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Two electrons in a quantum dot: a semiclassical approach

Stanisław Klama†§ and Eugene G Mishchenko‡

† Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznań, Poland

‡ L D Landau Institute for Theoretical Physics, Russian Academy of Sciences, Kosygina 2, 117334 Moscow, Russia

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Abstract. The spectra of two electrons in a parabolic quantum dot in a magnetic field are obtained using the WKB approximation. No restrictions are imposed on the value of the electron–electron interaction. A simple approximation allowing an exact solution to be obtained for the interaction between two electrons in a quantum dot is proposed. It reproduces all of the qualitative features of the two-electron spectrum. Quantitatively, it is in good agreement with the WKB solution for the range of parameters of experimental interest.

1. Introduction

The electronic properties of two-dimensional quantum dots are of considerable current interest. In particular, spectra of few-electron structures have been probed by a variety of experimental methods, in particular optical spectroscopy [1, 2], capacitance spectroscopy [3], and transport measurements [4, 5]. The theoretical studies are based on the model electron confinement, usually described by a parabolic potential. Although this model has proved to be in good agreement with experiment [1, 4–6], the main problem is that of how to take into account the electron–electron interaction. Known approaches include numerical diagonalization [7, 8], Monte Carlo simulations [9], Hartree–Fock or RPA calculations [8, 6, 10, 11], perturbation series expansion in powers of the electron–electron interaction [12], and numerical solution of the Schrödinger equation [13].

The theoretical and experimental results relating to the quantum dots problem which have been obtained so far have been presented in an excellent review article by Johnson (see [14] and references therein).

Here, we derive the solution of the Schrödinger equation of a two-electron parabolic dot in an external magnetic field, making use of the WKB approximation. We also propose a simple model which proves to be in quantitative agreement (within several per cent) with the WKB solution. Despite the initial approximations (such as assuming a parabolic confinement potential), it seems to be sufficient for producing a proper description of the experimental data. The model is based on the effective one-electron potential and admits an exact solution.

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2. WKB solution

In experimentally realized dots, the motion in the z-direction is always frozen, and we can treat the dots as two-dimensional discs using a parabolic confinement potential, as usual. Let us assume that the magnetic field is applied perpendicularly to the xy-plane. In the magnetic field, the Hamiltonian of two interacting electrons of effective masses m^* can be separated into the centre-of-mass and relative-motion parts as follows:

$$\mathcal{H}_R = \frac{1}{2M}\left(\boldsymbol{P} + \frac{Q}{c}\boldsymbol{A}(\boldsymbol{R})\right)^2 + \tfrac{1}{2}M\omega_0^2 R^2 \tag{1}$$

$$\mathcal{H}_r = \frac{1}{2\mu}\left(\boldsymbol{p} + \frac{q}{c}\boldsymbol{A}(\boldsymbol{r})\right)^2 + \tfrac{1}{2}\mu\omega_0^2 r^2 + \frac{e^2}{\epsilon}\frac{1}{|\boldsymbol{r}|} \tag{2}$$

where $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ and $\boldsymbol{p} = \frac{1}{2}(\boldsymbol{p}_1 - \boldsymbol{p}_2)$ are the relative coordinates, $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2)$ and $\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2$ are the centre-of-mass coordinates, $M = 2m^*$ and $Q = 2e$ are the total mass and charge, respectively, $\mu = m^*/2$ and $q = e/2$ are the reduced mass and charge, respectively, ω_0 is the characteristic confinement frequency, and $\boldsymbol{p} = -\mathrm{i}\nabla_r$, $\boldsymbol{P} = -\mathrm{i}\nabla_R$. Due to this separability, the wave function of the system considered reads simply as $\Psi(\boldsymbol{r}, \boldsymbol{R}) = \Phi(\boldsymbol{R})\phi(\boldsymbol{r})$, and the Schrödinger equation splits into two independent equations.

