Semiconductor quantum wells with BenDaniel–Duke boundary conditions: approximate analytical results

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Abstract
The Schrödinger equation for a particle moving in a square well potential with BenDaniel–Duke boundary conditions is solved. Using algebraic approximations for trigonometric functions, the transcendental equations of the bound states energy are transformed into tractable, algebraic equations. For the ground state and the first excited state, they are cubic equations; we obtain simple formulas for their physically interesting roots. The case of higher excited states is also analysed. Our results have direct applications in the physics of type I and type II semiconductor heterostructures.

Keywords: semiconductor heterojunctions, quantum wells, BenDaniel–Duke boundary conditions, type I and type II semiconductors

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

1. Introduction
This paper is devoted to the study of a simple problem of quantum mechanics: the movement of a particle with position-dependent mass (PDM) in a finite square well. The physical situation modelled by such a potential can be an electron in the conduction band of a semiconductor moving in a heterostructure, let us say BAB, i.e. a thin layer of a semiconductor A sandwiched between two somewhat larger semiconductors of identical composition, B ([1], p 66). So, simple as it is, this problem involves two important issues: the PDM quantum physics and semiconductor heterostructures. Let us shortly comment on these points.

As the effective mass of a charge carrier in a semiconductor depends on the charge carrier—lattice interaction, it changes if the lattice composition or the symmetry changes. So,
excepting the case of a charge moving in a perfect crystal, the effective mass of an electron or hole is, rigorously speaking, position-dependent.

The roots of the position dependent effective mass concept are to be found in the pioneering works of Wannier (1937) and Slater (1949) (see reference 1 in [2]). Recent papers give explicit methods to obtain explicit solutions of the Schrödinger equation with PDM, for various forms of this dependence and for several classes of potentials [3–5].

However, in practical situations usually encountered in the physics of semiconductor junctions of two materials, A and B, the simplest and more popular form of position dependence of the effective mass is a step function: the effective mass has a constant value in the material A and another, constant value, in the material B. In such a case, the most convenient approach for obtaining the wave functions or the envelope functions in a heterostructure—for instance, a quantum well (QW) or quantum dot (QD)—is to solve the Schrödinger equation with BenDaniel–Duke boundary conditions for the wave function [1, 6].

The transition from the complex problem of a real semiconductor (for instance Kane theory), to the simple problem of a particle moving in a square well with BenDaniel–Duke boundary conditions is indicated, for instance, in chapter III of Bastard’s book [6]. This simple problem provides however a realistic description of states near the high-symmetry points in the Brillouin zone of a large class of semiconductors. ‘It (i.e. ‘the simple problem’) often leads to analytical results and leaves the user with the feeling that he can trace back, in a relatively transparent way, the physical origin of the numerical results.’ ([6], p 63).

The boundary conditions for the wave functions or envelope functions at interfaces generate the eigenvalue equations for energy; of course, different boundary conditions generate different eigenvalue equations. They are transcendental equations, involving algebraic, trigonometric, hyperbolic or even more complicated functions. With few exceptions (for instance, the Lambert equation), their solutions, which cannot be expressed as a finite combinations of elementary functions, are not systematically studied.

However, in some situations, quite accurate analytical approximate solutions can be obtained. This happens in the case of laser dressed potentials [7, 8], of some applications of the Floquet theory [9] or in the ‘algebraization’ of some transcendental equations for eigenenergies of the bound state solutions of the Schrödinger equation with a quite large class of potentials [10, 11]. The ‘algebraization’ consists in replacing the trigonometric functions with appropriate algebraic approximations of these functions; in this way, the transcendental eigenvalue equations can be transformed in algebraic, tractable equations. The method was introduced by de Alcantara-Bonfim and Griffiths [10] and used in [11] in the context of nanophysics; it generated explicit and simple solutions for the ground state energy of a particle with position independent mass (PIM) in a square well, inter alia.

We can present now the main contributions of our paper to the aforementioned problems. Technically speaking, we shall solve the Schrödinger equation for a particle moving in a square well, with BenDaniel–Duke boundary conditions. The interesting part of this calculation is to obtain the wave vectors (and the energies) of bound states; obtaining the form of wave functions is a trivial exercise. The wave vectors are solutions of a couple of transcendental equations, somewhat more complicated than those obtained with usual boundary conditions (corresponding to a PIM). Actually, in the PIM case, they involve only the strength of the well, P—a parameter which depends both on the potential (on the depth and the length of the well) and on the mass of the particle. In the PDM case, the eigenvalue equations contain a new parameter, the ratio between the mass of the charge carrier inside and outside the well: \( \beta = m_i/m_r \). These exact transcendental equations are replaced with approximate algebraic equations, as just described in the previous paragraph.
The algebraic equations obtained in this way are simpler for the ground state and the first excited states, and more complicated for higher energies. In the first case, we obtain simple and accurate expressions, for both the $\beta < 1$ and $\beta > 1$. The relevance of these results for type I and type II heterointerfaces are discussed.

