ENERGY SPECTRA OF TWO ELECTRONS
IN A CIRCULAR QUANTUM DOT

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ABSTRACT:

The electron interaction energy of two interacting electrons in a circular quantum dot (with hard wall confinement) is investigated in the framework of the semi-classical Wentzel-Kramers-Brillouin (WKB) approximation. The two electrons are assumed to be in an infinitely deep well of radius $r_0$, in a simple configuration with one electron fixed at the origin. The corresponding Schrödinger equation, with hard wall boundary conditions, is also solved exactly by numerical integration. It is observed that the agreement between the two energy values is quite good, suggesting that the WKB approximation works well for such a confined quantum system as well. This may provide motivation to extend this to more realistic confined potentials.
1. Introduction

Advances in submicron technology have made it possible to realize artificial nanostructures, where electrons can be confined on a scale comparable to their de Broglie wavelengths. These quantum dots, or artificial atoms as they are called, containing only a few electrons, exhibit unusual optical and transport properties, because of the discrete energy levels of the confined electrons. Quantum dots have been extensively investigated both experimentally and theoretically. 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. Such quantum dots can be fabricated with two types of confinement potential — the ‘soft’ confinement potential, accomplished by electric and / or magnetic fields, or a ‘hard’ confinement in pillar-shaped quantum dots.

To study the behaviour of single electron tunneling, it is essential to derive the eigen-solutions of the system of interacting electrons confined in an ultrasmall quantum dot. Different theoretical methods have been used to study the problem of two electrons in a two-dimensional quantum dot, both with a soft wall (parabolic confinement) as well as a 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. Consequently, this field of research is of vital importance to modern electronic devices.

Merkt, Huser and Wagner 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 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 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 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 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\textsuperscript{10}. Akman and Tomak\textsuperscript{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\textsuperscript{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, the energy spectrum of two interacting electrons confined in a rigid disc of radius $r_0$, is investigated within the effective mass approximation, using the WKB method. The dot is considered in the two-dimensional limit of thin discs. The simplest model of quantum confinement is assumed, viz., infinitely deep well of radius $r_0$.

2. Theory

We apply the WKB method to the case of two particles, confined in a thin, circular, two-dimensional disc of radius $r_0$, lying in the $xy$ plane. The Hamiltonian for such a system is then given by

$$H = -\frac{\hbar^2}{2\mu^*} \nabla_1^2 - \frac{\hbar^2}{2\mu^*} \nabla_2^2 + V(r_1) + V(r_2) + V(|r_1 - r_2|)$$  \hspace{1cm} (1)

where $\mu^*$ is the effective mass. In two dimensions, the radial distance $r$ and the angle $\theta$ are given by

$$r = \sqrt{x^2 + y^2}, \quad \theta = \tan^{-1}\left(\frac{y}{x}\right)$$  \hspace{1cm} (2)

We shall consider here the same configuration as that considered by Matulis, Fjaerestad and Chao\textsuperscript{7}, that is one electron is fixed at the centre of the disc-like quantum dot. Substituting the radial wavefunction $\psi(r)$ by

$$\psi(r) = \frac{u(r)}{\sqrt{r}}$$  \hspace{1cm} (3)

the radial Schrödinger equation can be written as an effective one-dimensional equation

$$\frac{d^2u(r)}{dr^2} + \Gamma^2(r)u(r) = 0$$  \hspace{1cm} (4)

where

$$\Gamma^2(r) = \frac{2\mu^*}{\hbar^2} \left\{ E - \frac{1}{r} - \frac{(m^2 - 1/4)\hbar^2}{2\mu^* r^2} \right\}$$  \hspace{1cm} (5)
and $m$ stands for the azimuthal quantum number. The Coulomb repulsion term $\frac{1}{r}$ is responsible for the rich structure of the energy spectrum of the quantum dot. To apply the semiclassical Wentzel-Kramers-Brillouin (WKB) approximation, the $0 < r < \infty$ space is conformally mapped to the $-\infty < w < \infty$ space, by substituting

$$r = e^w$$

This mapping prevents the left turning point to be negative for attractive potentials (for the case $m = 0$).

