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Effective mass theory of a two-dimensional quantum dot in the presence of magnetic field

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Abstract. The effective mass of electrons in low-dimensional semiconductors is position-dependent. The standard kinetic energy operator of quantum mechanics for this position-dependent mass is non-Hermitian and needs to be modified. This is achieved by imposing the BenDaniel–Duke (BDD) boundary condition. We have investigated the role of this boundary condition for semiconductor quantum dots (QDs) in one, two and three dimensions. In these systems the effective mass m_{i} inside the dot of size R is different from the mass m_{o} outside. Hence a crucial factor in determining the electronic spectrum is the mass discontinuity factor $\beta = m_{\mathrm{i}}/m_{\mathrm{o}}$. We have proposed a novel quantum scale, σ, which is a dimensionless parameter proportional to $\beta^2 R^2 V_0$, where V_0 represents the barrier height. We show both by numerical calculations and asymptotic analysis that the ground state energy and the surface charge density, $(\rho(R))$, can be large and dependent on σ. We also show that the dependence of the ground state energy on the size of the dot is infraquadratic. We also study the system in the presence of magnetic field B. The BDD condition introduces a magnetic length-dependent term $(\sqrt{\hbar/eB})$ into σ and hence the ground state energy. We demonstrate that the significance of BDD condition is pronounced at large R and large magnetic fields. In many cases the results using the BDD condition is significantly different from the non-Hermitian treatment of the problem.

Keywords. Effective mass theory; BenDaniel–Duke; quantum dot; electron; magnetic field.

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1. Introduction

Low-dimensional systems have become technologically significant and their electronic structure is often understood on the basis of effective mass theory (EMT). In this paper, we use EMT to study the ground state energy and carrier charge density for semiconductor quantum dot (QD). We discuss our approach with the two-dimensional (2D) case as an illustration. The one- and three-dimensional cases can be treated similarly and only the results are discussed. The 2D case is a matter of interest in studies on quantum Hall effect, shell filling and capacitance.

Our goal in this paper is modest and does not involve many electron effects. It is to unravel the effect of the BenDaniel–Duke (BDD) boundary condition [1] on this system both in the absence and presence of a magnetic field. The BDD condition is invoked when the effective mass inside the QD is different from the mass outside. Rather surprisingly, the BDD condition has not been probed inspite of a very large number of studies on the 2D system.

The vertically stacked $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ or $Al_xGa_{1-x}As/In_xGa_{1-x}As/Al_xGa_{1-x}As$ is a reasonable experimental realization of the 2D QD. The central layer, namely GaAs or $In_xGa_{1-x}As$ is the 2D well with electron effective masses as low as $0.06m_{\rm o}$, $m_{\rm o}$ being the bare electron mass. 2D QD is also formed in experiments on single electron capacitance spectroscopy (SECS) and gated transport spectroscopy (GTS) and has been studied extensively [2].

In §2 we introduce the EMT Hamiltonian for an electron in two-dimensional potential and discuss the BenDaniel–Duke boundary condition [1].

In §3 we carry out the asymptotic analysis that brings out the essential features of the variation of ground state energy E. In this context we introduce a novel dimensionless parameter σ which is proportional to $\beta^2 R^2 V_0$. We call it the mass modified strength of the potential. We also define a penetration depth δ demonstrating that the finite barrier of size R is equivalent to an infinite barrier of size $R + \delta$. We also chart the dependence of surface charge density with β.

In §4 we study the effects of a uniform magnetic field on the QD. We redefine $\sigma_{\rm m}$, the strength of the potential, in the presence of the magnetic field.

In §5 we carry out a comparison of results obtained for one-dimensional [3] and three-dimensional quantum dots [4] with results obtained in this work. We conclude that the non-imposition of the BenDaniel–Duke boundary condition leads to erroneous results. We summarize our work and suggest directions for future work.