Of course, similar issues of elementary quantum mechanical problems with BenDaniel–Duke boundary conditions have been already discussed in literature. In two recent papers, Singh and co-workers [12, 13] obtained approximate solutions for the ground state wave vector replacing the trigonometric functions in the eigenvalue equation with the first few terms in their series expansions.

We consider that this paper is useful for teaching physics at tertiary level for several reasons: (1) the problem is mathematically very simple, essentially a Schrödinger equation for a square potential; (2) however, it involves a quite unfamiliar, but important concept, namely the PDM; (3) it shows that not only wave functions, but also enveloping functions satisfy the Schrödinger equation; (4) it is discussed in the framework of semiconductor nanostructures, a field of great interest for applied and theoretical physics; (5) it uses a simple mathematical approach to find approximate analytical solutions of transcendental equations; (6) it illustrates the concept of type I and type II semiconductors (see figure 1); (7) it suggests themes of research accessible to undergraduate students (for instance applying the same approach to QDs); (8) it makes use of a simple way of finding the real roots of a cubic equation, a subject rarely discussed in undergraduate physics.

Figure 1. Schematic representation of the conduction $E_c$ and valence $E_v$ bands for type I (a) and type II (b) semiconductors.
The structure of this paper is the following. Section 2 will be devoted to the presentation of basic theory: we shall write the Schrödinger equation for a PDM, namely in the simplest case, when the position dependence is given by a step function; we shall write the normalised wave functions, inside and outside the well, for even and odd states, and the eigenvalue equations for energy—in fact, for the wave vector. Section 3 contains most of the original part of our paper. We use an algebraic approximation for \( \cos x \), proposed by de Alcantara-Bonfim–Griffiths (dABG) [10], and another one, proposed by us, for \( \sin x/x \); in this way, the eigenvalue equations become tractable, algebraic equations—more precisely, cubic equations. We obtain simple formulas for the wave vector of the ground state and of the first excited state, if \( \beta < 1 \) and if \( \beta > 1 \). If the limit \( \beta \to 1 \) is taken, in each of these cases, the results from [10] are obtained. We obtain also simple formulas for shallow wells, irrespective of the parity of state and of the value of \( \beta \). The case of excited states of higher order \( (n > 2) \) is shortly discussed: the eigenvalue equation can be approximated with a quartic algebraic equation. The results of this section are relevant for type I heterointerfaces. In section 4, they are adapted to the case of type II heterointerfaces and to QDs; also, the condition of validity of the envelope function approximation are discussed.

The last section is devoted to conclusions. As we systematically use formulas for the real roots of a cubic equation, where several authors propose slightly different approaches, we collect in an appendix the minimal theoretical tools to be used in the specific cases studied in this paper.

2. Basic theory

We shall solve the Schrödinger equation for an electron moving in a square well, described by the potential:

\[
V(x) = \begin{cases} 
0, & |x| \leq L/2 \\
V_0 > 0, & |x| > L/2 
\end{cases}
\]

considering that its mass is position-dependent. More exactly, the mass inside the well, \( m_i \), and the mass outside the well, \( m_o \), are different:

\[
m(x) = \begin{cases} 
m_i, & |x| \leq L/2 \\
m_o, & |x| > L/2 
\end{cases}
\]

So, the Schrödinger equation for bound states is:

\[
H^\psi = \left[ -\frac{\hbar^2}{2} \frac{d}{dx} \left( \frac{1}{m(x)} \frac{d}{dx} \right) + V(x) \right] \psi_n = E_n \psi_n.
\]

Its physically acceptable solutions, i.e. the wave functions, have to satisfy two conditions: the continuity of the wave functions and the continuity of the probability currents density at the interface. The first one is encountered in all quantum mechanical problems, but the second one is specific to the case of the position dependent mass [1], defined by equation (2), and takes the form:

\[
\frac{1}{m_i} \frac{d \psi_{in}}{dx} \bigg|_{x=-L/2} = \frac{1}{m_o} \frac{d \psi_{out}}{dx} \bigg|_{x=-L/2},
\]

where \( \psi_{in}, \psi_{out} \) are the wave functions inside, respectively outside the well. The equation (4) is known as the BenDaniel–Duke boundary condition.
The $n$th bound state has a unique energy, $E_n$, but two wave vectors, one inside the well, $k_{\text{in},n}$, and another one outside, $k_{\text{out},n}$:

$$E_n = \frac{\hbar^2 k_{\text{in},n}^2}{2m_i}, \quad V_0 - E_n = \frac{\hbar^2 k_{\text{out},n}^2}{2m_o}. \quad (5)$$

Due to the parity of the potential, $V(x) = V(-x)$, the wave functions can be chosen to be symmetric or antisymmetric.

