 - 4\omega_x^2 \right) + 2 \right]. \tag{11}$$

Now, it is easy to see that by setting $\omega_y = 2\omega_x$ and $\psi(\eta_1, \eta_2) = g_1(\eta_1)g_2(\eta_2)$ into (11) one gets two ordinary differential equations of the identical form

$$\left[-\frac{d^2}{d\eta_j^2} - \varepsilon^{\mathbf{r}}\eta_j^2 + \omega_x^2\eta_j^6 + \beta_j \right] g_j(\eta_j) = 0, \qquad j = 1, 2 \qquad (12)$$

that are coupled by the condition $\beta_1 + \beta_2 = 2$ to be satisfied by the separation constants β_1 and β_2. The integrability is explained by the fact that in the case of $\omega_y : \omega_x = 2$ an operator commuting with the Hamiltonian (11) exists in the form [11]

$$\Lambda = \{\hat{L}_z, \hat{p}_x\} + 2\omega_x^2 yx^2 - \frac{y}{\rho}, \qquad (13)$$

where the bracket { } denotes the anticommutator. The operator Λ commutes with the x-reflection but anticommutes with the y-reflection operator, and its eigenvalue is given by $\delta = (\beta_1 - \beta_2)/2$. Therefore, the eigenstates corresponding to $\delta \neq 0$, i.e. $\beta_1 \neq \beta_2$, are doubly degenerate with respect to the sign of δ, and those with $\delta = 0$, i.e. $\beta_1 = \beta_2$, are non-degenerate.

The bound states of the QD correspond to the values of $\varepsilon^{\mathbf{r}}$ and β_j such that the functions $\psi(\eta_1, \eta_2)$ vanish, as $|\eta_1|, \eta_2 \to \infty$. The eigenfunctions of (12) which vanish at infinity can be ordered by the quantum number n_j that counts its nodal points on $-\infty < \eta_j < \infty$, and will be denoted by $g^{(n_j)}(\eta_j, \beta_j)$. The reflection symmetry of (12) divides $g^{(n_j)}(\eta_j, \beta_j)$ into two parity types, depending on n_j being even or odd. As the inverse coordinate transformation,

$$\eta_1 = \frac{x}{|x|}\sqrt{\rho + y} \qquad \text{and} \qquad \eta_2 = \sqrt{\rho - y},$$

shows discontinuity of in the η_1 coordinate at the positive y-axis, the condition emerges that the solution of (10) be a product of functions of the same parity in η_1 and η_2, since only such products have the appropriate continuity properties in the whole space. In the case of $\delta = 0$, which corresponds to the functions $g(\eta_j, \beta_j)$ having the same number of nodal points, the singlet state (s) with (x, y)-parity $(+, +)$ is represented by the product of functions being even in η_1 and η_2, while the triplet state (t) with $(-, +)$ is represented by the product of odd functions. For $\delta \neq 0$, the solutions of (10) with well-defined (x, y)-parity are easily constructed as

$$\psi_{(\pm)}^{(n_1, n_2)}(\eta_1, \eta_2) = g^{(n_1)}(\eta_1, \beta_1)g^{(n_2)}(\eta_2, \beta_2) \pm g^{(n_1)}(\eta_2, \beta_1)g^{(n_2)}(\eta_1, \beta_2), \quad (14)$$

where the sign (+) corresponds to the singlet/triplet state with $(x, y)-$ parity $(+, +)/(-, +)$, and the sign (−) to the triplet/singlet state with $(+, -)/(-, -)$ in the case of n_1 and n_2 being even/odd.

In order to visualize the manifestation of degeneracies discussed above, we consider the behaviour of bound-state energies for varying anisotropy ω_x/ω_y. The numerical calculation have been performed with the help of the linear Rayleigh–Ritz method using the basis of two-dimensional harmonic oscillator eigenstates ('exact diagonalization'). The energies of low-lying states of the relative motion, $\varepsilon^{\mathbf{r}}$, are plotted in figure 1, for a fixed frequency $\omega_x = 0.5$ in function of the parameter ω_y. It can be observed how the states with spatial parity, $(+, -)$, $(-, +)$ become degenerate with those of $(+, +)$, $(-, -)$, respectively, in the case discussed above, i.e. $\omega_y : \omega_x = 2$, and in the case equivalent to it after exchange $x \rightleftarrows y$, i.e. $\omega_x : \omega_y = 2$. The visible degeneracy of the spectrum at $\omega_y = \omega_x = 0.5$ corresponds to a circular symmetry of the harmonic potential.

