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An approximate approach to the quantum well in the presence of electric field and BenDaniel–Duke boundary condition

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Abstract

Very few problems are analytically solvable in quantum mechanics. We present an analytical approximation to the expression for quantized energies of a semiconductor quantum well placed in a constant electric field. The system is studied under the influence of the BenDaniel–Duke boundary condition. We obtain approximated scaling laws to understand the exact numerical results obtained. We study the size dependence, field dependence and charge densities on the mass ratio of electron outside and inside the well. We relate the obtained results to quantum confinement Stark effect. The approach is suitable to discuss in an undergraduate classroom.

Keywords: quantum mechanics, effective mass theory, approximation methods

(Some figures may appear in colour only in the online journal)

1. Introduction

The technological importance of low-dimensional semiconductor systems can hardly be overstated [1–3]. Due to the extremely small size of a quantum dot (QD), the charge carriers in it are essentially trapped and can be modelled by the well-known problem of particle-in-a-box. Further, the effective mass theory (EMT) must be considered to investigate the properties of the system in which the effective mass of the particle inside the well is different from one outside the well. Despite a long history, the effect of EMT on boundary condition, namely,

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BenDaniel–Duke (BDD) boundary condition [4] has not been studied extensively. Recent advances in the synthesis of QDs with precise control over its shape and size has led to possible applications of QDs in bio-sensing for probing properties of bio-molecules and effective drug delivery, for photonics in the development of optical display, for photovoltaic cells for example quantum dot solar cells and for several other applications. In the context of many of these applications, it is desirable to study the effect of external electric field applied to quantum dots with BDD.

An infinite one-dimensional quantum well is a standard textbook exercise in an undergraduate quantum mechanics course. Linear perturbation (e.g. particle in a gravitational or electric field) is often used to illustrate the importance of boundary conditions and the perturbation theory. As a first step to studying the effect of electric field on confined systems, in section 2, we model the conduction band of the quantum dot as a one-dimensional quantum well with externally applied electric field. One may also model the valence band as a potential barrier in an electric field but we currently present the modeling of the conduction band alone. We incorporate mass discontinuity of the quantum well by using the BDD boundary conditions instead of the conventional boundary conditions of wavefunction continuity. Thus the mass ratio $\beta = m_i/m_o$ plays an important role where m_i is the mass inside and m_o is the mass outside the well respectively.

The approximate methods to study the behavior of the system under BDD without the influence of the external field have been studied earlier [5, 6]. In section 3, we go beyond the standard numerical results and obtain an approximate analytical expression for the energy levels, which is valid in the limit of high potential barrier and strong electric field. Consider the well of length L. Wavefunction decays exponentially outside L. As it is well known that this can be viewed as infinite well with width $(L + 2\delta)$ [7]. In section 3, this appealing picture is reconstructed in the present case with $L + 2\delta$ as an effective length. In the infinite well, energy $E \propto 1/L^2$. On the other hand, in a finite well $E \propto 1/(L + 2\delta)^2$. Thus one can build a complete pedagogy at the undergraduate level.

Section 4 consists of numerical results and understands it with the help of approximated analytical expression obtained in the previous section. Finally we obtain the well-known quadratic variation of energy relative to the average potential with variation in the electric field. The last section constitutes the discussion.

2. Quantum well under the influence of an electric field

Consider a nanostructure in which a material with a lower bandgap is sandwiched between the same materials on two sides with a higher bandgap (e.g. GaAlAs/GaAs/GaAlAs). The boundary of the materials are chosen such that charges are confined in the x direction and free in the perpendicular direction. Using the envelope function approach approximation, wavefunction in the x and y, z direction can be described by the finite well and the Bloch functions respectively [8, 9]. Thus, such nanostructures can be modeled as a finite well in one direction and we are going to refer to it as a one-dimensional finite well.