The symmetric wave functions, describing the even states, are:

$$\psi_{2n}(x, 0 < x \leq L/2) = A_{2n} \cos k_{\text{in},2n}x$$
$$\psi_{2n}(x, x > L/2) = B_{2n} \exp(-k_{\text{out},2n}x)'$$
$$\psi_{2n}(x < 0) = \psi_{2n}(-x). \quad (6)$$

The ground state wave function is, of course, $\psi_0(x)$. The antisymmetric wave functions, describing the odd states, are:

$$\psi_{2n+1}(x, 0 < x \leq L/2) = A_{2n+1} \sin k_{\text{in},2n+1}x$$
$$\psi_{2n+1}(x, x > L/2) = B_{2n+1} \exp(-k_{\text{out},2n+1}x)'$$
$$\psi_{2n+1}(x < 0) = -\psi_{2n+1}(-x). \quad (8)$$

The continuity of these functions in $x = L/2$ gives:

$$B_{2n} = A_{2n} \cos \frac{k_{\text{in},2n}L}{2} \exp\left(\frac{k_{\text{out},2n}L}{2}\right). \quad (10)$$

$$B_{2n+1} = A_{2n+1} \sin \frac{k_{\text{in},2n+1}L}{2} \exp\left(\frac{k_{\text{out},2n+1}L}{2}\right). \quad (11)$$

So, the wave function outside the well is:

$$\psi_{2n}(x > L/2) = A_{2n} \cos \frac{k_{\text{in},2n}L}{2} \exp\left[-k_{\text{out},2n}\left(x - \frac{L}{2}\right)\right]. \quad (12)$$

$$\psi_{2n+1}(x > L/2) = A_{2n+1} \sin \frac{k_{\text{in},2n+1}L}{2} \times \exp\left[-k_{\text{out},2n+1}\left(x - \frac{L}{2}\right)\right]. \quad (13)$$

The wave functions are normalised if:

$$\frac{1}{A_{2n}^2} = \frac{L}{2} \left(1 + \frac{\sin k_{\text{in},2n}L}{k_{\text{in},2n}L} + \frac{1 + \cos k_{\text{in},2n}L}{k_{\text{out},2n}L}\right), \quad (14)$$

$$\frac{1}{A_{2n+1}^2} = \frac{L}{2} \left(1 - \frac{\sin k_{\text{in},2n+1}L}{k_{\text{in},2n+1}L} + \frac{1 - \cos k_{\text{in},2n+1}L}{k_{\text{out},2n+1}L}\right). \quad (15)$$

These results generalise the formula (24) in [12] and the equations (25.3e, o) in Flügge[14].

It is convenient to use the potential strength $P$ (introduced by Pitkanen [15], who actually used $\alpha$, instead of $P$) and its inverse, $p$:
\[ P = \sqrt{\frac{L^2}{2\hbar^2}m_0V_0} = \frac{1}{p} \]  
(16)

and to define also \( \varepsilon_n, \beta \) and \( \Phi_n \) as:

\[ \varepsilon_n = \frac{E_n}{V_0} \]  
(17)

\[ \beta = \frac{m_i}{m_0} \]  
(18)

\[ \Phi_n = k_{n,\text{in}}\frac{L}{2} \]  
(19)

\( P, \varepsilon_n, \beta \) and \( \Phi_n \) are dimensionless quantities; \( \Phi_n \) will be sometimes called dimensionless wave vector.

It is easy to see that:

\[ k_{\text{in},n}\frac{L}{2} = P\sqrt{\varepsilon_n}, \]  
(20)

\[ k_{\text{out},n}\frac{L}{2} = P\sqrt{\frac{1 - \varepsilon_n}{\beta}}, \]  
(21)

\[ k_{\text{in},n}^2 + \beta k_{\text{out},n}^2 = \frac{1}{(pL/2)^2}. \]  
(22)

Let us mention that, if the mass is constant, i.e. if \( m_i = m_0 \), the eigenvalue equations are (see for instance [6], p 3, equations (15) and (16)):

\[ \tan \frac{k_{\text{in},2n}L}{2} = \frac{k_{\text{out},2n}}{k_{\text{in},2n}}, \text{ even states}, \]  
(23)

\[ \tan \frac{k_{\text{in},2n+1}L}{2} = -\frac{k_{\text{in},2n}}{k_{\text{out},2n}}, \text{ odd states}. \]  
(24)

If the mass is position-dependent, according to (2), the eigenvalue equations obtained from the Schrödinger equation, with BenDaniel–Duke boundary conditions have the form:

\[ \tan \frac{k_{\text{in},2n}L}{2} = \frac{m_i}{m_o} \frac{k_{\text{out},2n}}{k_{\text{in},2n}} = \beta \frac{k_{\text{out},2n}}{k_{\text{in},2n}}, \text{ even states}, \]  
(25)

\[ \tan \frac{k_{\text{in},2n+1}L}{2} = -\frac{m_i}{m_o} \frac{k_{\text{in},2n+1}}{k_{\text{out},2n+1}} = -\frac{1}{\beta} \frac{k_{\text{in},2n+1}}{k_{\text{out},2n+1}}, \text{ odd states}. \]  
(26)