In the following we will discuss the spectrum of the anisotropic QD in the case of $\omega_y : \omega_x = 2$, which can be determined by solving a coupled pair of one-dimensional equations (12). A simple scheme based on the FM will be used for the numerical determination of the solutions in the above case. The exact solution will be provided for particular values of ω_x.
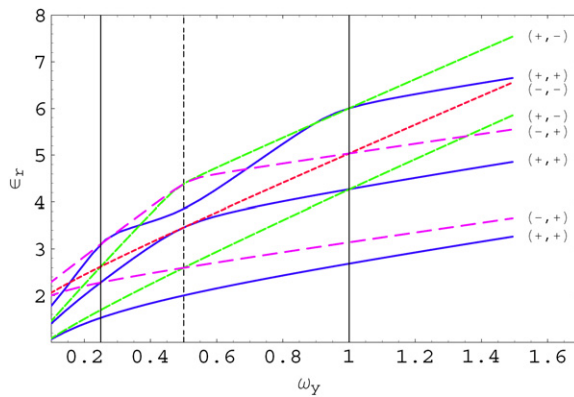
Figure 1. The behaviour of the relative motion energy levels of a QD at $\omega_x = 0.5$ in function of ω_y. The vertical lines correspond to the cases $\omega_x : \omega_y = 2$ and $\omega_y : \omega_x = 2$. The circularly symmetric case of $\omega_y = \omega_x$ is marked by the broken line.

3. Exact solutions

Let us to come to the main purpose of this paper which is the demonstration that the problem of a 2D QD, confined by the potential $\omega_x^2 x^2 + \omega_y^2 y^2$, is quasi-solvable for $\omega_y : \omega_x = 2$, i.e., some of the solutions of the relative motion equation (8) can be found algebraically for certain values of ω_x. We are looking for a solution of the form $\psi(\eta_1, \eta_2) = g(\eta_1, \beta_1)g(\eta_2, \beta_2)$, where $\beta_1 + \beta_2 = 2$, and $g(\eta_j, \beta_j)$ fulfils the ordinary differential equation (12). As the form of equation (12) is similar to that of the sextic anharmonic oscillator, the quasi exact solutions can be represented as [18]

$$g(\eta_j, \beta_j) = e^{-\frac{\omega_x \eta_j^4}{4}} \sum_{i=0}^{\infty} a_i^{(j)} \eta_j^{2i+\nu}, \tag{15}$$

where $a_0^{(j)} \neq 0$ and $\nu = 0, 1$ correspond to the even- and odd-parity cases, respectively. Substituting (15) into (12) and comparing the coefficients of like powers of η_j, one gets the three-term recursion relation for the expansion coefficients $a_i^{(j)}$ in the form

$$A_i a_{i+1}^{(j)} + B_i^{(j)} a_i^{(j)} + C_i a_{i-1}^{(j)} = 0, \tag{16}$$

where

$$A_i = (2i + \nu + 1)(2i + \nu + 2)$$
$$B_i^{(j)} = -\beta_j \tag{17}$$
$$C_i = \varepsilon^{\mathbf{r}} + (1 - 4i - 2\nu)\omega_x$$

with $a_i^{(j)} = 0$ for $i < 0$. It turns out that the QD equation (8) is exactly solvable if the series in the representations (15) for both $g(\eta_1, \beta_1)$ and $g(\eta_2, \beta_2)$ terminate after a finite number of terms. This gives the three conditions

$$\varepsilon^{\mathbf{r}} = \omega_x(3 + 4n + 2\nu) \tag{18}$$
$$a_{n+1}^{(1)}(\omega_x, \varepsilon^{\mathbf{r}}, \beta_1) = 0 \qquad \text{and} \qquad a_{n+1}^{(2)}(\omega_x, \varepsilon^{\mathbf{r}}, \beta_2) = 0, \tag{19}$$