The Hamiltonian of an electron in such kind of one-dimensional well of length L using the effective mass theory is given by

$$H = \frac{-\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d}{dx}\right) + V(x). \qquad (1)$$

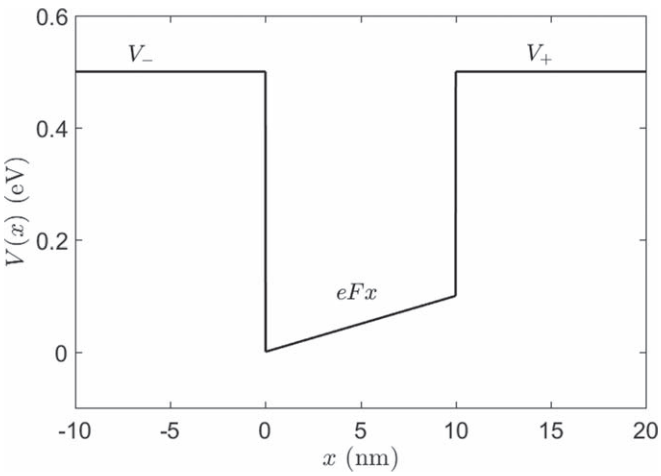

Figure 1. Quantum well with applied electric field $F = 10^7$ V/m, $V_- = V_+ = 0.5$ eV,

The mass distribution of the electron is taken as a step function:

$$m(x) = \begin{cases} m_i & 0 < x < L \\ m_o & x < 0 \text{ or } x > L \end{cases} \tag{2}$$

where m_i is the bare mass of the electron. We define $\beta = m_i/m_o$. If an electric field (F) is applied inside the well, as shown in figure 1, the potential becomes

$$V(x) = \begin{cases} V_- & x < 0 \\ eFx & 0 < x < L. \\ V_+ & x > L \end{cases} \tag{3}$$

The Schrodinger equation can be solved to obtain the bound states. For $x < 0$

$$-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d\,\psi}{dx}\right) + (V_- - E)\,\psi = 0 \tag{4}$$

and for $x > L$

$$-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d\,\psi}{dx}\right) + (V_+ - E)\,\psi = 0. \tag{5}$$

The equations (4) and (5) can be rewritten as

$$\psi'' - \kappa_- \psi = 0 \text{ and } \psi'' - \kappa_+ \psi = 0$$

where

$$\kappa_\pm = \sqrt{\frac{2m_o}{\hbar^2}(V_\pm - E)}.$$

A general solution to this differential equation is

$$\psi = c_1 e^{-k_+ x} + c_4 e^{k_- x}.$$

For $x < 0$, $c_1 = 0$. Therefore $\psi = c_4 e^{k_- x}$ and for $x > L$, $\psi = c_1 e^{-k_+ x}$.

Inside the well the Schrodinger equation in the presence of electric field inside the well becomes

$$-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d\,\psi}{dx}\right) + (eFx - E)\,\psi = 0. \tag{6}$$

Let us define

$$\xi = \frac{eFx}{\alpha} - \frac{E}{\alpha} \tag{7}$$

where $\alpha = \left(\frac{\hbar^2 e^2 F^2}{2\beta m_o}\right)^{1/3}$. Using these definitions, equation (6) reduces to

$$\frac{d^2\psi}{d\xi^2} - \xi\psi = 0. \tag{8}$$

The solution of the above equation is well known in literature, which is the Airy's functions [10]:

$$\psi = c_2 Ai(\xi) + c_3 Bi(\xi). \tag{9}$$

Note that $Ai(\xi)$ is oscillatory for $\xi < 0$ and dies exponentially for $\xi > 0$. It is $Bi(\xi)$ on the other hand that is oscillatory for $\xi > 0$ but grows exponentially for $\xi > 0$ [11]. Unlike the standard infinite quantum well in literature, the well discussed here has a finite barrier width and electric field exists in this finite region. Thus we may not take $c_3 = 0$ [12].

The wavefunction can be written as

$$\psi = \begin{cases} c_4 e^{\kappa_- x} & x < 0 \\ c_2 Ai\left(\frac{eFx - E}{\alpha}\right) + c_3 Bi\left(\frac{eFx - E}{\alpha}\right) & 0 < x < L. \\ c_1 e^{-\kappa_+ x} & x > L \end{cases} \tag{10}$$

We make an important change here. In addition to the boundary condition of continuity of wavefunction, we use the BDD boundary condition [4], namely

$$\frac{\psi'(0^-)}{m_o} = \frac{\psi'(0^+)}{m_i} \tag{11}$$

$$\frac{\psi'(L^-)}{m_i} = \frac{\psi'(L^+)}{m_o} \tag{12}$$

where the superscripts $-$ and $+$ denote the left and right hand limit respectively. Above equations yield

$$-\frac{c_2}{c_3} = \frac{Bi'\left(\frac{eFL-E}{\alpha}\right) + \frac{\alpha\beta\kappa_+}{eF}Bi\left(\frac{eFL-E}{\alpha}\right)}{Ai'\left(\frac{eFL-E}{\alpha}\right) + \frac{\alpha\beta\kappa_+}{eF}Ai\left(\frac{eFL-E}{\alpha}\right)} = \frac{\frac{\alpha\beta\kappa_-}{eF}Bi\left(\frac{-E}{\alpha}\right) - Bi'\left(\frac{-E}{\alpha}\right)}{\frac{\alpha\beta\kappa_-}{eF}Ai\left(\frac{-E}{\alpha}\right) - Ai'\left(\frac{-E}{\alpha}\right)}. \tag{13}$$

