Energy spectra of two electrons in a circular quantum dot

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Abstract

The energy spectrum of two interacting electrons in a flat circular quantum dot is investigated. While the centre of motion can be treated exactly, the Wentzel-Kramers-Brillouin (WKB) approximation has been applied to study the relative motion. The energies are seen to agree well with the exact numerical results.
I. Introduction

Advances in submicron technology have made it possible to manufacture quantum dots containing only a few electrons [1]. Quantum dots have been extensively investigated both experimentally and theoretically [1-4]. Ever since the integral and fractional quantum Hall effects were discovered in two-dimensional electron systems under a high magnetic field, two-dimensional studies have been the subject of intense investigation in quantum solid state physics and quantum field theory. In two-dimensional quantum dots the electrons are confined in a circular region, such that the motion perpendicular to the plane of confinement is essentially frozen out.

Different theoretical methods have been used to study the problem of two electrons in a two-dimensional quantum dot, both with soft wall (parabolic confinement) as well as hard wall (rigid circular wall at a radius $r_0$) in-plane confinement. Physical examples of electrons being confined in such a thin layer can be found in the vicinity of junctions between insulators and semiconductors, between layers of semiconductors, and between a vacuum and liquid Helium.

Merkt, Huser and Wagner [5] have calculated the energy spectra of two electrons in a two-dimensional harmonic quantum dot, in the effective mass approximation, as a function of the dot size and the strength of a magnetic field directed perpendicularly to the dot plane. Matulis and Peeters [6] have proposed a convergent renormalized perturbation series in powers of the electron-electron interaction for calculating the energy of a quantum dot. They have used this method to calculate the ground and several excited states of a quantum dot consisting of two electrons. Matulis, Fjaerestad and Chao [7] have solved the Schrödinger equation for the ground state of two electrons in a two-dimensional circular quantum dot, with hard confinement potential, using a renormalized perturbation series approach, which interpolates between the perturbation solutions in the weak interaction regime and the asymptotic solutions in the strong interaction regime. They assumed that one electron was fixed at the origin. Zhu et al [8] have made use of the expansion in a power series to obtain the eigen solutions of two electrons in a parabolic quantum dot. McKinney and Watson [9] have applied the dimensional perturbation theory to the two-electron D-dimensional quantum dot, obtaining values for the ground- and excited-state energies. The charge- and spin-density excitation spectra for two electrons in a two-dimensional circular hard-wall confined quantum dot have been calculated by Brataas, Hanke and Chao [10]. Akman and Tomak [11] have performed the exact numerical diagonalization of the Hamiltonian of a 2D circular quantum dot for 2, 3, and 4 interacting electrons. Adamowski et al [12] have studied two electrons confined in quantum dots under an assumption of a Gaussian confining potential and its parabolic approximation. They have calculated the energy levels of singlet and triplet states as functions of the range and depth of the confining potential in the two-dimensional (circular) and three-dimensional (spherical) quantum dots. There have been several other investigations on the properties of circular quantum dots.

In the present work, we investigate the energy spectrum of 2 interacting electrons confined
in a rigid disc of radius $r_0$, within the effective mass approximation, using the WKB method. We consider the dots in the two-dimensional limit of thin discs. We take the simplest model of quantum confinement, viz., infinite square well of radius $r_0$.

First we formulate the WKB method for the case when the two particles are confined in a circular region. The Hamiltonian for 2 particles of masses $\mu_1$ and $\mu_2$, in a central force potential $V(r)$, is given by

$$\begin{align*}
-H &= -\frac{\hbar^2}{2\mu_1}\nabla^2_1 - \frac{\hbar^2}{2\mu_2}\nabla^2_2 + V(r_1 - r_2) 
\end{align*}$$