We choose the gauge described by the vector potential $A_\varphi = rB/2$, $A_r = A_z = 0$. In the planar polar coordinates, the Hamiltonian (2) of the relative motion takes the form

$$\mathcal{H}_r = -\frac{1}{2\mu}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right] + \frac{1}{2}\mu\Omega^2 r^2 - \frac{\mathrm{i}}{2}\omega_c\frac{\partial}{\partial\varphi} + \frac{e^2}{\epsilon r} \tag{3}$$

with the cyclotron frequency given by $\omega_c = eB/m^*c$, and the renormalized confinement frequency given by $\Omega^2 = \omega_0^2 + \omega_c^2/4$. A dielectric constant, ϵ, concerns the host semiconductor. After making the substitution $\phi(\boldsymbol{r}) = r^{-1/2}\chi(r)\mathrm{e}^{\mathrm{i}m\varphi}$, we obtain

$$\frac{\mathrm{d}^2\chi(r)}{\mathrm{d}r^2} + \left(2\mu E - m\mu\omega_c - \frac{m^2 - \frac{1}{4}}{r^2} - \mu^2\Omega^2 r^2 - \frac{2\mu e^2}{\epsilon}\frac{1}{r}\right)\chi(r) = 0 \tag{4}$$

where $m = 0, \pm1, \pm2, \ldots$ denotes the azimuthal quantum number.

The centre-of-mass wave function $\Phi(\boldsymbol{R})$ obeys equation (4) without the Coulomb potential. With the last term in the brackets omitted, equation (4) is easily solved in terms of the confluent hypergeometric function. The spectrum is

$$E_c = (2N + |\mathcal{M}| + 1)\Omega + \tfrac{1}{2}\mathcal{M}\omega_c \qquad N = 0, 1, 2, \ldots \qquad \mathcal{M} = 0, \pm1, \pm2, \ldots. \tag{5}$$

In the following we concentrate on the relative motion only. The electron energy spectrum is given by the sum of E_c and the energy of the relative motion. After making the substitution $r = \sqrt{2}\ell x$, where $\ell^2 = 1/m^*\Omega$, we get from equation (4)

$$\frac{\mathrm{d}^2\chi(x)}{\mathrm{d}x^2} + \left(\varepsilon - x^2 - \frac{\beta}{x} - \frac{\gamma}{x^2}\right)\chi(x) = 0 \tag{6}$$

with

$$\varepsilon = (2E - m\omega_c)/\Omega \qquad \gamma = m^2 - \tfrac{1}{4} \qquad \beta = \sqrt{2}\ell/\epsilon a_B \qquad a_B = 1/m^* e^2. \tag{7}$$

We solve equation (6) within the WKB approximation. Equation (6) contains the irregular point $x = 0$. According to the general WKB theory for equations with irregularities

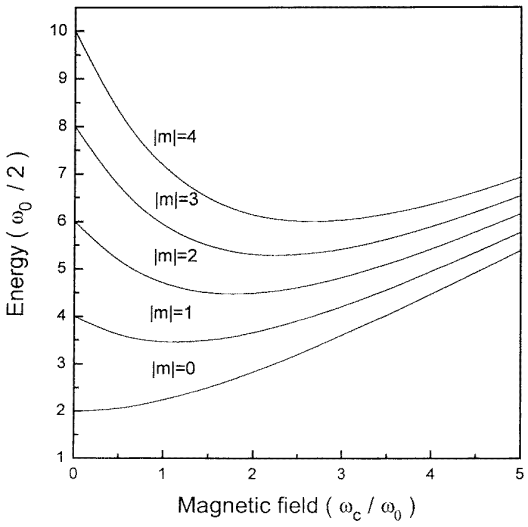

Figure 1. The spectrum of a two-electron quantum dot in the WKB approximation for $n = 0$ and $m = 0, 1, 2, 3, 4$, and in the absence of electron–electron interaction, $\beta = 0$.

[15], one needs to make the substitution $\gamma \to \gamma + \frac{1}{4}$. Thereafter, the semiclassical spectrum of the system can be obtained from the Bohr–Sommerfeld condition

$$\int_b^a \left(\varepsilon - x^2 - \frac{\beta}{x} - \frac{m^2}{x^2}\right)^{1/2} \mathrm{d}x = \pi(n + \tfrac{1}{2}) \qquad n = 0, 1, 2 \ldots \tag{8}$$

where the turning points a, b are determined by the positive roots of the algebraic equation

$$x^4 - \varepsilon x^2 + \beta x + m^2 = 0. \tag{9}$$

Equation (9) can be solved with the help of its cubic resolvent (see e.g. [16])

$$z^3 - 2\varepsilon z^2 + (\varepsilon^2 - 4m^2)z - \beta^2 = 0. \tag{10}$$

The solutions z_1, z_2, z_3 of the cubic resolvent (10) for equation (9) are given by Cardano's formulae:

$$\begin{aligned} z_1 &= \frac{2\varepsilon}{3} - 2\,\mathrm{Re}\left(\frac{q}{2} - \mathrm{i}\sqrt{D}\right)^{1/3} \\ z_2 &= \frac{2\varepsilon}{3} - \mathrm{Re}\left[\left(\frac{q}{2} - \mathrm{i}\sqrt{D}\right)^{1/3}\left(-1 + \mathrm{i}\sqrt{3}\right)\right] \\ z_3 &= \frac{2\varepsilon}{3} - \mathrm{Re}\left[\left(\frac{q}{2} - \mathrm{i}\sqrt{D}\right)^{1/3}\left(-1 - \mathrm{i}\sqrt{3}\right)\right] \end{aligned} \tag{11}$$

where

$$\begin{aligned} q &= \frac{2}{27}\varepsilon^3 - \frac{8}{3}\varepsilon m^2 - \beta^2 \\ D &= \frac{4m^2}{27}\left(\varepsilon^2 - 4m^2\right)^2 + \frac{\beta^2}{2}\left(q + \frac{\beta^2}{2}\right). \end{aligned}$$

Note that the branch of the cubic root in equations (11) has to be chosen in such a way that $\arg(y^{1/3}) = \arg(y)/3$. Using the solutions (11), we express the positive roots (turning points) of equation (9) as follows:

$$\begin{aligned} a &= \left(\sqrt{z_3} + \sqrt{z_2} - \sqrt{z_1}\right)/2 \\ b &= \left(\sqrt{z_3} - \sqrt{z_2} + \sqrt{z_1}\right)/2 \end{aligned}$$

and the negative ones as follows:

$$c = \left(-\sqrt{z_3} + \sqrt{z_2} + \sqrt{z_1}\right)/2$$
$$d = \left(-\sqrt{z_3} - \sqrt{z_2} - \sqrt{z_1}\right)/2.$$

The integral (8) written in the form

$$\int_b^a \frac{-x^4 + \varepsilon x^2 - \beta x - m^2}{\sqrt{(a-x)(x-b)(x-c)(x-d)}} \frac{\mathrm{d}x}{x}$$

can be easily expressed in terms of complete Legendre elliptic integrals of the first, $F(\pi/2, k)$, and third, $\Pi(\pi/2, s, k)$, kinds [17]. The Bohr–Sommerfeld condition (8) then gives the transcendental equation for the electron relative-motion spectrum $\varepsilon = \varepsilon_{n,m}$:

$$-\tfrac{3}{4}\beta I_0 + \tfrac{1}{2}\varepsilon I_1 - m^2 I_2 = \pi(n + \tfrac{1}{2}) \tag{12}$$

with

$$I_0 = \frac{2}{\sqrt{(a-c)(b-d)}} F(\pi/2, k)$$
$$I_1 = \frac{2}{\sqrt{(a-c)(b-d)}} \left[(b-c)\Pi\left(\frac{\pi}{2}, \frac{a-b}{a-c}, k\right) + cF(\pi/2, k)\right]$$
$$I_2 = \frac{2}{\sqrt{(a-c)(b-d)}} \left[\frac{c-b}{bc}\Pi\left(\frac{\pi}{2}, \frac{c(a-b)}{b(a-c)}, k\right) + \frac{1}{c}F(\pi/2, k)\right]$$

where

$$k^2 = \frac{(a-b)(c-d)}{(a-c)(b-d)}.$$

The solution of equation (12) can be easily carried out numerically. For the non-interacting electrons ($\beta = 0$), the numerical WKB solution coincides precisely with the exact solution of the type given by (5), and is presented in figure 1 as a function of the ratio ω_c/ω_0.

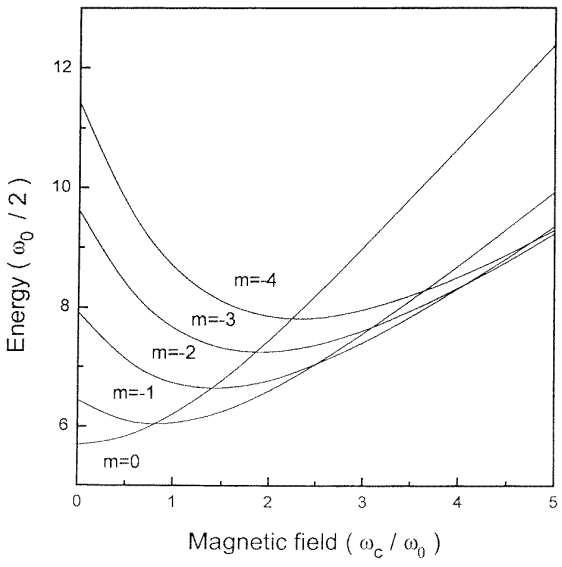

Figure 2. The spectrum of a two-electron quantum dot in the WKB approximation for $n = 0$ and $m = 0, -1, -2, -3, -4$, and finite electron–electron interaction $\beta = 3$. The ground state shifts to the states with higher angular momentum as the magnetic field increases.