2. Basic formalism

We consider a two-dimensional quantum well of radius R [1]. An electron in this well is described using effective mass theory by the Hamiltonian

$$\widehat{H} = -\frac{\hbar^2}{2}\nabla \cdot \left(\frac{1}{m^*(r)}\nabla\right) + V(r). \tag{1}$$

For a position-dependent mass the appropriate Hermitian kinetic energy operator is given by the first term on the right-hand side of eq. (1). The electron effective mass inside the well, $m_{\rm i}$, is constant but differs from the mass outside the well, $m_{\rm o}$. A useful parameter is the ratio $\beta = m_{\rm i}/m_{\rm o}$ of the effective masses. The potential $V(r)$ for our problem is given by

$$V(r) = \begin{cases} 0 & \text{if } r \le R \\ V_0 & \text{if } r > R \end{cases}, \tag{2}$$

where the barrier height V_0 is typically between 1 eV and 10 eV. Using separation of variables the wave function for an electron in this quantum well can be written in the form:

$$\Psi(r,\phi) = g(r)\Phi(\phi), \tag{3}$$

where the symbols have their usual meaning. The ground state wave function will be independent of ϕ and angular moment index l. Hence the equation for partial wave functions $g(r)$ inside the well is

$$\frac{1}{g}\left(\frac{\mathrm{d}^2 g}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}g}{\mathrm{d}r}\right) = -k_{\mathrm{i}}^2, \quad k_{\mathrm{i}} = \sqrt{\frac{2m_{\mathrm{i}}E}{\hbar^2}}. \tag{4}$$

Equation (4) is the Bessel equation of integer of order l [5]. The solution is

$$g(r) = A_{\mathrm{i}} J_0(k_{\mathrm{i}} r) + B_{\mathrm{i}} Y_0(k_{\mathrm{i}} r). \tag{5}$$

However, Y_0 blows up as r approaches zero. Hence we choose $B_{\mathrm{i}} = 0$. The wave function inside the well therefore is

$$\Psi_{\mathrm{i}} = A_{\mathrm{i}} J_0(k_{\mathrm{i}} r). \tag{6}$$

One can similarly argue that the wave function outside is

$$\Psi_{\mathrm{o}} = A_{\mathrm{o}} \frac{\mathrm{e}^{-k_{\mathrm{o}} r}}{\sqrt{r}}, \quad k_{\mathrm{o}} = \sqrt{\frac{2m_{\mathrm{o}}(V_0 - E)}{\hbar^2}}. \tag{7}$$

We use BenDaniel–Duke boundary conditions to account for different effective electron mass inside and outside the well, namely

$$\Psi_{\mathrm{i}}(R) = \Psi_{\mathrm{o}}(R) \tag{8}$$

$$\frac{1}{m_{\mathrm{i}}}\frac{\partial \Psi_{\mathrm{i}}(R)}{\partial r} = \frac{1}{m_{\mathrm{o}}}\frac{\partial \Psi_{\mathrm{o}}(R)}{\partial r}. \tag{9}$$

Using eqs (6) and (7) and noting that $J_0'(x) = -J_1(x)$ we obtain [6]

$$\frac{J_1(k_{\mathrm{i}}R)}{J_0(k_{\mathrm{i}}R)} = \beta \frac{2k_{\mathrm{o}}R + 1}{2k_{\mathrm{i}}R}. \tag{10}$$

3. Asymptotic analysis

For very large V_0, the solution of eq. (10) for the ground state will be close to the solution for the case when V_0 is infinite and thus may be approximated as

$$k_{\mathrm{i}}R = \alpha_0 - \epsilon, \tag{11}$$

where α_0 (=2.40483) is the smallest positive zero of $J_0(x)$ and ϵ is a small positive quantity. If we substitute eq. (11) in eq. (10) and linearize the resulting equation, we get

$$\epsilon \backsimeq \frac{\alpha_0}{\sqrt{\sigma}}, \tag{12}$$

where we have introduced a parameter σ given by

$$\sqrt{\sigma} = \beta R \sqrt{\frac{2m_{\mathrm{o}}}{\hbar^2}\left(V_0 - \frac{\hbar^2\alpha_0^2}{2m_{\mathrm{i}}R^2}\right)} + \frac{\beta}{2}. \tag{13}$$

We now find the energy of the ground state. Using eq. (4)

$$E = \frac{\alpha_0^2\hbar^2}{2\beta m_{\mathrm{o}}R^2}\left(1 - \frac{1}{\sqrt{\sigma}}\right)^2. \tag{14}$$