The Hamiltonian in (1) can be separated into the relative motion and the centre-of-mass motion as

$$
H = H_R + H_r
$$

with

$$
H_R = -\frac{\hbar^2}{2\mu_R}\nabla^2_R 
$$

$$
H_r = -\frac{\hbar^2}{2\mu_r}\nabla^2_r + V(r)
$$

where the centre-of-mass co-ordinate

$$R = \frac{\mu_1 r_1 + \mu_2 r_2}{\mu_1 + \mu_2}
$$

and the relative co-ordinate

$$r = |r_1 - r_2|
$$

$\mu_R$ and $\mu_r$ are the total mass and reduced mass respectively, given by

$$
\mu_R = \mu_1 + \mu_2
$$

$$
\mu_r = \frac{\mu_1 \mu_2}{\mu_1 + \mu_2}
$$

The spatial part of the wave function is symmetric (antisymmetric) with respect to particle permutation for even (odd) azimuthal quantum number $m$. Since Pauli exclusion principle requires the total wave function to be antisymmetric, therefore we must have spin singlet ($s = 0$) and spin triplet ($s = 1$) states for even and odd $m$ respectively. Thus the 2-particle wave function can be separated as

$$
\psi(r_1, r_2) = \Phi(R)\psi(r)
$$
Assuming the medium to be isotropic, the $\theta$ dependence can be approximated by a plane wave, viz., $\exp(\im \theta)$. So each state is denoted by four quantum numbers $|n_R, m_R, n_r, m_r\rangle$. The Schrödinger is now separable giving

$$-\frac{\hbar^2}{2\mu_R} \nabla_R^2 \Phi(R) = E_R \Phi(R) \tag{10}$$

and

$$-\frac{\hbar^2}{2\mu_r} \nabla_r^2 \psi(r) + V(r) \psi(r) = E_r \psi(r) \tag{11}$$

In the above equation $E_R$ denotes the centre-of-mass energy and $E_r$ represents the relative energy.

We assume the system consisting of 2 electrons to be confined in a disc of radius $r_0$, by a rigid wall. Because of the quantum confinement, the centre-of-mass and relative motions can no longer be separated. Since $\mu_1 = \mu_2$, hence

$$R = \frac{r_1 + r_2}{2} \tag{12}$$

Assuming an infinite deep well model, the confinement implies

$$V(\sigma_i) = \infty \quad \sigma_i > r_0$$

$$V(\sigma_i) = 0 \quad \sigma_i < r_0 \tag{13}$$

for $\sigma_i = R, r$.

Further substituting

$$\Phi(R) = \frac{u_R(R)}{\sqrt{R}} \tag{14}$$

$$\psi(r) = \frac{u_r(r)}{\sqrt{r}} \tag{15}$$

the radial Schrödinger equations reduce to the effective one-dimensional analogue

$$\frac{d^2u_R(R)}{dR^2} + \Gamma^2_{R}(R)u_R(R) = 0 \tag{16}$$

$$\frac{d^2u_r(r)}{dr^2} + \Gamma^2_{r}(r)u_r(r) = 0 \tag{17}$$

where

$$\Gamma^2_{R}(R) = \sqrt{\frac{2\mu_R}{\hbar^2} \left\{ E_R - \frac{m^2_R \hbar^2}{2\mu_R R^2} \right\}} \tag{18}$$

$$\Gamma^2_{r}(r) = \sqrt{\frac{2\mu_r}{\hbar^2} \left\{ E_r - \frac{1}{r} - \frac{m^2_r \hbar^2}{2\mu_r r^2} \right\}} \tag{19}$$
In the above expressions we have used $m_R$ and $m_r$ for the azimuthal quantum numbers for the centre-of-mass motion and relative motions respectively.

Thus the centre-of-mass Hamiltonian $H_R$ is a purely single electron Hamiltonian, which can be solved exactly. It is the part $H_r$, involving the important Coulomb repulsion, which is responsible for the rich structure of the energy spectrum. To study the energy spectrum of this part applying the semiclassical Wentzel-Kramers-Brillouin (WKB) approximation, we conformally map the $0 < r < \infty$ space to the $-\infty < x < \infty$ space, by substituting

$$r = e^x$$

In 2 dimensions, conformal mapping modifies the centrifugal barrier term $(m^2 - 1/4)\frac{\hbar^2}{2\mu r^2}$ to $m^2\frac{\hbar^2}{2\mu r^2}$, i.e. replaces $(m^2 - 1/4)$ by $m^2$. The situation might be compared with Langer modification in 3 dimension, where the centrifugal term $\frac{l(l+1)\hbar^2}{4\mu r^2}$ is replaced by $\frac{l(l+1/2)\hbar^2}{4\mu r^2}$.