Roots of the above equation give the quantized energy states of the system which can be obtained numerically. In the next section we obtain an approximate analytical solution which is valid for large barrier heights.

3. An analytical approach

One must accept the fact that not every problem in physics can be solved analytically. Often, judicious use of approximations is used to derive an expression to see the effect of various variables present in the problem. The approach presented here is doable at the level of lowerdivision courses. At the end of this section, we shall be able to separate the effect of confinement and electric field on the energy levels of the charged particles.

We assume the asymptotic form of the Airy functions [13]. After truncating higher order terms,

$$Ai(-z) = \frac{1}{\sqrt{\pi\sqrt{z}}}\sin(\zeta + \pi/4) \tag{14}$$

$$Ai'(-z) = -\sqrt{\frac{\sqrt{z}}{\pi}}\cos(\zeta + \pi/4) \tag{15}$$

$$Bi(-z) = \frac{1}{\sqrt{\pi\sqrt{z}}}\cos(\zeta + \pi/4) \tag{16}$$

$$Bi'(-z) = \sqrt{\frac{\sqrt{z}}{\pi}}\sin(\zeta + \pi/4) \tag{17}$$

where

$$\zeta = \frac{2}{3}z^{\frac{3}{2}}.$$

We assume $V \gg E$ (see table A1 in the appendix) so that $\kappa_- \approx \sqrt{2mV_-}/\hbar$ and $\kappa_+ \approx \sqrt{2mV_+}/\hbar$. We define $eF/\alpha\beta\kappa_+ = \mathcal{G}_+$ and $eF/\alpha\beta\kappa_- = \mathcal{G}_-$. Equation (13) can be written as

$$\frac{\mathcal{G}_-\sqrt{z_1}\tan(\zeta_1 + \pi/4) - 1}{\tan(\zeta_1 + \pi/4) + \mathcal{G}_-\sqrt{z_1}} = \frac{\mathcal{G}_+\sqrt{z_2}\tan(\zeta_2 + \pi/4) + 1}{\mathcal{G}_+\sqrt{z_2} - \tan(\zeta_2 + \pi/4)} \tag{18}$$

where $z_1 = -\mathrm{E}/\alpha$ and $z_2 = (eFL - \mathrm{E})/\alpha$ and ζ is as defined before. Let us assume $G\sqrt{z} = \tan(\gamma)$, hence $\gamma = \tan^{-1}(\mathcal{G}\sqrt{z}) \approx \mathcal{G}\sqrt{z}$. Using this approximation for both the arguments in the above equation, an estimate is obtained:

$$\frac{\tan(a) + \tan(\gamma_1)}{1 - \tan(a)\tan(\gamma_1)} = \frac{\tan(b) - \tan(\gamma_2)}{1 + \tan(b)\tan(\gamma_2)} \tag{19}$$

where $a = \zeta_1 + \pi/4$ and $b = \zeta_2 + \pi/4$. Above form can be further reduced to

$$a + \gamma_1 = b - \gamma_2 + n\pi.$$

Hence

$$\left(\mathcal{G}_- + \mathcal{G}_+\left(1 - \frac{eFL}{E}\right)^{\frac{1}{2}}\right)\sqrt{\frac{E}{\alpha}} = \frac{2}{3}\left(\frac{E}{\alpha}\right)^{\frac{3}{2}}\left[\left(1 - \frac{eFL}{E}\right)^{\frac{3}{2}} - 1\right] + n\pi. \tag{20}$$

We consider the case when $eFL \gg E$. We can apply binomial approximation in eFL/E, up to second order. Equation (20) evolves into

$$\mathcal{G}_- + \mathcal{G}_+\left(1 - \frac{eFL}{2E} - \frac{1}{8}\left(\frac{eFL}{E}\right)^2\right) = \frac{2}{3}\frac{E}{\alpha}\left(-\frac{3}{2}\left(\frac{eFL}{E}\right) + \frac{3}{8}\left(\frac{eFL}{E}\right)^2\right) + n\pi\sqrt{\frac{\alpha}{E}}. \tag{21}$$