Thus the Schrödinger eqn. (4) gets transformed to

$$\frac{d^2\chi(w)}{dw^2} + \Gamma^2(w)\chi(w) = 0$$

where

$$\Gamma^2(w) = \left\{ \frac{2\mu r^2}{\hbar^2}e^{2w}[E - V(w)] - m^2 \right\}$$

with

$$\chi(w) = \psi(r) = e^{-w/2}u(w)$$

In terms of the original variable $r$,

$$\int^w \Gamma(w)dw = \int^r \Gamma(r)dr$$

where

$$\Gamma^2(r) = \frac{2\mu^*}{\hbar^2}[E - V_1(r)]$$

and

$$V_1(r) = V(r) + \frac{m^2\hbar^2}{2\mu^*r^2} \quad m = 0, \pm1, \pm2, \ldots$$

Thus in two dimensions, conformal mapping replaces $(m^2 - 1/4)$ by $m^2$ (Yi et al\textsuperscript{13}). In other words, the centrifugal barrier term $\frac{(m^2 - 1/4)\hbar^2}{2\mu^*r^2}$ is modified to $\frac{m^2\hbar^2}{2\mu^*r^2}$. The situation might be compared with Langer modification in three dimensions, where the centrifugal term $\frac{l(l+1)\hbar^2}{2\mu^*r^2}$ is replaced by $\frac{l(l+1/2)\hbar^2}{2\mu^*r^2}$. Henceforth, for convenience of calculations, the units used are $\hbar = 1$.

Assuming an infinite deep well model, the hard wall confinement condition implies

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

$$V(r) = 0 \quad r < r_0$$

The radial solution $u(r)$ satisfies the Schrödinger equation,

$$-\frac{1}{2\mu^*} \frac{d^2u}{dr^2} + \left\{ \frac{1}{r} + \frac{m^2}{2\mu^*r^2} \right\}u = Eu$$

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Substituting
\[ \rho = \mu^* r \tag{15} \]
\[ e = \frac{E}{\mu^*} \tag{16} \]
equation (14) reduces to
\[ \frac{d^2 u}{d\rho^2} + \Gamma^2(\rho) u = 0 \tag{17} \]
where
\[ \Gamma^2(\rho) = 2 \{ e - V \} \tag{18} \]
\[ V = \frac{1}{\rho} + \frac{m^2}{2\rho^2} \tag{19} \]
The impenetrable circular wall imposes the additional boundary condition
\[ u(r_0) = 0 \tag{20} \]
It may be mentioned here that the region of space \( 0 \leq \rho \leq r_0 \) may be divided into 2 sections
i) Region I : \( 0 \leq \rho \leq \rho_t \) where \( V > e \)
ii) Region II : \( \rho_t \leq \rho < r_0 \) where \( e > V \)
where \( \rho_t \) is the classical turning point, obtained by putting \( \Gamma^2(\rho) = 0 \).

A WKB ansatz is assumed for the solution of the Schrödinger equation in region I, and the solution in region II is obtained with the help of the WKB connection formulae on either side of the turning point as,
\[ u_I(\rho) = \frac{A}{\sqrt{\kappa(\rho)}} \exp \left\{ - \int_{\rho}^{\rho_t} \kappa d\rho \right\} \tag{21} \]
\[ u_{II}(\rho) = \frac{2A}{\sqrt{\Gamma(\rho)}} \sin \left\{ \int_{\rho_t}^{\rho} \Gamma(\rho) d\rho + \frac{\pi}{4} \right\} \tag{22} \]
where
\[ \kappa^2(\rho) = -\Gamma^2(\rho) \tag{23} \]
Imposition of the condition \( u_{II}(r_0) = 0 \) gives the WKB quantization rules as
\[ \alpha = \left( n_r + \frac{3}{4} \right) \pi \quad n_r = 0, 1, 2, \ldots \tag{24} \]
where \( \alpha \) is calculated to be\(^{15} \)
\[ \alpha = \int_{\rho_t}^{r_0} \left[ 2 \left\{ e - \frac{1}{\rho} - \frac{m^2}{2\rho^2} \right\} \right]^{1/2} d\rho \]
\[
E \left( WKB \right) = \sqrt{2er_0^2 - 2r_0 - m^2 + |m| \sin^{-1} \frac{r_0 + m^2}{r_0 \sqrt{1 + 2em^2}} - |m| \frac{\pi}{2}} - \frac{1}{\sqrt{2e}} \ln \left| \sqrt{2er_{00}^2 + 2er_0 - 12e\rho_t} - 1 \right|
\]

with

\[
\rho_t = \frac{1 + \sqrt{1 + 2em^2}}{2e}
\]

\[
r_{00} = 2er_0^2 - 2r_0 - m^2
\]