Henceforth, for convenience of calculations, we shall work in units $\hbar = 1$.

The centre-of-mass motion is given by the Schrödinger equation (16), viz.,

$$\frac{\hbar^2}{2\mu_R} \frac{d^2 u_R}{dR^2} + \left[ E_R - (m_R^2 - 1/4)\frac{\hbar^2}{2\mu_R R^2} \right] u_R = 0 \quad (21)$$

If we substitute

$$u_R = R^{1/2} \chi(R) \quad (22)$$

$$\rho_R = \frac{\sqrt{2\mu_E R}}{\hbar} R \quad (23)$$

then it is easy to observe that $\chi(R)$ satisfies the Bessel differential equation. Hence the solution of (22) is given by

$$u_R = R^{1/2} j_{\pm m_R} \left( \sqrt{2\mu_E R} \right) \quad (24)$$

So the confined energies are obtained from the zeroes of the Bessel function. If $\xi_n$ is the $n$-th zero of the Bessel function, then the energies are given by

$$E_{nR} = \frac{\xi_n^2 \hbar^2}{2\mu_R E_R \rho_R^2} \quad (25)$$

To formulate the WKB quantization rules for the relative motion of a circular quantum dot consisting of two electrons in the $xy$ plane, we proceed as follows. The radial solution $u_r$ satisfies
the Schrödinger equation (17), viz.,

$$-\frac{1}{2\mu_r} \frac{d^2 u_r}{dr^2} + \left\{ \frac{1}{r} + \frac{m_r^2}{2\mu_r r^2} \right\} u_r = E_r u_r$$  \hspace{1cm} (26)

Substituting

$$\rho_r = \mu_r r$$  \hspace{1cm} (27)
$$e_r = \frac{E_r}{\mu_r}$$  \hspace{1cm} (28)

equation (26) reduces to

$$\frac{d^2 u_r}{d\rho_r^2} + \Gamma^2(\rho_r) u_r = 0$$  \hspace{1cm} (29)

where

$$\Gamma^2(\rho_r) = 2 \{ e_r - V \}$$  \hspace{1cm} (30)
$$V = \frac{2}{\rho_r} + \frac{m_r^2}{\rho_r^2}$$  \hspace{1cm} (31)

The impenetrable circular wall imposes the additional boundary condition

$$u(r_0) = 0$$  \hspace{1cm} (32)

It may be mentioned here that the region of space $0 \leq \rho_r \leq r_0$ may be divided into 2 sections

i) Region I : $0 \leq \rho_r \leq \rho_t$ where $V > e_r$

ii) Region II : $\rho_t \leq \rho_r \leq r_0$ where $e_r > V$

where $\rho_t$ is the classical turning point, obtained by putting $\Gamma^2(\rho_r) = 0$.

We assume a WKB ansatz for the solution of the Schrödinger equation in region I, and obtain the solution in region II with the help of the WKB connection formulae [15] on either side of the turning point as,

$$u_{rI}(\rho_r) = \frac{A}{\sqrt{\kappa(\rho_r)}} \exp \left\{ - \int_{\rho_t}^{\rho_r} \kappa d\rho_r \right\}$$  \hspace{1cm} (33)

$$u_{rII}(\rho_r) = \frac{2A}{\sqrt{\Gamma(\rho_r)}} \sin \left\{ \int_{\rho_t}^{\rho_r} \Gamma(\rho_r) d\rho_r + \frac{\pi}{4} \right\}$$  \hspace{1cm} (34)

where

$$\kappa^2(\rho_r) = -\Gamma^2(\rho_r)$$  \hspace{1cm} (35)

Imposition of the condition $u_{rII}(r_0) = 0$ gives the WKB quantization rules as

$$\alpha_r = n_r + \frac{3}{4} \pi \quad n_r = 0, 1, 2, \cdots$$  \hspace{1cm} (36)
where
\[
\alpha_r = \int_{\rho_t}^{r_0} \left[ 2 \left\{ \frac{e_r - \frac{1}{\rho_r} - \frac{m_r^2}{\rho_r^2}}{\rho_r^2} \right\} \right]^{1/2} d\rho_r
\] (37)
\[
= \sqrt{2e_r r_0^2 - 2r_0 - m_r^2} + |m_r| \sin^{-1} \frac{r_0 + m_r^2}{r_0 \sqrt{1 + 2e_r m_r^2}} - \frac{|m_r| \pi}{2}
- \frac{1}{\sqrt{2e_r}} \ln \left| \frac{\sqrt{2e_r r_{00} + 2e_r r_0} - 1}{2e_r \rho_t - 1} \right|
\] (38)
with
\[
\rho_t = \frac{1 + \sqrt{1 + 2e_r m_r^2}}{2e_r}
\] (39)
\[
r_{00} = 2e_r r_0^3 - 2r_0 - m_r^2
\] (40)