where n denotes the number of the highest non-vanishing term which appears to be necessarily the same in both series. Using the recurrence relation (16), the coefficients of the series may

be conveniently represented in the form

$$a_{n+1}^{(j)}(\omega_x, \varepsilon^{\mathbf{r}}, \beta_j) = \frac{(-1)^{n+1}a_0^{(j)}}{(2(n+1)+\nu)!} P_n^{(j)}(\varepsilon^{\mathbf{r}}, \beta_j, \omega_x)$$

$$= \frac{(-1)^{n+1}a_0^{(j)}}{(2(n+1)+\nu)!} Det \begin{pmatrix} B_0^{(j)} & A_0 & \ldots & \ldots & 0 \\ C_1 & B_1^{(j)} & A_1 & \ldots & 0 \\ 0 & C_2 & B_2^{(j)} & A_2 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & \ldots & C_{n-1} & B_{n-1}^{(j)} & A_{n-1} \\ 0 & \ldots & \ldots & C_n & B_n^{(j)} \end{pmatrix}, \quad j = 1, 2.$$

(20)

By calculating the above determinant for a chosen value of n, the polynomials $P_n^{(j)}$ may be easily determined and expressed in terms of β_j and $\varepsilon^{\mathbf{r}}$ upon taking (18) into account. As an illustration we list here the first four polynomials:

$$P_1^{(j)}(\varepsilon^{\mathbf{r}}, \beta_j) = -\frac{4\varepsilon^{\mathbf{r}}(1+\nu)(2+\nu)}{7+2\nu} + \beta_j^2$$

(21)

$$P_2^{(j)}(\varepsilon^{\mathbf{r}}, \beta_j) = \frac{4\varepsilon^{\mathbf{r}}(16+\nu(13+3\nu))\beta_j}{11+2\nu} - \beta_j^3$$

(22)

$$P_3^{(j)}(\varepsilon^{\mathbf{r}}, \beta_j) = \frac{48\varepsilon^{\mathbf{r}2}(1+\nu)(2+\nu)(5+\nu)(6+\nu)}{(15+2\nu)^2} - \frac{8\varepsilon^{\mathbf{r}}(30+\nu(17+3\nu))\beta_j^2}{15+2\nu} + \beta_j^4$$

(23)

$$P_4^{(j)}(\varepsilon^{\mathbf{r}}, \beta_j) = -\frac{16\varepsilon^{\mathbf{r}2}(2944+\nu(3404+\nu(1451+5\nu(50+3\nu))))\beta_j}{(19+2\nu)^2}$$

$$+ \frac{40\varepsilon^{\mathbf{r}}(16+\nu(7+\nu))\beta_j^3}{19+2\nu} - \beta_j^5$$

(24)

The values of $\varepsilon^{\mathbf{r}}, \beta_1, \beta_2$, for which a closed-form solution of a given parity ν exists, are determined by solving the algebraic equations $P_n^{(1)}(\varepsilon^{\mathbf{r}}, \beta_1) = 0$ and $P_n^{(2)}(\varepsilon^{\mathbf{r}}, \beta_2) = 0$, simultaneously with the imposition of $\beta_1 + \beta_2 = 2$ at a chosen value of n. The solution may be explicitly determined by calculating the coefficients $a_i^{(j)}$ in the functions $g(\eta_j, \beta_j)$ via (20) for $j = 1, 2$. We may notice that for a fixed confinement potential with a specific value of the frequency ω_x determined by (18), there is only one solution that is exactly known. This is a consequence of the fact that the energy $\varepsilon^{\mathbf{r}}$ enters equation (18) as a coefficient of the quadratic term in the potential, which is in difference with the case of the sextic oscillator Schrödinger equation, where several solutions may be analytically determined at specific values of the anharmonicity parameter [18].