The spectra of the interacting electrons are shown in figure 2 for $\beta = 3$. As the magnetic field increases, the ground state $n = 0, m = 0$ shifts to the levels with higher angular momentum $n = 0$, $m = -1, -2, -3, \ldots$. This happens because the Coulomb energy gets smaller when the angular momentum $|m|$ increases along with the average distance between electrons. The spectra presented in figures 1 and 2 correspond to the previous results [18–20] obtained by different (mainly numerical) methods.

3. Harmonic approximation

Now, we propose a model which has been found to give a good approximation of the above results. The potential energy in the WKB approximation (see also (6) after making the substitution $\gamma \to \gamma + \frac{1}{4}$)

$$V(x) = x^2 + \frac{\beta}{x} + \frac{m^2}{x^2} \tag{13}$$

has its minimum value at $x = x_0$, where $V(x_0) = 2x_0^2 + \beta/2x_0$, and increases when $x \to 0, \infty$. Above, x_0 is the positive root of the equation

$$x^4 - \tfrac{1}{2}\beta x - m^2 = 0.$$

We replace $V(x)$ by its harmonic approximation, allowing exact solution of the Schrödinger equation (6). Then, the expression (13) with its Taylor's expansion up to a quadratic term near the minimum value is replaced by

$$V(x) = V(x_0) + 4\left(1 - \frac{\beta}{8x_0^3}\right)x^2. \tag{14}$$

The result is the linear oscillator spectrum

$$E = E(n, m) = \left[x_0^2 + \frac{\beta}{4x_0} + (2n + 1)\left(1 - \frac{\beta}{8x_0^3}\right)^{1/2}\right]\Omega + \tfrac{1}{2}m\omega_c. \tag{15}$$

Note that the spectrum (15) for noninteracting electrons ($\beta = 0$) coincides with its exact value $E(n, m) = (2n + |m| + 1)\Omega + \frac{1}{2}m\omega_c$.

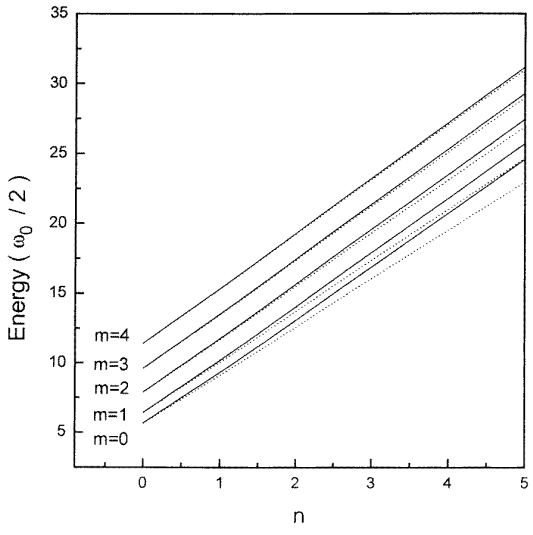

Figure 3. The linear oscillator approximation (15) for $\beta = 3$ and zero magnetic field, $\omega_c = 0$, and various quantum numbers n, m. The WKB solution is also shown (dotted curves) to allow an assessment to be made of the accuracy of the formula (15).

To compare the WKB solution with the interpolation formula (15), both spectra are shown in figure 3 for the absence of a magnetic field. Naturally enough, the approximation (15) is better for smaller n and larger m. Nonzero magnetic field, obviously, does not render this approximation less accurate, because it results only in a rescaling of the confinement frequency and the adding of a diamagnetic term into the Hamiltonian (3). Therefore, the most important effect of the magnetic field, i.e., the shift of the ground state to the higher angular moments in order to decrease the Coulomb electron–electron repulsion [3, 18], is also represented in terms of the approximate formula (15). The corresponding data mainly coincide with those presented in figure 2, and are not given here for brevity.

4. Summary

The electron–electron interaction of two electrons in a quantum dot can be taken into account using a simple approximation which allows exact solutions to be obtained. To allow us to estimate the accuracy of this approximation, the WKB solution is also derived. The error is not larger than a few per cent. In view of the initial approximations, such as that of assuming a parabolic confinement potential, such precision seems to be sufficient.

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