We shall consider that both \( m_i, m_o \) are positive; this case corresponds to type I QDs. So, \( \beta > 0 \) and replacing \( k_{\text{in}}L/2 \) with \( \Phi_{2n} \) for even states and with \( \Phi_{2n+1} \) for odd states, we can put the equations (25) and (26) in a more convenient form:

\[ \Phi_{2n}\tan \Phi_{2n} = \frac{\sqrt{\beta}}{p}\sqrt{1 - p^2\Phi_{2n}^2}, n = 0, 1, \ldots \text{ even states}, \]  
(27)

\[ \Phi_{2n+1}\cot \Phi_{2n+1} = -\frac{\sqrt{\beta}}{p}\sqrt{1 - p^2\Phi_{2n+1}^2}, n = 0, 1, \ldots \text{ odd states}. \]  
(28)
or, equivalently:

\[
\cos \Phi_{2n} = (-1)^n \frac{p}{\sqrt{\beta + (1 - \beta)p^2\Phi_{2n}^2}}, \quad n = 0, 1, \ldots \text{ even states},
\]

\[
\sin \Phi_{2n+1} = (-1)^n \frac{p}{\sqrt{\beta + (1 - \beta)p^2\Phi_{2n+1}^2}}, \quad n = 0, 1, \ldots \text{ odd states}. \tag{30}
\]

For \( \beta = 1 \), they take the form of the well-known equations for the energy eigenvalues of the finite square well. Approximate analytical solutions of these equations were obtained for deep wells \( p \ll 1 \) [19] and in the general case [10, 11, 16].

If \( 0 < \beta < 1 \) \( (\beta > 1) \), the rhs of equations (29) and (30) is a monotonically decreasing (increasing) function of \( \Phi \); in both cases, the roots of these equations can be obtained using the same approach.

In this paper, we shall obtain precise analytical approximations for the energy of the first two states, i.e. for the ground state and for the first excited state, considering the cases \( \beta < 1 \) and \( \beta > 1 \) separately. For moderate and deep wells, the formulas are both simple and accurate. In the limit \( \beta \to 1 \), we shall obtain the result of de Alcantara Bonfim and Griffiths, equation (17) of [10]. The case of shallow wells is also discussed in detail, for both cases \( \beta \ll 1 \).

### 3. Approximate analytical solutions for eigenvalue equations

#### 3.1. The first even state

According to equation (29), the dimensionless momentum of the first even state, which is also the ground state, is the first root of the equation:

\[
\frac{\cos \Phi_0}{\Phi_0} = \frac{p}{\sqrt{\beta + (1 - \beta)p^2\Phi_0^2}}, \quad 0 < \Phi_0 < \frac{\pi}{2}. \tag{31}
\]

We shall discuss separately the cases \( \beta > 1 \) and \( \beta < 1 \).

##### 3.1.1. The case \( \beta > 1 \)

We shall examine this case in detail, as the approach used here will be followed with minor changes in the other three cases (even state, \( \beta < 1 \); odd state, \( \beta < 1 \) and \( \beta > 1 \)).

It is useful to introduce the new parameters \( \gamma_\gamma, g_\gamma, A_\gamma^2 \) :

\[
\gamma_\gamma = \beta - 1, \quad g_\gamma = \frac{1}{\gamma_\gamma}, \quad A_\gamma^2 = \frac{p^2\beta}{\beta - 1} = p^2\beta g_\gamma.
\]

The eigenvalue equation can be written now in a simpler form:

\[
\frac{\cos \Phi_0}{\Phi_0} = \frac{1}{\sqrt{\gamma_\gamma} \sqrt{A_\gamma^2 - \Phi_0^2}}, \quad 0 < \Phi_0 < \frac{\pi}{2}. \tag{33}
\]

In the most interesting cases, \( P \) is quite large (the wells are quite deep), and according to equation (32), \( A_\gamma \) is even larger, so it is more convenient to use \( A_\gamma \) instead of \( P \), as ‘large parameter’.

We shall replace the exact, transcendental equation equation (33) with an approximate, algebraic equation, using one of the formulas proposed in [10] for \( \cos x \):
Reference [10] gives two values for $c$, namely

$$c = 1 - \frac{8}{\pi^2} = 0.18943 \text{ or } 0.2120126. \quad (35)$$

The relative errors of the algebraic approximation of $\cos$ are plotted in figure 2. For $0 < x \leq 0.7$, the both approximations are excellent, with relative errors of about $10^{-3}$, but for $0.7 < x \leq \pi/2$, the second one is better; even in this case, the error increases until about 3.7% for $x \leq \pi / 2$. So, the value $c = 0.2120126$ seems to be more appropriate. In the same time, larger values of $c$, for instance $c = 0.22$ or $c = 0.23$, give better precision at larger values of $x$. We shall keep the value of $c$ undefined in our formulas for the roots; eventually, it can be adapted according to the value of the specific root. The advantage of using a very precise value of $c$ is not really obvious.