In order to solve this equation, we define $\mathcal{P} = \dfrac{eFL}{\alpha}$ and $\epsilon = \sqrt{\frac{E}{\alpha}}$. On simplifying we get

$$(\mathcal{P} + \mathcal{G}_- + \mathcal{G}_+)\epsilon^4 - (n\pi)\epsilon^3 - \left(\frac{\mathcal{P}\mathcal{G}_+}{2} + \frac{\mathcal{P}^2}{4}\right)\epsilon^2 - \frac{\mathcal{P}^2\mathcal{G}_+}{8} = 0. \tag{22}$$

The order of magnitude of the last term is lesser than the other terms (see table A2 in the appendix for the justification of the approximation). Hence, dropping the constant term, we end up with a simple quadratic equation. The solution of this quadratic equation gives the approximate analytical expression for quantized energy as

$$\epsilon = \sqrt{\frac{E}{\alpha}} = \frac{n\pi \pm \sqrt{(n\pi)^2 + 4(\mathcal{P} + \mathcal{G}_+ + \mathcal{G}_-)\left(\frac{\mathcal{P}\mathcal{G}_+}{2} + \frac{\mathcal{P}^2}{2}\right)}}{2(\mathcal{P} + \mathcal{G}_+ + \mathcal{G}_-)} \tag{23}$$

$$\Rightarrow E = \frac{2\alpha n^2\pi^2}{4A^2}(1 + \mathcal{A}\mathcal{B} + (1 + 2\mathcal{A}\mathcal{B})^{1/2}) \tag{24}$$

where $\mathcal{A} = \mathcal{P} + \mathcal{G}_+ + \mathcal{G}_-$ and $\mathcal{B} = \frac{\mathcal{P}^2}{4} + \frac{\mathcal{P}\mathcal{G}_+}{(n\pi)^2}$=. The term $\mathcal{A}\mathcal{B}$ is smaller in comparison to the other terms Once more we do binomial approximation to obtain

$$E = \frac{\alpha n^2\pi^2}{\mathcal{A}^2}(1 + \mathcal{A}\mathcal{B}). \tag{25}$$

Plugging back the respective expressions for α, $\mathcal{A}$ and $\mathcal{B}$ yields the final expression:

$$E = \frac{n^2\pi^2\hbar^2 e^2F^2}{2\beta m_o(eFL)^2}\left(1 + \frac{1}{L\beta\kappa_+}\left(1 + \sqrt{\frac{V_+}{V_-}}\ \right)\right)^{-2} \times \left(1 + \frac{1}{(n\pi)^2}\left(\frac{eFL}{\alpha}\right)^3\left(1 + \frac{2}{L\beta\kappa_+}\right)\left(1 + \frac{1}{L\beta\kappa_+}\sqrt{\frac{V_+}{V_-}}\ \right)\right). \tag{26}$$

The final expression for the energy eigenvalues for the system is thus given by equation (26). To further investigate the dependence of the energy on the width of the well, electric field and mass ratio, we consider a special case pertaining to $V_+ = V_- = V$. Equation (26) can be further simplified as

$$E = \frac{n^2\pi^2\hbar^2}{2\beta m_o}\frac{1}{L^2} + eFL - \frac{12eF}{\kappa_+^2\beta^2}\frac{1}{L} - \frac{16eF}{\beta^3\kappa_+^3}\frac{1}{L^2} - \frac{2n^2\pi^2\hbar^2}{\beta^2 m_o\kappa_+}\frac{1}{L^3} \tag{27}$$

where $\kappa_+ \approx \sqrt{2mV}/\hbar$

$$E = \frac{n^2\pi^2\hbar^2}{2\beta m_o}\frac{1}{L^2}\left[1 - \frac{4}{\sqrt{\sigma}}\right] + eFL\left[1 - \frac{4}{\sigma}\left(3 + \frac{4}{\sqrt{\sigma}}\right)\right] \tag{28}$$

where $\sigma = \beta\kappa_+L$. We have separated the confinement effect and the electric field effect in the above expression. Further for $\sigma \gg 1$, we can write the first term of equation (28) as

$$\frac{n^2\pi^2\hbar^2}{2m_i(L + 2\delta)^2}$$

where

$$\delta = L/\sqrt{\sigma}$$

which is same as equation (21) of Singh and Kumar [14].