We calculate the exact analytical energies of the system for the centre-of-mass motion from the zeroes of the Bessel function [16]. The results are explicitly given in Table 1.

For the relative motion we calculate the WKB energies \( E_r(WKB) \) with the help of the formalism given above. For simplicity of calculations we take \( \mu_1 = \mu_2 = 1/2 \). Hence \( \mu_R = 1, \mu_r = 1/4 \). To test the validity of our approach, we compare our results with the exact numerical energies \( E_r(exact) \) for different values of the confining radius, in Table 2 \((n_r = 0, m_r = 0)\), Table 3 \((n_r = 0, m_r = 1)\), and Table 4 \((n_r = 1, m_r = 1)\). The exact energies are obtained by numerical integration of the Schrödinger equation using Numerov’s method and the logarithmic mesh. Considering the semiclassical nature of the WKB approximation, the agreement between the two values is found to be excellent, improving further as the region of confinement increases.

To conclude we have found the confined energies of two interacting electrons in a circular quantum dot of radius \( r_0 \). Our semiclassical WKB approach gives excellent results when compared with exact numerical values. In this work we have considered the simplest model of the confined two-electron system, by assuming an infinite confining potential. We shall deal with more complicated potentials in our future work.

Table 1. Exact energies of the system for the centre-of-mass motion \( (E_R(n_R, m_R)) \)
<table>
<thead>
<tr>
<th>$r_0$</th>
<th>$E_R(0,0)$</th>
<th>$E_R(0,1)$</th>
<th>$E_R(1,0)$</th>
<th>$E_R(1,1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>72.2901</td>
<td>183.525</td>
<td>380.891</td>
<td>615.231</td>
</tr>
<tr>
<td>0.5</td>
<td>11.5664</td>
<td>29.3640</td>
<td>60.9426</td>
<td>98.4370</td>
</tr>
<tr>
<td>1.0</td>
<td>2.89160</td>
<td>7.34100</td>
<td>15.2356</td>
<td>24.6092</td>
</tr>
<tr>
<td>1.5</td>
<td>1.28516</td>
<td>3.26267</td>
<td>6.77139</td>
<td>10.9374</td>
</tr>
<tr>
<td>2.0</td>
<td>0.72290</td>
<td>1.83525</td>
<td>3.80891</td>
<td>6.15231</td>
</tr>
<tr>
<td>3.0</td>
<td>0.32129</td>
<td>0.81567</td>
<td>1.69285</td>
<td>2.73436</td>
</tr>
<tr>
<td>4.0</td>
<td>0.18072</td>
<td>0.45881</td>
<td>0.95223</td>
<td>1.53808</td>
</tr>
<tr>
<td>5.0</td>
<td>0.11566</td>
<td>0.29364</td>
<td>0.60942</td>
<td>0.98437</td>
</tr>
<tr>
<td>6.0</td>
<td>0.08073</td>
<td>0.20392</td>
<td>0.42321</td>
<td>0.68359</td>
</tr>
<tr>
<td>8.0</td>
<td>0.04518</td>
<td>0.11470</td>
<td>0.23805</td>
<td>0.38452</td>
</tr>
<tr>
<td>10.0</td>
<td>0.02892</td>
<td>0.07341</td>
<td>0.15263</td>
<td>0.24609</td>
</tr>
<tr>
<td>15.0</td>
<td>0.01285</td>
<td>0.03263</td>
<td>0.06771</td>
<td>0.10937</td>
</tr>
</tbody>
</table>

Table 2. Energy of the ground state ($n_r = 0$, $m_r = 0$)