So, we get for the algebraic approximation of the eigenvalue equation:

$$\frac{1}{\Phi_0} \left( 1 - \frac{(2\Phi_0)}{\pi} \right)^2 = \frac{1}{\sqrt{\pi} \sqrt{A_z^2 - \Phi_0^2}}. \quad (36)$$

With

$$\Phi_0^2 = z \quad (37)$$

it can be written as:

$$z^3 + \left( \frac{1}{16} \pi^4 g_s A_z^2 - A_z^2 - \frac{1}{2} \pi^2 \right) z^2 + \frac{\pi^2}{2} \left( \frac{\pi^2}{8} g_s A_z^2 + \frac{1}{8} \pi^2 \right) z - \frac{1}{16} \pi^4 A_z^2 = 0. \quad (38)$$
Following the approach outlined in the appendix, let us put:

\[ a_{2>} = \left( \frac{1}{16} \pi^4 c g_\geq - A^2_\geq - \frac{1}{2} \pi^2 \right), \]  
\[ a_{1>} = \frac{\pi^2}{2} \left( \frac{\pi^2}{8} g_\geq + A^2_\geq + \frac{1}{8} \pi^2 \right), \]  
\[ a_{0>} = \left( - \frac{1}{16} \pi^4 A^2_\geq \right), \]  
\[ p_{1>} = -\frac{1}{3} (A^4_\geq + P_1 A^2_\geq + P_{0>}), \]  

where \( P_1 > \) is a linear, and \( P_{0>} \) a quadratic polynomial in \( g_\geq \). 

In the last equation, the index \( c \) in \( p_{c>} \) is for cos, suggesting the even symmetry of this state.

If the well is not too shallow, \( A_\geq > 1 \) and it is convenient to define the ‘small’ parameter \( \alpha_\geq > \):

\[ \alpha_\geq = \frac{1}{A_\geq}, \]  

so we can write:

\[ p_{c>} = -\frac{A^4_\geq}{3} (1 + P_1 \alpha^2_\geq + P_{0>} \alpha^2_\geq). \]

Similarly, defining \( Q_{K>} \) through the formula:

\[ q_{c>} = \frac{2}{27} A^6_\geq Q_{K>}, \]  
\[ = \frac{2}{27} A^6_\geq (1 + Q_{2>} \alpha^2_\geq + Q_{1>} \alpha^4_\geq + Q_{0>} \alpha^6_\geq), \]

where:

\[ Q_{2>} = -\frac{3\pi^4}{4} \left( 1 + \frac{1}{4} \pi^2 c g_\geq \right), \]  
\[ Q_{1>} = \frac{3^2 \pi^4}{2^4} \left[ \frac{\pi^4}{2^4 \cdot 3} g^2_\geq = \frac{\pi^2}{2 \cdot 3} c + \frac{1}{3} \right], \]  
\[ Q_{0>} = -\frac{\pi^6}{2^6} \left[ \frac{\pi^6}{2^6} c^3 g^3_\geq - \frac{3^2 \pi^2 c}{2^3} \left( \frac{\pi^2 c}{3} + 1 \right) g^2_\geq + \frac{3^2 \left( 5 \pi^2 c}{2^3 \cdot 3} + 1 \right) g_\geq c + \frac{1}{3} \right], \]

we obtain the following expression for \( K_{c>} \):

\[ K_{c>} = \frac{Q_{K>}}{|P_{K>}|^{1/2}}, \]  
\[ = \frac{1 + Q_{2>} \alpha^2_\geq + Q_{1>} \alpha^4_\geq + Q_{0>} \alpha^6_\geq}{|1 + P_1 \alpha^2_\geq + P_{0>} \alpha^2_\geq|^{1/2}}. \]
In fact, the index $K$ in $Q_K$ was chosen because $Q_K$ is the part of $q_\alpha$ which enters effectively in the simplest form of $K_\alpha$. For deep wells, $\alpha_\alpha \to 0$; consequently $P_\alpha \to 0$ and:

$$K_\alpha = \frac{1 + Q_{2\alpha_\alpha}^2 + Q_{4\alpha_\alpha}^4 + Q_{6\alpha_\alpha}^6}{(1 + P_{1\alpha_\alpha}^2 + P_{0\alpha_\alpha}^4)^{3/2}}.$$  

(50)

It is fortunate, for the precision and simplicity of our formulas, that the quadratic and quartic terms of its series expansion in $\alpha_\alpha$ are zero, and

$$K_\alpha = 1 - \frac{3\pi^6}{2^7}g_\alpha\left(1 + \frac{\pi^2}{4}\right)\alpha_\alpha^6 + \cdots.$$  

(51)

The equation has three real roots; we shall choose the root which is compatible with the condition $0 < \Phi < \pi/2$, or $z < \pi^2/4$. Putting:

$$K_\alpha = 1 - Z_\alpha, Z_\alpha \ll 1$$  

(52)

we find easily:

$$y_1 = \sin\left(\frac{1}{3}\arcsin(1 - Z) - \frac{\pi}{3}\right) = -\frac{1}{2} - \frac{\sqrt{Z}}{3} + \cdots,$$  