We consider here the lowest exact solutions of for the 2D asymmetric QD generated through setting $n = 1, 2, 3, 4, \ldots$, etc. In the simplest case of $\nu = 0$ and $n = 1$, we have the equations $P_1^{(j)}(\varepsilon^{\mathbf{r}}, \beta_j) = -\frac{8\varepsilon^{\mathbf{r}}}{7} + \beta_j^2 = 0$, which upon the condition $\beta_1 + \beta_2 = 2$, are solved by $\beta_j = 1, \varepsilon^{\mathbf{r}} = 7/8$, corresponding to the functions $g^{(0)}(\eta_j, 1) = e^{-\frac{\eta_j^4}{32}}\left(1 + \frac{\eta_j^2}{2}\right)$ that are nodeless. This yields the normalized exact solution of (8) in cartesian coordinates in the form

$$\psi^{(0,0)}(x, y) = \frac{1}{2\sqrt{\left(12\pi\sqrt{2} + \Gamma\left[-\frac{1}{4}\right]^2 + 2\Gamma\left[\frac{1}{4}\right]^2\right)}} e^{-\frac{x^2}{16}-\frac{y^2}{8}}\left(1 + \frac{1}{4}x^2 + \rho\right),$$

(25)

which corresponds to the ground state. Further examples obtained in this way, for both the ground and excited states, are given in table 1 with the corresponding values of $\omega_x, |\delta|$ and $\varepsilon^{\mathbf{r}}$.
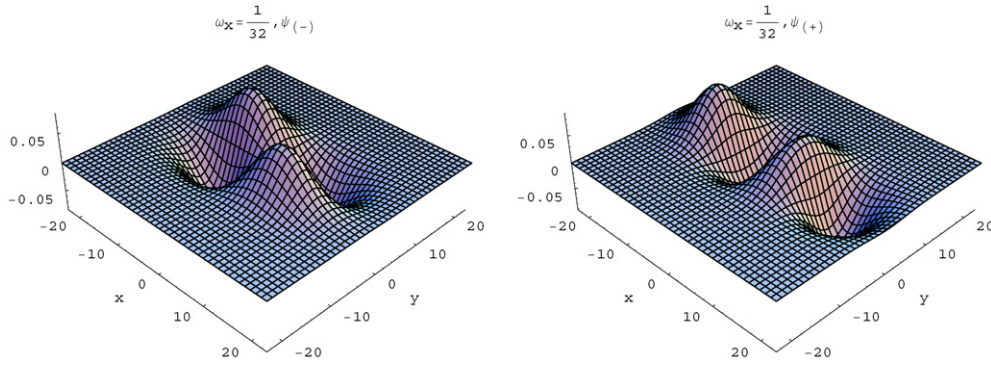
Figure 2. The exact wavefunctions $\psi_{(\pm)}$ corresponding to the degenerate level of the relative motion energy $\varepsilon^{\mathbf{r}} = \frac{13}{32}$.

Table 1. Confinement frequencies, ω_x, and the corresponding exact values of the relative motion energy, $\varepsilon^{\mathbf{r}}$, in the case of $\omega_y : \omega_x = 2$ at a given parity ν for several values of n.

n	ν	ω_x	spin	Symmetry parity	$|\delta|$	$\varepsilon^{\mathbf{r}}$	(n_1, n_2)
1	0	$\frac{1}{8}$	(s)	$(+, +)$	0	$\frac{7}{8}$	$(0, 0)$
2		$\frac{1}{64}$	(s)	$(+, +)$	0	$\frac{11}{64}$	$(0, 0)$
		$\frac{1}{16}$	(s), (t)	$(+, +), (+, -)$	1	$\frac{11}{16}$	$(2, 0)$
3		$\frac{1}{120}(5 + 2\sqrt{5})$	(s)	$(+, +)$	0	$\frac{1}{8}(5 + 2\sqrt{5})$	$(2, 2)$
		$\frac{1}{120}(5 - 2\sqrt{5})$	(s)	$(+, +)$	0	$\frac{1}{8}(5 - 2\sqrt{5})$	$(0, 0)$
		$\frac{1}{240}(5 + \sqrt{5})$	(s), (t)	$(+, +), (+, -)$	$\frac{1}{2}(\sqrt{5} + 1)$	$\frac{1}{16}(5 + \sqrt{5})$	$(0, 4)$
		$\frac{1}{240}(5 - \sqrt{5})$	(s), (t)	$(+, +), (+, -)$	$\frac{1}{2}(\sqrt{5} - 1)$	$\frac{1}{16}(5 - \sqrt{5})$	$(2, 0)$
1	1	$\frac{1}{24}$	(t)	$(-, +)$	0	$\frac{3}{8}$	$(1, 1)$
2		$\frac{1}{128}$	(t)	$(-, +)$	0	$\frac{13}{128}$	$(1, 1)$
		$\frac{1}{32}$	(s),(t)	$(-, -), (-, +)$	1	$\frac{13}{32}$	$(3, 1)$