<table>
<thead>
<tr>
<th>$r_0$</th>
<th>$E_r(WKB)$</th>
<th>$E_r(exact)$</th>
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</thead>
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<tr>
<td>0.4</td>
<td>47.031</td>
<td>44.505</td>
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<tr>
<td>0.6</td>
<td>22.989</td>
<td>21.589</td>
</tr>
<tr>
<td>0.7</td>
<td>17.608</td>
<td>16.513</td>
</tr>
<tr>
<td>0.8</td>
<td>14.013</td>
<td>13.135</td>
</tr>
<tr>
<td>0.9</td>
<td>11.479</td>
<td>10.762</td>
</tr>
<tr>
<td>1.0</td>
<td>9.6186</td>
<td>9.0240</td>
</tr>
<tr>
<td>1.5</td>
<td>4.9446</td>
<td>4.6693</td>
</tr>
<tr>
<td>2.0</td>
<td>3.1283</td>
<td>2.9776</td>
</tr>
<tr>
<td>3.0</td>
<td>1.6742</td>
<td>1.6152</td>
</tr>
<tr>
<td>4.0</td>
<td>1.0895</td>
<td>1.0610</td>
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<tr>
<td>5.0</td>
<td>0.78678</td>
<td>0.7712</td>
</tr>
<tr>
<td>6.0</td>
<td>0.60592</td>
<td>0.59663</td>
</tr>
<tr>
<td>9.0</td>
<td>0.34399</td>
<td>0.34126</td>
</tr>
<tr>
<td>10.0</td>
<td>0.29788</td>
<td>0.29592</td>
</tr>
<tr>
<td>12.0</td>
<td>0.23288</td>
<td>0.23180</td>
</tr>
</tbody>
</table>
### Table 3. Energy of the excited state having $n_r = 0, m_r = 1$

<table>
<thead>
<tr>
<th>$r_0$</th>
<th>$E_r$ (WKB)</th>
<th>$E_r$ (exact)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>65.835</td>
<td>66.613</td>
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<tr>
<td>1.0</td>
<td>18.479</td>
<td>18.646</td>
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<tr>
<td>1.5</td>
<td>9.0618</td>
<td>9.1573</td>
</tr>
<tr>
<td>2.0</td>
<td>5.6020</td>
<td>5.6328</td>
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<tr>
<td>3.0</td>
<td>2.9121</td>
<td>2.9225</td>
</tr>
<tr>
<td>5.0</td>
<td>1.3404</td>
<td>1.3428</td>
</tr>
<tr>
<td>6.0</td>
<td>1.0288</td>
<td>1.0303</td>
</tr>
<tr>
<td>8.0</td>
<td>0.68606</td>
<td>0.68676</td>
</tr>
<tr>
<td>10</td>
<td>0.50576</td>
<td>0.50621</td>
</tr>
<tr>
<td>15</td>
<td>0.29604</td>
<td>0.29629</td>
</tr>
<tr>
<td>20</td>
<td>0.20500</td>
<td>0.20518</td>
</tr>
</tbody>
</table>

### Table 4. Energy of the excited state having $n_r = 1, m_r = 1$

<table>
<thead>
<tr>
<th>$r_0$</th>
<th>$E_r$ (WKB)</th>
<th>$E_r$ (exact)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>206.42</td>
<td>206.51</td>
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<tr>
<td>1.0</td>
<td>54.222</td>
<td>54.208</td>
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<td>1.2</td>
<td>38.375</td>
<td>38.356</td>
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<td>25.249</td>
<td>25.227</td>
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<td>14.842</td>
<td>14.821</td>
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<td>3.0</td>
<td>7.1557</td>
<td>7.1399</td>
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<tr>
<td>4.0</td>
<td>4.3329</td>
<td>4.3209</td>
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<tr>
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<td>2.9659</td>
<td>2.9567</td>
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<tr>
<td>6.0</td>
<td>2.1910</td>
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<td>8.0</td>
<td>1.3763</td>
<td>1.3714</td>
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<tr>
<td>10</td>
<td>0.96993</td>
<td>0.96643</td>
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<td>15</td>
<td>0.52556</td>
<td>0.52379</td>
</tr>
<tr>
<td>20</td>
<td>0.34602</td>
<td>0.34496</td>
</tr>
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References