(53)

$$y_2 = \sin\left(\frac{1}{3}\arcsin(1 - Z) + \frac{\pi}{3}\right) = 1 - \frac{Z}{9} + \cdots,$$  

(54)

$$y_3 = -\sin\left(\frac{1}{3}\arcsin(1 - Z)\right) = -\frac{1}{2} + \frac{\sqrt{Z}}{6} + \cdots.$$  

(55)

Finally, using the formula equation (A.18):

$$z_1 = \sqrt{\frac{4|\alpha_\alpha|^3}{3}}y_1 - \frac{1}{3}a_{2\alpha_\alpha}$$  

(56)

and introducing the notation:

$$C = \frac{\pi^2}{2c}$$  

(57)

we get (later on we shall drop the index 1 of $z_1$):

$$z(\beta > 1) = \frac{\pi^2}{4} - \frac{\pi^3}{8}\sqrt{1 + \frac{\alpha_\alpha^2}{2\sqrt{g_\alpha}}} + \frac{\pi^4}{32}(1 + C)(\sqrt{g_\alpha} \alpha_\alpha^4)^2$$

$$+ \frac{\pi^5}{32}(1 + C \sqrt{g_\alpha} \alpha_\alpha^4)\sqrt{1 + \frac{\alpha_\alpha^2}{2\sqrt{g_\alpha}}} + \frac{\pi^6}{128}g_\alpha(1 + C)(\frac{1}{2} + C \sqrt{g_\alpha} \alpha_\alpha^4)^2 + \cdots.$$  

(58)

If the depth of the well increases indefinitely, $\alpha_\alpha \to 0$ and $z_1 \to \pi^2/4$, $\Phi_0 \to \pi/2$, as requested. Indeed, in a finite well, the energy of a bound state is smaller than the corresponding energy in an infinite one, so the first term in $\sqrt{g_\alpha} \alpha_\alpha^4$ in the previous formula is negative.
It is useful to write (58) in terms of more physical parameters, \( p \) and \( \beta \). In order to do this, let us notice that:

\[
g_{\gamma} \alpha^2 = \frac{p^2}{\beta}, \quad \alpha^2 = \frac{\beta - 1}{\beta} p^2 \tag{59}
\]

so equation (58) takes the form:

\[
z(\beta > 1) = -\frac{\pi^2}{4} - \frac{\pi^3}{8} \sqrt{1 + \frac{C}{2} \frac{p}{\beta^{3/2}}} + \frac{\pi^4}{32} (1 + C) \frac{p^2}{\beta} \\
+ \frac{\pi^5}{32} \sqrt{1 + \frac{C}{2}} (\beta + \frac{C}{2} - 1) \frac{p^3}{\beta^{3/2}} + \frac{\pi^6}{128} (1 + C) \left( \beta + \frac{C}{2} - 1 \right) \frac{p^4}{\beta^2} + \ldots
\tag{60}
\]

and:

\[
z(\beta = 1) = -\frac{\pi^2}{4} - \frac{\pi^3}{8} \sqrt{1 + \frac{C}{2} p} + \frac{\pi^4}{32} (1 + C) p^2 \\
+ \frac{\pi^5}{32} \sqrt{1 + \frac{C}{2} \frac{p^3}{2}} + \frac{\pi^6}{128} \frac{C}{2} (1 + C) p^4 + \ldots
\tag{61}
\]

It is a simple exercise to check that the previous formula coincides with the first three terms of the power series given by equation (17) of [10].

For the other two roots given by equation (A.18), \( z_2, z_3 \) the ‘large’ parameter \( A_\beta \) does not disappear, so the condition \( z^2 < \pi^2/4 \) cannot be fulfilled.

If the parameter \( \alpha_\gamma \), cannot be considered ‘small’, the formulas (42) and (49), used according to the algorithm given in the appendix, will give the root of the cubic equation (38).

3.1.2. The case \( \beta < 1 \). If \( \beta < 1 \), the eigenvalue equation for the dimensionless wave vector is:

\[
\cos \Phi_0 = \frac{1}{\sqrt{\gamma_\zeta} \sqrt{A_\zeta^2 + \Phi_0^2}} , \quad 0 < \Phi_0 < \frac{\pi}{2}
\tag{62}
\]

with the following definitions for the parameters:

\[
\gamma_\zeta = 1 - \beta, \quad \frac{1}{\gamma_\zeta} = g_{\zeta}, A_\zeta^2 = \frac{P^2}{1 - \beta} = P^2 \gamma_\zeta.
\tag{63}
\]