3. Results and Discussion

The WKB energies \( E(WKB) \) for the system were calculated for various values of the confining radius, with the help of the equations given above. The exact energies \( E(exact) \) are obtained by numerical integration of the Schrödinger equation using Numerov’s method and the logarithmic mesh. The effective mass has been taken as \( \mu^* = \frac{1}{4} \).

To test the validity of our approach, our WKB results are compared with the exact numerical energies for different values of the confining radius \( r_0 \), in Table 1 \((n_r = 0, m = 0)\), Table 2 \((n_r = 0, m = 1)\), and Table 3 \((n_r = 1, m = 1)\). 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. It may be mentioned here that though the infinitely deep well circular quantum dot with two electrons was investigated by Goff and Stébé\(^{16}\) and Matulis, Fjaerestad and Chao\(^7\), their discussions were restricted to the ground state only, whereas the analysis presented in this paper is valid for excited states as well. Moreover, the approach used here is totally different from either of these cases.

To conclude the confined energies are obtained for two interacting electrons in a circular quantum dot of radius \( r_0 \), with one electron fixed at the origin. The semiclassical WKB approach adopted here gives excellent results when compared with exact numerical values. In this work the simplest model of the confined two-electron system is considered, by assuming an infinitely deep well for the confining potential. The authors hope to deal with more complicated potentials in future.
Table 1. Energy of the ground state ($n_r = 0, m = 0$)

| $r_0$ | $E_{WKB}$ | $E_{exact}$ |
|-------|-----------|------------|
| 0.4   | 47.031    | 44.505     |
| 0.6   | 22.989    | 21.589     |
| 0.7   | 17.608    | 16.513     |
| 0.8   | 14.013    | 13.135     |
| 0.9   | 11.479    | 10.762     |
| 1.0   | 9.6186    | 9.0240     |
| 1.5   | 4.9446    | 4.6693     |
| 2.0   | 3.1283    | 2.9776     |
| 3.0   | 1.6742    | 1.6152     |
| 4.0   | 1.0895    | 1.0610     |
| 5.0   | 0.78678   | 0.7712     |
| 6.0   | 0.60592   | 0.59663    |
| 9.0   | 0.34399   | 0.34126    |
| 10    | 0.29788   | 0.29592    |
| 12    | 0.23288   | 0.23180    |

Table 2. Energy of the excited state having $n_r = 0, m = 1$.

| $r_0$ | $E_{WKB}$ | $E_{exact}$ |
|-------|-----------|------------|
| 0.5   | 65.835    | 66.613     |
| 1.0   | 18.479    | 18.646     |
| 1.5   | 9.0618    | 9.1573     |
| 2.0   | 5.6020    | 5.6328     |
| 3.0   | 2.9121    | 2.9225     |
| 5.0   | 1.3404    | 1.3428     |
| 6.0   | 1.0288    | 1.0303     |
| 8.0   | 0.68606   | 0.68676    |
| 10    | 0.50576   | 0.50621    |
| 15    | 0.29604   | 0.29629    |
| 20    | 0.20500   | 0.20518    |
Table 3. Energy of the excited state having \((n_r = 1, m = 1)\).

| \(r_0\) | \(E(WKB)\) | \(E(exact)\) |
|--------|-------------|---------------|
| 0.5    | 206.42      | 206.51        |
| 1.0    | 54.222      | 54.208        |
| 1.2    | 38.375      | 38.356        |
| 1.5    | 25.249      | 25.227        |
| 2.0    | 14.842      | 14.821        |
| 3.0    | 7.1557      | 7.1399        |
| 4.0    | 4.3329      | 4.3209        |
| 5.0    | 2.9659      | 2.9567        |
| 6.0    | 2.1910      | 2.1837        |
| 8.0    | 1.3763      | 1.3714        |
| 10     | 0.96993     | 0.96643       |
| 15     | 0.52556     | 0.52379       |
| 20     | 0.34602     | 0.34496       |

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