In figures 2 and 3, we have plotted the normalized wavefunctions $\psi_{(\pm)}$, that correspond to the pairs of degenerate states, obtained for $\omega_x = 1/32$ and $\omega_x = 1/16$, respectively.

4. Fröbenius method

Now we develop a numerical scheme based on the Fröbenius method (FM) for obtaining the approximate energies of an asymmetric QD (8) in the integrable case of $\omega_y : \omega_x = 2$. The method consists of expanding the solution of a differential equation into power series [19], and was originally applied by Barakat and Rosner [13] to compute the spectrum of one-dimensional quartic oscillator confined by impenetrable walls at $x = \pm R$. The energy eigenvalues of the system have been obtained numerically as zeros of a function, calculated from its power series representation. Moreover, it has been shown that the bound-state energies of the confined system approach rapidly those of the unconfined oscillator for increasing R [13–15]. Here we show that solving the two separated equations (12) with the help of the power series representation (15) simultaneously with the condition $\beta_1 + \beta_2 = 2$ enables us to determine
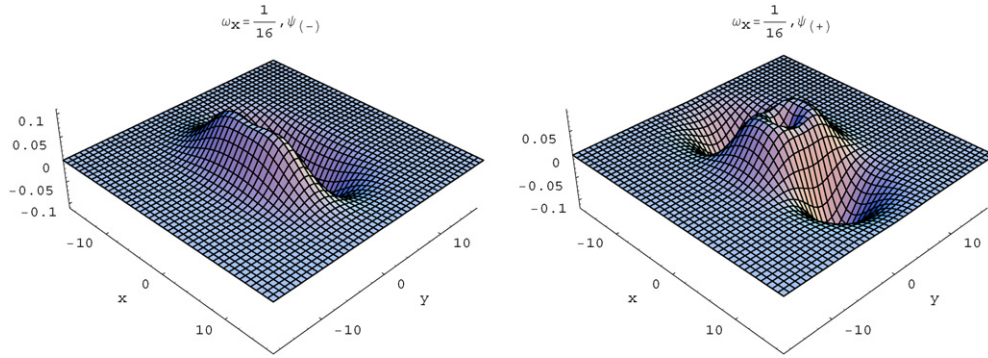
Figure 3. The exact wavefunctions $\psi_{(\pm)}$ corresponding to the degenerate level of the relative motion energy $\varepsilon^{\mathbf{r}} = \frac{11}{16}$.

Table 2. Convergence of the energy eigenvalue and the corresponding separation constant determined by the FM. The underlined numbers agree with the exact results.

K	R	$\varepsilon^{\mathbf{r}}_{FM}$	δ
60	5	0.687 443 2520	0.999 811 134
70		0.687 502 4844	1.000 007 959
90	5.5	0.687 500 0837	1.000 000 296
100		0.687 500 0006	1.000 000 002
120		0.687 500 0008	1.000 000 003
140	6	0.6875000000	1.000 000 000

effectively the energy levels of the QD to very high precision. With the boundary conditions imposed on the functions $g_j(\eta_j)$ at the points $\eta_j = R$, namely $g(R, \beta_j) = 0$, the above problem reduces to finding common zeros $[\delta, \varepsilon^{\mathbf{r}}]$ of the functions $g(R, 1 + \delta)$ and $g(R, 1 - \delta)$. The functions $g(R, 1 \pm \delta)$ can be calculated numerically with an arbitrary accuracy from the power series representations