Undergraduate students are familiar with the textbook example of infinite well in which energy goes as $1/L^2$. Here we have reconstructed the analogy in the finite well which can be thought as an infinite well of length $L + 2\delta$. In literature δ is called penetration depth [14, 7]. In such a well, according to equation (28), confinement part of the energy goes as $1/(L + 2\delta)^2$ and linear in electric field strength. This kind of interpretation is well suited for the students where one can separately see the confinment and electric field effects in the first and second terms of the equation (28).

The effect of BDD condition is also evident here. Due to finiteness of the well, charge can penetrate the boundary and presence of β (BDD boundary condition) enhances this penetration. This perticular aspect will be absent had we have only replaced m by m^*in building the Hamiltonian in the beginning of this section. In the following section, we will compare the equation (28) with the numerical results (equation (13)).

4. Results

4.1. Energy variation with length

Since we attempt to model a semiconductor nanocrystals, an appropriate range of L and β is: $L \sim 1$–100 Å, $\beta \sim 0.05$–1 and V_-or $V_+ \sim 0.1$–5 eV, while the appropriate range of applied field is usually $F \sim 10^5$–10^7 V/m. In order to verify the asymptotic analysis, in figure 2, we plot the variation of the ground and first excited state energies (E_0 and E_1 respectively) obtained from the exact numerical solution (equation (13)) and from the asymptotic analysis (equation (28)). We consider two different cases of $\beta = 0.5$ and 1 as shown in the figure 2. Note that $\beta = 1$ refers to the case when mass is not discontinuous, thus, the absence of BDD in the calculations.

The asymptotic solution, despite various approximations and basic order of magnitude analysis is able to provide a very accurate match with the exact solution in desirable range of L and β. When BDD condition is not applied ($\beta = 1$), results from the approximation and the exact numerical analysis are almost identical (relative error is 1%). Relative error increases for for the lower β value i.e. when the particle effectively feels lighter inside the well. The effect of BDD condition is evident. Energy almost doubles when β is changed from 1 (no BDD) to 0.1 (BDD effect). That indicates that applying the BDD condition has a strong effect on the system. In the following sections, we present only the numerically exact results.

4.2. Transition energies

Transition energies are important from the point of view of experiments. In figure 3 we plot the differences between the ground state and first excited state (ΔE_{01}), second and the first excited state (ΔE_{21}), and between second excited and ground state energies (ΔE_{20}). In all the cases, transition energies decreases with increasing well length L. On the transition energies, the effect of lowering the value of β is more pronounced than increasing the electric field. For example, in the case of $\beta = 0.1$, the curves of electric field 10^7 V/m is indistinguishable from 10^6 V/m. This can be explained with the help of approximate expression equation (28) where the electric field dependent second term does not depend on β. Once again the asymptotic analysis proved to be a versatile tool in explaining the physics of the problem.

4.3. Variation of energy with electric field

When an electric field is applied, the conventional square potential in the quantum well acquires a tilt as shown in figure 1. Figure 4 shows the variation of ground state and first excited state energy levels with variation in applied electric field using exact solution (obtained in terms of Airy functions as given by (13)). Clearly, as the applied external field increases the energy value of either state increases. Such a trend is observed for all desired values of β and L.

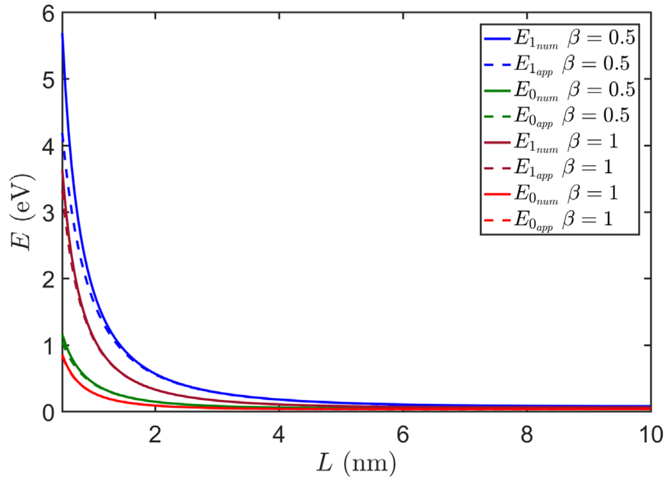

Figure 2. Variation of E_0, E_1 obtained through exact solution (denoted by subscript 'numerical') and asymptotic analysis (denoted by subscript 'app') for two different cases of β being 0.5 and 1; where F $= 10^7$ V/m and $V_+ = V_- = 5$ eV. Note that $\beta = 1$ implies no BDD.