We confirm that $\sqrt{\sigma}$ increases almost linearly with R and β and the asymptotic analysis holds for $R > 5$ nm (see eq. (11)). From eq. (14) it follows that the energy is large for small R and small β. The former is the standard quantum confinement argument. The latter is the effect of BDD. Note that for $V_0 \to \infty$, and $\beta \to 1$, we obtain the infinite well result. The behaviour of ground state energy is depicted in figure 1. We also observe that this dependence is infraquadratic and is similar to the relation obtained in one-dimensional [3] and three-dimensional [4] quantum dots. Note that $\beta = 1$ corresponds to the absence of BDD condition. The BDD for $\beta = 0.1$ makes a substantial difference to the results. Further, inspection of figure 1 reveals that with decreasing value of β, the behaviour increasingly departs from the quadratic behaviour. We have

$$E \propto \frac{1}{R^\gamma}, \tag{15}$$

where γ takes values $1.98, 1.90, 1.81$ and 1.42 for $\beta = 5.0, 1.0, 0.5$ and 0.1 respectively, by the Levenberg–Marquardt fit. We may rewrite E approximately as

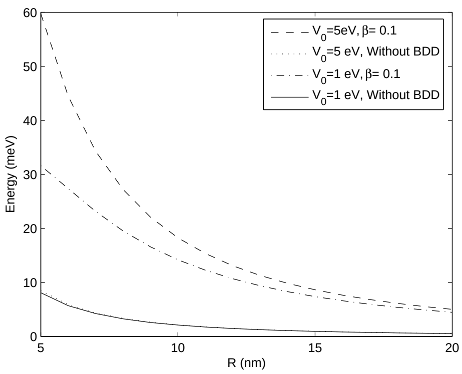

Figure 1. The dependence of ground state energy on the radius of the well in the absence of the magnetic field for two barrier heights, namely $V = 1$ eV and 5 eV. The energy values increase with lower values of β. The non-BDD results for $V = 5$ eV are indistinguishable from $V = 1$ eV.

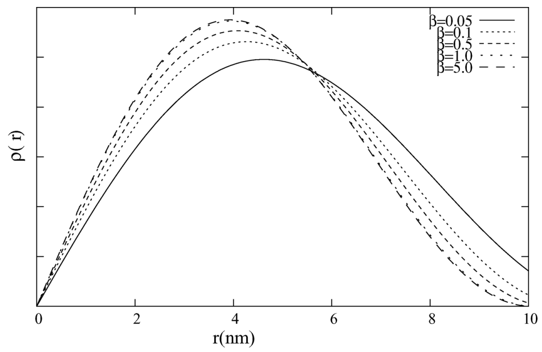

Figure 2. A typical charge density $\rho(r)$ inside a nanostructure of size $R =$ 10 nm and barrier height $V_0 = 5$ eV. Note that for small β, $\rho(r)$ is large at the surface ($r = R$). Note that $B = 0$.

$$E \backsimeq \frac{\alpha_0^2 \hbar^2}{2m_{\mathrm{i}}(R+\delta)^2}, \tag{16}$$

where $\delta = R/\sqrt{\sigma}$ is the penetration depth. A quantity of interest is the radial charge density $\rho(r)$.

$$\rho(r) = r g^2(r), \tag{17}$$

where the carrier charge e has been ignored. Figure 2 depicts the variation of $\rho(r)$ with r for different β. The barrier potential is chosen to be $V_0 = 5$ eV and radius of well $R = 10$ nm. As easily seen in figure 2 the value of equilibrium charge density at the surface $r = R$ falls rapidly with increasing β. For increasingly small values of β the peak in charge density moves towards the edge of the well. Physically, we can also see that for small β, that is small effective mass inside the well, the particle is 'spread out'. Also for higher β, $\rho(R) \to 0$, while $\rho(r)$ attains its maximum value approximately near $r = R/2$.

4. Magnetic field

A large number of experiments focus their attention on various properties of quantum dots in a magnetic field [2]. However, their theoretical understanding is still in its infancy. We assume the same model as in the preceding sections.