$$g(\eta_j, \beta_j) = \sum_{i=0}^{K} b_i^{(j)} \eta_j^{2i+\nu}, \tag{26}$$

truncated at a suitably high order K. The obtained approximations to $g(R, 1 \pm \delta)$ are polynomials in the variables $\varepsilon^{\mathbf{r}}$ and δ, which can be taken to advantage in determining the numerical values of their common zeros. Since the exact bound-states of the QD correspond to the functions $g(\eta_j, 1 \pm \delta)$ that vanish at $\eta_j \to \infty$, we expect the solution of the parabolically confined problem to approach the desired solution of the unconfined system, as the confinement range R increases. For the demonstration of convergence, we apply the above scheme to the QD with $\omega_x = 1/16$, for which the exact solution is known (see table 1). Table 2 shows how the numerical values $[\delta, \varepsilon^{\mathbf{r}}_{FM}]$, obtained for the confined system, approach the exact ones, as the truncation order K in the power series (26) and the confinement range R increase.

We have also applied the FM for determining the precise values of energies for the states that are not amenable to exact solution at various $\omega_y : \omega_x = 2$. The stability of numerical results was achieved by increasing K and R until the energy $\varepsilon^{\mathbf{r}}_{FM}$ and the corresponding separation eigenvalue δ stay fixed to the quoted accuracy, which determines the energy of the relative motion of a QD to that accuracy. The bound-state energies determined by the FM
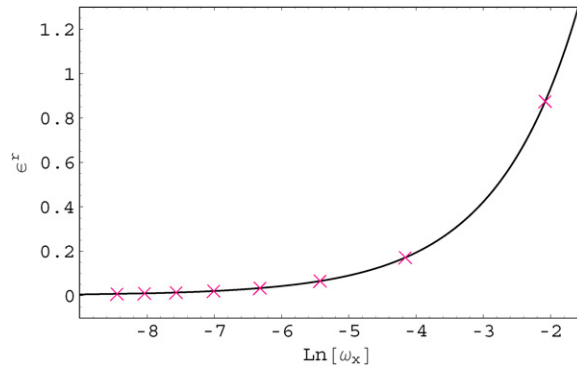
Figure 4. The relative motion ground state energy $\varepsilon^{\mathbf{r}}$ of a QD as a function of $\text{Ln}\,\omega_x$ ($\omega_y : \omega_x = 2$) determined by the FM. A few values of energy, for which closed-form solutions exist are marked with crosses.

Table 3. Low-lying bound-state energies at various confinement frequencies ω_x, as determined by the FM. The existing exact solution are marked bold.

ω_x	$\varepsilon_{\text{FM}}^{\mathbf{r}(+,+)}$	$\varepsilon_{\text{FM}}^{\mathbf{r}(-,+)}$	$\varepsilon_{\text{FM}}^{\mathbf{r}(+,+)(+,-)}$	$\varepsilon_{\text{FM}}^{\mathbf{r}(-,-),(-,+)}$
1/64	**0.171 875 00**	0.172 678 376	0.220 586 977	0.225 979 324
1/32	0.293 674 143	0.297 716 776	0.386 949 414	**0.406 250 00**
1/24	0.367 590 598	**0.375 000 00**	0.490 314 824	0.521 041 536
1/16	0.505 362 736	0.521 827 040	**0.687 500 00**	0.743 921 450
1/8	**0.875 000 00**	0.931 629 324	1.241 576 361	1.386 478 626
1/6	1.100 931 183	1.191 668 135	1.595 014 888	1.803 819 570
1/2	2.681 851 499	3.142 358 616	4.266 819 742	5.035 425 098
1	4.773 351 606	5.921 649 105	8.099 126 926	9.762 556 072
2	8.623 556 558	11.317 113 654	15.569 391 839	19.083 841 664

are listen in table 3 up to 8-digit accuracy at particular values of ω_x. The states for which the exact solution exists are marked bold, their energies can be shown to agree with the exact values to practically unlimited accuracy. The plot of ground state energy in function of Ln ω_x is displayed in figure 4, where we have marked a few of exact values of energy, which correspond to the closed-form solutions discussed in the previous Section.

We may notice that the other integrable case, that of circular symmetry, where the problem reduces to the radial equation for the relative motion, can be also treated within the FM. In that case the solutions has a generalized power series representation and the highly accurate values of energies can be determined with a small computational effort by the scheme developed recently in our previous work [16].