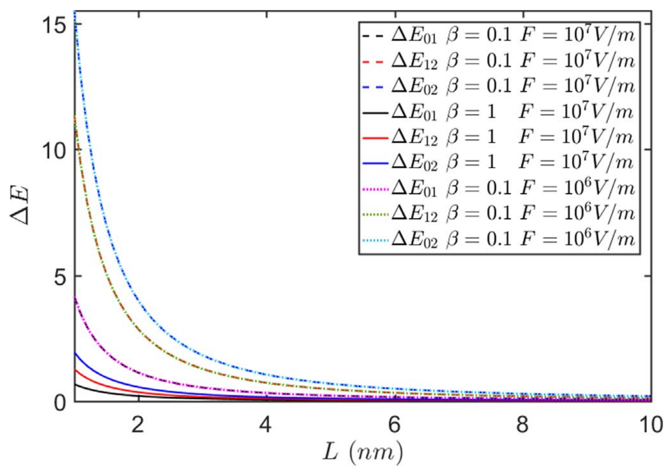

Figure 3. Variation of transition energies with the well length for $\beta = 0.1$,1 and two values of electric field 10^6 and 10^7 V/m. Barrier height is taken to be 1 eV.

4.4. Ground state vs β

It is also interesting to note the variation of the ground state energy with the increase in the value of β. Figure 5 shows that the energy eigenvalue increases as the mass ratio decreases. Such variation in the energy value with the mass ratio is noteworthy since it is usually not accounted for in conventional variational methods or studied in reduced mass models.

4.5. Effect of electric field and mass ratio on the charge density distribution

We investigate the variation of the charge density ($\rho = e|\psi|^2$) with variation in the mass ratio β and the variation in the electric field applied externally. Figure 6 shows the distinct charge

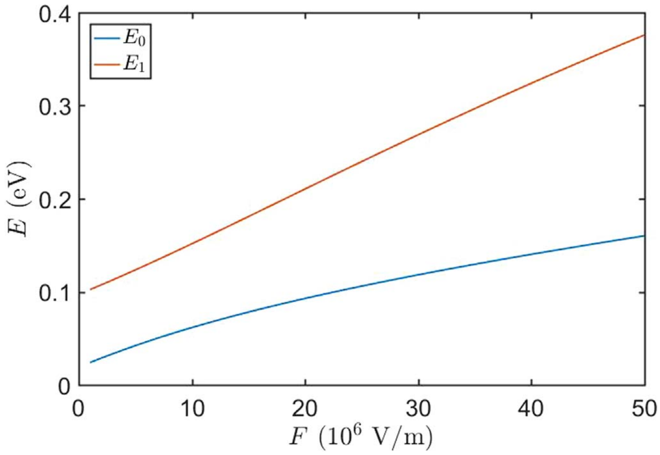

Figure 4. Variation of E_0 and E_1 with an externally applied electric field of strength F. Other parameters are kept constant as: $\beta = 0.07$, $V_+ = V_- = 0.5$ eV and $L = 10$ nm.

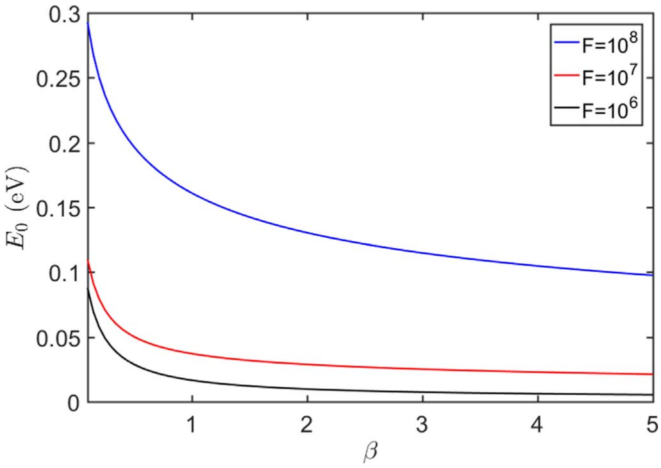

Figure 5. Variation of ground state energy E_0 with β for $L = 3$ nm, $V_+ = V_- = 5$ eV for three different values of F.

density distribution corresponding to the ground state for three different values of the mass ratio. Also, the corresponding energy values are indicated by dashed lines in the figure.