Using the dABG algebraization for \( \cos \Phi_0 \), we get the algebraic equation:

\[
\frac{1}{\Phi_0} \left( 1 - \frac{2 \Phi_0}{\pi} \right)^2 = \frac{1}{\sqrt{\gamma_\zeta} \sqrt{A_\zeta^2 + \Phi_0^2}}
\tag{64}
\]
It becomes, with

$$\Phi_0^2 = z$$

(65)

a cubic equation:

$$z^3 + \left(A_\zeta^2 - \frac{1}{2} \pi^2 - \frac{1}{16} \pi^4 g_\zeta\right) z^2 + \frac{\pi^2}{2} \left(\frac{1}{8} \pi^2 - A_\zeta^2 - \frac{\pi^2}{8} \zeta g_\zeta\right)$$

$$\times z + \frac{1}{16} \pi^4 A_\zeta^2 = 0, \quad \beta < 1.$$

(66)

Similar to the case $\beta > 1$, let us put:

$$a_{2<}(A_\zeta^2, g_\zeta) = A_\zeta^2 - \frac{1}{2} \pi^2 - \frac{1}{16} \pi^4 g_\zeta,$$  

(67)

$$a_{1<}(A_\zeta^2, g_\zeta) = \frac{\pi^2}{2} \left(\frac{1}{8} \pi^2 - A_\zeta^2 - \frac{\pi^2}{8} g_\zeta\right),$$  

(68)

$$a_{0<}(A_\zeta^2, g_\zeta) = \frac{1}{16} \pi^4 A_\zeta^2.$$  

(69)

Let us notice that:

$$a_{2<}(A_\zeta^2, g_\zeta) = a_{2>}(A_\zeta^2 \rightarrow -A_\zeta^2, g_\zeta \rightarrow g_\zeta)$$

$$a_{1<}(A_\zeta^2, g_\zeta) = a_{1>}(A_\zeta^2 \rightarrow -A_\zeta^2, g_\zeta \rightarrow g_\zeta)$$  

$$a_{0<}(A_\zeta^2) = a_{0>}(A_\zeta^2 \rightarrow -A_\zeta^2).$$  

(70)

As in equation (58), the parameters $g_\zeta, \alpha_\zeta$ enter only through the monoms $g_\zeta A_\zeta^2$ and $\alpha_\zeta^2$ at various powers. The roots of equation (66) can be obtained from equation (58) making the following substitutions:

$$g_\zeta \rightarrow g_\zeta, \quad \alpha_\zeta^2 \rightarrow -\alpha_\zeta^2.$$  

(71)

The result is:

$$z(\beta < 1) = \frac{\pi^2}{4} - \frac{1}{8} \pi^3 \sqrt{g_\zeta \left(1 + \frac{C}{2}\right)} \alpha_\zeta + \frac{1}{32} \pi^4 g_\zeta (1 + C) \alpha_\zeta^2$$

$$+ \frac{\pi^5}{32} \left(1 - \frac{C g_\zeta}{2}\right) \sqrt{g_\zeta \left(1 + \frac{C}{2}\right)} \alpha_\zeta^3 - \frac{\pi^6}{128} g_\zeta (1 + C) \left(1 - \frac{C}{2} g_\zeta\right) \alpha_\zeta^4 + \cdots.$$  

(72)

In order to write the previous equation in terms of $p$ and $\beta$, let us notice, similarly to the previous case, that

$$\sqrt{g_\zeta} \alpha_\zeta = \frac{p}{\sqrt{\beta}}, \quad \alpha_\zeta^2 = p^2 \frac{1 - \beta}{\beta}.$$  

(73)
Replacing these monoms in (70), we obtain an equation having exactly the form (72)

\[ z(p, \beta < 1) = \frac{\pi^2}{4} - \frac{\pi^3}{8} \sqrt{\frac{C + 1}{2}} + 1 \cdot \frac{p^2}{\beta} \]

\[ - \frac{\pi^5}{32} \sqrt{\frac{C + 1}{2}} \left( \beta + \frac{C}{2} - 1 \right) \frac{p^3}{\beta^{3/2}} \]

\[ + \frac{\pi^6}{128} (C + 1) \left( \beta + \frac{C}{2} - 1 \right) \frac{p^4}{\beta^2} + \cdots \]  

(74)

3.2. The case of a shallow well

It is well-known that, for \( \beta = 1 \), any square well, even a very shallow one, has at least one bound state; if the well keeps only one state, this state is an even one. We shall see that this property remains valid if \( \beta \neq 1 \).

A shallow well corresponds to small values of \( P \) and large values of \( p \). In this case, replacing in the eigenvalue equation the zero order approximation for \( \cos \Phi_0 \), i.e. \( \cos \Phi_0 \approx 1 \), one obtains

\[ \frac{1}{\Phi_0^2} = \frac{p^2}{\beta + (1 - \beta)p^2\Phi_0^2}. \]  

(75)

Its solution is independent of \( \beta \):

\[ \Phi_0 = \frac{1}{p} = P. \]  

(76)

The relative error of this solution is about \(-10^{-2}\) for \( P = 0.1 \) and becomes about \(-3.7 \times 10^{-2}\) for \( P = 0.2 \).