On the example of a QD with confinement frequency $\omega_x = \frac{1}{64}$, we use the exact ground-state energy and the very precise numerical values for higher bound-states determined by the FM (see table 3) to check the convergence of the popular numerical methods applied directly to the two dimensional Schrödinger equation (8). First, we consider the Rayleigh-Ritz (RR) method with the basis set of the two dimensional harmonic oscillator eigenstates, calculating the approximate values of energies by separate diagonalization of the matrix Hamiltonian corresponding to the eigenfunctions with definite $(x, y)-$ parity in a manner similar to that used in [11]. In table 4 the obtained values of energies $\varepsilon_{RR}^{\mathbf{r}}$ are presented for increasing

Table 4. Convergence of low-lying states energy eigenvalues calculated by the Rayleigh-Ritz method for a QD with $\omega_x = 1/64$. The underlined numbers agree with the exact result or that determined by the FM.

D	$\varepsilon_{RR}^{\mathbf{r}(+,+)}$	$\varepsilon_{RR}^{\mathbf{r}(-,+)}$	$\varepsilon_{RR}^{\mathbf{r}(+,+)}$	$\varepsilon_{RR}^{\mathbf{r}(+,-)}$	$\varepsilon_{RR}^{\mathbf{r}(-,-)}$	$\varepsilon_{RR}^{\mathbf{r}(-,+)}$
25	0.171 8911	0.172 6898	0.220 6744	0.220 6004	0.225 9834	0.226 0368
64	0.171 8856	0.172 6830	0.220 6472	0.220 5919	0.225 9803	0.225 9999
144	0.171 8823	0.172 6804	0.220 6274	0.220 5891	0.225 9796	0.225 9878
256	0.171 8805	0.172 6795	0.220 6169	0.220 5881	0.225 9795	0.225 9839

Table 5. Same as in table 4 but calculated by the DVR method.

d	R	$\varepsilon_{DVR}^{\mathbf{r}}$					
256	30	0.171 9120	0.172 7763	0.220 6480	0.221 4837	0.226 0438	0.227 7602
400		0.171 9294	0.172 7757	0.220 6258	0.221 5710	0.226 0337	0.227 7544
	35	0.171 8335	0.172 6833	0.220 4264	0.220 6146	0.225 9909	0.226 0835
576		0.171 8460	0.172 6824	0.220 4845	0.220 5998	0.225 9843	0.226 0752
900		0.171 8557	0.172 6815	0.220 5324	0.220 5924	0.225 9816	0.226 0703
	40	0.171 8483	0.172 6799	0.220 4538	0.220 5956	0.225 9819	0.225 9880

dimension D of the RR matrix. The same QD example is used for testing the DVR (discrete variable representation) method with the trigonometric basis for the square grid on a square whose sides have length R; $x_i = y_i = -R + 2Ri/N$, $i = 1, \ldots, N - 1$ (for details see [20]). The numerical values of energies $\varepsilon_{DVR}^{\mathbf{r}}$ obtained by diagonalization of the Hamiltonian matrix in the point grid representations with dimension $d = (N - 1)^2$, are presented in table 5 for several values of R and d. We may see that in both considered methods, the rough values of energies can be determined with the use of small basis sets but the convergence is rather slow although the computational effort increases quadratically with the size of the basis.

5. Concluding remarks

We discussed the case of a QD consisting of two interacting electrons confined in an anisotropic harmonic potential $V(x, y) = m_*\left(\omega_x^2 x^2 + \omega_y^2 y^2\right)/2$. In the case of $\omega_y : \omega_x = 2$ we developed a numerical scheme based on the Fröbenius method that allows an efficient determination of the spectrum. Moreover, we have shown that a closed-form analytical solutions for the relative motion can be obtained at particular values of ω_x. We illustrated using both the exact and the very precise values of energies determined by FM for testing the convergence of the Rayleigh-Ritz and DVR approximation methods. We have shown that both the methods determine well the approximate values of low-lying states energies but their convergence rates are quite slow.

The exact values of energies and the corresponding wavefunctions obtained in our work can be useful for investigating the performance of other approximation methods in the case of the asymmetric confinement. They can be also used to build the exact density functional and testing the possible ways of constructing approximations to it.

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