The Schrödinger equation inside the dot is

$$-\frac{\hbar^2}{2m_{\mathrm{i}}}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \Psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 \Psi}{\partial \phi^2}\right) + \frac{1}{2} i\hbar\omega_{\mathrm{ci}}\frac{\partial \Psi}{\partial \phi} + \frac{1}{8} m_{\mathrm{i}}\omega_{\mathrm{ci}}^2 r^2 \Psi = E\Psi, \tag{18}$$

where $\omega_{\mathrm{ci}} = eB/m_{\mathrm{i}}$ is the cyclotron frequency of the carrier inside the well. We ignore the spin term as its effect would be to simply shift the energy eigenvalues by a constant amount.

The equation for radial wave function is

$$\frac{\hbar^2}{2m_\mathrm{i}}\left(\frac{\mathrm{d}^2g}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}g}{\mathrm{d}r}\right)+\left(E-\frac{1}{8}m_\mathrm{i}\omega_\mathrm{ci}^2r^2\right)g=0. \tag{19}$$

The wave function for the ground state inside the well is

$$\Psi_\mathrm{i}=A_\mathrm{i}\,\exp\left(-\frac{eBr^2}{4\hbar}\right)J_0(k_\mathrm{i}'r),\quad k_\mathrm{i}'=\sqrt{\frac{2m_\mathrm{i}}{\hbar^2}\left(E-\frac{\hbar\omega_\mathrm{ci}}{2}\right)}. \tag{20}$$

Following the same analysis, the wave function for the ground state outside the well is

$$\Psi_\mathrm{o}=A_\mathrm{o}\exp\left(-\frac{eBr^2}{4\hbar}\right)\frac{\exp(-k_\mathrm{o}'r)}{\sqrt{r}},\quad k_\mathrm{o}'=\sqrt{\frac{2m_\mathrm{o}}{\hbar^2}\left(V_0-E+\frac{\hbar\omega_\mathrm{co}}{2}\right)}. \tag{21}$$

Using the BenDaniel–Duke boundary conditions, eqs (8) and (9), we obtain

$$k_\mathrm{i}'R\frac{J_1(k_\mathrm{i}'R)}{J_0(k_\mathrm{i}'R)}=\frac{\beta}{2}+\beta k_\mathrm{o}'R+\frac{eBR^2}{2\hbar}(\beta-1)\,. \tag{22}$$

The above expression reduces to eq. (10) when $B=0$. We follow the asymptotic analysis as done in §3 to arrive at the expression for ground state energy in the presence of magnetic field

$$E=\frac{\alpha_0^2\hbar^2}{2m_\mathrm{i}R^2}\left(1-\frac{1}{\sqrt{\sigma_\mathrm{m}}}\right)^2+\frac{\hbar\omega_\mathrm{ci}}{2} \tag{23}$$

$$\sqrt{\sigma_\mathrm{m}}=\frac{1}{2}\left(\frac{R}{L_\mathrm{m}}\right)^2(\beta-1)+\frac{\beta}{2}+\beta R\sqrt{\frac{2m_\mathrm{o}}{\hbar^2}\left(V_0+\frac{\hbar\omega_\mathrm{co}}{2}-\left(\frac{\hbar^2\alpha_0^2}{2\beta m_\mathrm{o}R^2}+\frac{\hbar\omega_\mathrm{ci}}{2}\right)\right)}, \tag{24}$$