The charge density distribution shown in figure 6 discloses several noteworthy features. First, we observe that the charge density distribution is continuous but not differentiable at the boundaries (at $x = 0$ and $x = L$), i.e. the slope of ρ changes abruptly, owing to the mass discontinuity. From the solution of equation (13) for fixed values of F, L and V_- $(=V_+)$, we note that the ground state, the first and the second excited state are the only bound states. The charge density distribution is skewed towards the left with increasing β. It is known that a charged particle trapped in a potential well tends to acquire lower potential. The more the charge density is skewed to the left, the lower the potential energy of the charge.

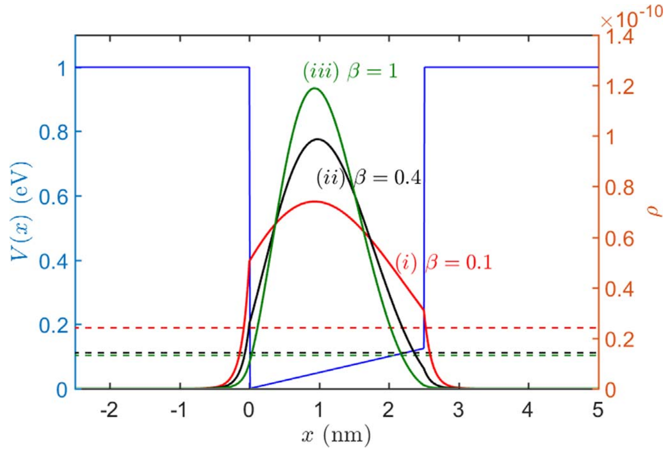

Figure 6. Charge density distributions (plotted along the right y-axis) for different values of β superimposed on the quantum well potential (blue solid line, plotted along the left y-axis). The solid lines (red, violet, green) represent the charge density distribution for different cases: (i)$\beta = 0.1$, (ii) $\beta = 0.4$ and (iii)$\beta = 1.2$ respectively; while the dashed lines (in corresponding colors) show the ground state energy level for each case. Other parameters are: $L = 2.5$ nm, $V_+ = V_- = 1$ eV, $F = 5 \times 10^7$ V/m.

We observe that with th increase in the value of β, the peak of the charge density distribution sharpens (peak becomes thinner and the peak value increases). This indicates that the probability of finding the charged particle at a particular location increases. From the uncertainty principle, we infer that if the position of the charged particle becomes more certain and the probability of finding it in a certain position increases, then the uncertainty in its momentum increases and the kinetic energy decreases. Also, the dashed lines which indicate the energy value of the ground state show that the energy of the ground state decreases with the increase in β. The same has been demonstrated by the plot of energy variation with β in figure 5.

If one increases the electric field, the peak of the charge density distribution would shift towards the lower potential (to the left) and also sharpens (peak value of ρ increases). As, discussed earlier, sharpening of the peak essentially implies lowering of the kinetic energy of the charged particle while the shift of the peak to the left implies lowering of the potential energy. On the whole, the energy of the charged particle is suppressed with increase in the electric field. Such suppression of the energy in the presence of an external electric field is known as quantum-confined Stark effect (QCSE) [15], discussed in detail in the next section.

4.6. Quantum-confined Stark effect (QCSE)

QCSE refers to suppression of the energy of the system of electron-hole pair confined in a potential well due to reduction in their Coulomb interaction in the presence of an external electric field. In their well-known study, Miller *et al* [15] have described the QCSE phenomena in great detail and have also presented a theoretical model for the same. They have shown that for high values of F, the suppression in the energy of the individual charged particles with respect to the average potential energy of the system is the dominant contribution to QCSE.

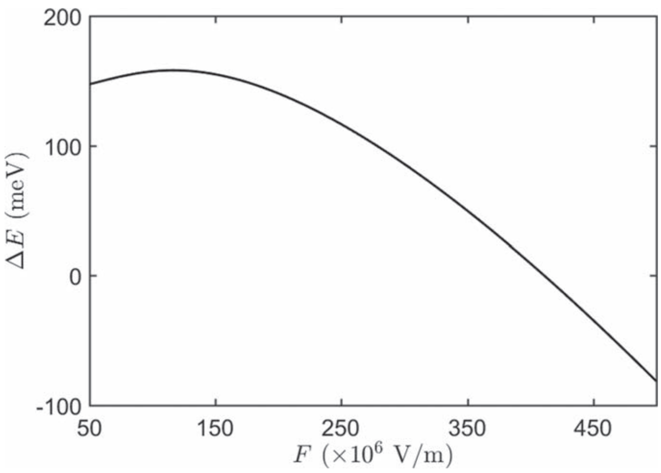

Figure 7. Variation of the ground state energy relative to the average potential energy of the quantum well (ΔE) with variation in the applied electric field (F).