where we define the magnetic length scale $L_\mathrm{m}=\sqrt{\hbar/eB}$. The value of L_m is 25 nm for $B=1$ T. Note that if the BDD condition is not applied then $\beta=1$ and the first term, which depends on magnetic length scale, drops out. However, since it is quadratic in R, it is bound to dominate over the linear term at large R. Numerical calculations show: (i) Similar to the non-magnetic case, the approximation to obtain eq. (23) is valid for $R>5$ nm. (ii) The third term in eq. (24) dominates the value of $\sqrt{\sigma_\mathrm{m}}$ and the first term makes a mere 10% (negative) contribution for $R\le 20$ nm. (iii) For large R the first term begins to dominate. For example, for $V_0=1$ eV, $B=10$ T and $\beta=0.1$ we find that $\sqrt{\sigma_\mathrm{m}}$ peaks at ≈37 nm and then declines. Thus introduction of magnetic field has two effects on electronic ground state energy. Firstly, as seen by the second term on the RHS of eq. (23), it increases by an amount $(\hbar\omega_\mathrm{ci}/2)$ which depends inversely on β. Secondly, σ_m affects the first term on RHS of eq. (23). As σ_m increases, energy increases. Also note that we have $\sigma_\mathrm{m}<\sigma$ for a given V_0 and R. Figure 3 shows how energy changes with R for different values of β and strength of potential well. Again we see that BDD makes a major difference and energy increases as β decreases.

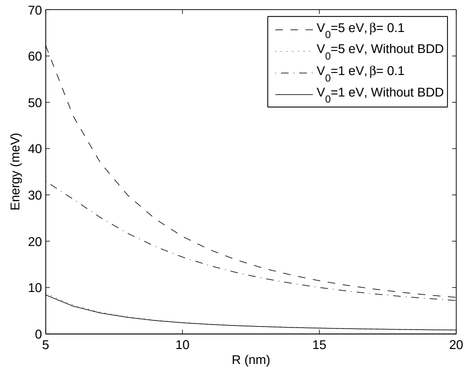

Figure 3. The dependence of ground state energy on the radius of the well in the presence of the magnetic field ($B = 5$ T) for $V = 5$ eV and 1 eV. We can see that BDD makes a major difference. The energy values increase with lower values of β. The non-BDD results for $V = 5$ eV are indistinguishable from $V = 1$ eV.

Table 1. The table depicts the comparison of the results of two-dimensional quantum well analysis done in this paper and the results of one- and three-dimensional quantum dots addressed in literature. The table shows energy ratio of 2D and 3D cases taking 1D as reference.

Dimension	1D	2D	3D
Size of the well	$-L/2 \le x \le L/2$	$r \le R$	$r \le R$
Ground state energy ($V_0 \to \infty$)	$\pi^2\hbar^2/2m_{\rm i}L^2$	$\alpha_0^2\hbar^2/2m_{\rm i}R^2$	$\pi^2\hbar^2/2m_{\rm i}R^2$
Ground state energy (V_0 finite)	$\pi^2\hbar^2/2m_{\rm i}(L+\delta)^2$	$\alpha_0^2\hbar^2/2m_{\rm i}(R+\delta)^2$	$\pi^2\hbar^2/2m_{\rm i}(R+\delta)^2$
Penetration depth (δ)	$L/\sqrt{\sigma}$	$R/\sqrt{\sigma}$	$R/\sqrt{\sigma}$
Strength of potential (σ)	$\sim(\beta k_{\rm o}L)^2$	$\sim(\beta k_{\rm o}R)^2$	$\sim(\beta k_{\rm o}R)^2$
Ratio of ground state energies ($L = 2R$; $V_0 \to \infty$)	1	2.34	4

5. Discussion

We compare the results between non-magnetic and magnetic cases. We find that energy is higher for magnetic case. Our calculations also show that the magnetic field does not cause much alteration in the charge density distribution. Table 1 encapsulates the comparison between one-, two- and three-dimensional cases. With this work the trilogy has been completed.

We have carried through an elaborate asymptotic analysis in order to make the effects of the BDD condition physically transparent. We have identified the strength of the potential term for both magnetic and non-magnetic cases as the relevant scale in the problem. Excited states have not been discussed since we wanted to keep the discussion simple and analytical. We hope to address excited states numerically in future work. It could then be used to discuss transitions and the BDD condition may affect the interpretation of data. Another area we hope to address is the role of multi-electrons in 2D QD. Finally, studies are underway on the diamagnetic dot in a magnetic field, a system studied recently by Kocsis *et al* [7]. In a recent work, Berry *et al* [8] discussed the circular dots with a boundary condition which depends on an azimuthal angle ϕ. It is possible but perhaps experimentally very difficult to realize this by having an exterior whose composition is continuously varying such that the mass outside becomes ϕ-dependent.

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