As discussed earlier, through figure 4, the absolute energy of the ground state seems to increase with increasing electric field. But through shifts in the charge density distribution, we infer that the energy of the charged particle decreases. Such contrast can easily be explained. Since increasing the value of electric field implies that we are adding energy to the entire system, the eigen-energy (of the ground state) will also increase. Such an increase of absolute energy of the ground state is evident form the curve in figure 4. Further, to understand the shift in charge density curves on increasing the electric field, it is important to investigate the variation of the energy of the charged particle alone, with variation in the electric field. One can obtain such information by analysing the change in energy of the ground state apart from the increase induced by the externally applied electric field [15]. We thus define ΔE as the difference in the energy of the ground state and the average potential energy of the system. Figure 7 shows the variation of ΔE with increasing electric field.

On excluding the effect of increasing average potential energy, we observe a suppression in the energy of the ground level, similar to that reported in several studies [15, 16]. As explained by the study of Miller *et al* [15], for electric field in the range $>3 \times 10^6 V/m$, the suppression of the energy of the individual electron (and hole) in the conduction (and valence) band is the dominant effect causing QCSE. Hence it is expected that the energy of the charged particle confined inside a quantum well will decrease with increasing electric field (excluding the increase in the average potential energy); which is well captured in our model.

5. Discussion

The paper discusses the quantum mechanics of a one-dimensional well in the presence of electric field. Though the problem is a textbook problem it is not discussed in detail when effective mass theory is properly applied. This brings the importance of the BenDaniel–Duke boundary condition on the energy levels. We have demonstrated that applying the condition significantly alters the transition energies and charge densities. We also derived an approximated expression for large quantum well which matches in some range with the exact results. The effect of various parameters such as length of the well, barrier height, mass ratio, and the electric field obtained from the numerical analysis but their trends can be well explained using the approximated analytical expression. At the end we also demonstrated the usefulness of BDD in QCSE. We hope that such exercises are useful in undergraduate classes to enrich the knowledge of quantum mechanics.

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Appendix A. Justification of approximations

We justify the approximation used in section 3.

1. $V \gg E$
   Let us consider a typical example where $V_- = V_+ = 0.8\,\text{eV}$, $L = 10\,\text{nm}$, $\beta = 0.07$ and $F = 8 \times 10^6\text{V/m}$. For these values, equation (13) can be solved numerically to obtain the quantized energy levels at 0.0272eV, 0.1108eV and 0.2825eV for the ground, first excited and second excited states respectively. We therefore consider the order of magnitude for energy eigenvalue of the system to be 0.1 eV.
   For $\beta = 0.5$, $L = 1\,\text{nm}$, $F = 10^7\,\text{V/m}$, $V = 1\,\text{eV}$, energy $E_0 = 0.27\,\text{eV}$. For $V = 0.1\,\text{eV}$ we get $E_0 = 0.11\,\text{eV}$ and for $V = 5\,\text{eV}$, $E_0 = 0.4\,\text{eV}$. So the assumption of $V \gg E$ is valid up to $V = 0.5\,\text{eV}$.
2. Neglecting constant term in equation (22) we see that the order of magnitude of the constant term $\mathcal{P}^2\mathcal{G}_+/8$ is much lesser than that of other terms (refer table 2).

Table A1. Order of magnitude of various terms.

Term	Order of magnitude (in SI units)
β	0.1
L	10^{-9}
E	10^{-20}
α	10^{-21}
eFL	10^{-21}

Table A2. Order of magnitude of various terms.

Term	Order of magnitude (in SI units)
$\mathcal{P}$	1
$\mathcal{G}_+$ and $\mathcal{G}_-$	0.1
$(\mathcal{P} + \mathcal{G}_- + \mathcal{G}_+)x^4$	10
$(n\pi)\,x^3$	10
$\left(\frac{\mathcal{P}\mathcal{G}_+}{2} + \frac{\mathcal{P}^2}{4}\right)x^2$	10
$\frac{\mathcal{P}^2\mathcal{G}_+}{8}$	0.1

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