A more precise expression for the root can be obtained using the parabolic approximation, i.e. \( \cos \Phi_0 \approx 1 - \frac{\Phi_0^2}{2} \), gives:

\[ \frac{\cos^2 \Phi_0}{\Phi_0^2} = \frac{(1 - \Phi_0^2/2)^2}{\Phi_0^2} = \frac{p^2}{\beta + (1 - \beta)p^2\Phi_0^2}. \]  

(77)

Putting:

\[ \Phi_0^2 = z, \quad 1 - \beta = \frac{1}{\gamma}, \quad \beta \gamma = \delta = \frac{\beta}{1 - \beta} \]  

(78)

the equation can be written as:

\[ z^3 + (\delta p^2 - 4)z^2 - 4\delta (1 + p^2)z + 4\delta p^2 = 0. \]  

(79)

We get:

\[ p_1 = -\frac{16}{3} \left( 1 + \frac{3}{4} \beta \gamma + \frac{1}{4} p^2 \beta \gamma + \frac{1}{16} (p^2 \beta \gamma)^2 \right). \]  

(80)

\[ q_c = \frac{128}{27} \left( 1 + \frac{9}{32} \beta \gamma - \frac{15}{32} p^2 \beta \gamma - \frac{9}{32} (\beta \gamma)^2 \right), \quad \frac{1}{64} (p^2 \beta \gamma)^2 \right), \]  

(81)
As $P \ll 1$, $K$ is well approximated by:

$$K = \frac{1 + \frac{9}{4}\beta\gamma - \frac{15}{32}P^2\beta\gamma - \frac{9}{32}(\beta\gamma P)^2 - \frac{3}{32}(P^2\beta\gamma)^2 - \frac{1}{64}(P^2\beta\gamma)^3}{\sqrt{1 + \frac{3}{4}\beta\gamma + \frac{1}{4}P^2\beta\gamma + \frac{1}{16}(P^2\beta\gamma)^2}^{1/2}}.$$  

(82)

As $P \ll 1$, $K$ is well approximated by:

$$K = \sqrt{d} \left(1 + \frac{9}{4}\beta\gamma\right) + \frac{3}{32}\beta\gamma(4 - 5\sqrt{d} + 9\beta\gamma)P^2 + \cdots,$$  

(83)

where we used the notation:

$$d = \sqrt{\frac{3}{4}\beta\gamma + 1}$$  

(84)

and presumed that the physically reasonable condition:

$$\frac{3}{4}\beta\gamma + 1 > 0.$$  

(85)

The roots can be easily obtained, using the same method used in the previous subsections. If the condition (85) is not satisfied, and $p(P = 0) > 0$, the expression under modulus in equation (82) changes its sign and a similar series expansion for $K$ can be obtained.

3.3. The first odd state

3.3.1. The case $\beta > 1$. The exact eigenvalue equation for the first odd state—which is also the first excited state—can be written as:

$$\sin \Phi_1 \Phi_1 = \frac{1}{\sqrt{\gamma} \sqrt{\lambda^2 - \Phi_1^2}} \frac{\pi}{2} < \Phi_1 < \pi.$$  

(86)

As the shape of the function $\sin \Phi_1 \Phi_1$ on the interval $[0, \pi]$ is quite similar with the shape of $\cos \Phi_1$ on the interval $[0, \pi/2]$, we can try an algebraization for $\sin \Phi_1 \Phi_1$ similar to that proposed by de Alcantara Bonfim and Griffiths [10] for $\cos \Phi_1$.
\[
\frac{\sin \Phi_1}{\Phi_1} \approx 1 - \left(\frac{\Phi_1}{\pi}\right)^2 \frac{1}{\sqrt{1 + a\Phi_1^2}}.
\]  
(87)

Plotting the function
\[
F(a; x) = \frac{\sin x \sqrt{1 + ax^2}}{x(1 - (x/a)^2)} - 1
\]  
(88)

for several values of \(a\), we can see that the error of this approximation is of the order \(10^{-2}\) and varies quite strongly (for the same value of \(a\)) if \(x\) moves on the interval \([0, \pi]\); so, fixing \(a\) to a very precise value seems a procedure of questionable usefulness. Let us mention again that the physically interesting root of equation (87) belongs to the interval \((\pi/2, \pi)\). More precise could be an iterative process, namely obtaining a root \(x(a)\) for a fixed \(a\) and repeating the calculation of this root using a new value, \(a_0\), given by graphical inspection of the condition \(F(a_0; x(a)) = 0\) in figure 3. In our numerical verifications, we chose the value \(a = 0.2\).

So, replacing equation (87) in the lhs of the equation (86), and putting:
\[
\Phi_1^2 = z
\]  
(89)

we obtain a cubic equation:
\[
z^3 - (A_2^2 + 2\pi^2)z^2 + \pi^2(2A_2^2 + \pi^2 + \pi^2ag)z + \pi^4(g - A_2^2) = 0.
\]  
(90)

Let us define:
\[
a_2 > = -(A_2^2 + 2\pi^2),
\]  
(91)
\[
a_1 > = \pi^2(2A_2^2 + \pi^2 + \pi^2ag),
\]  
(92)
\[
a_0 > = \pi^4(g - A_2^2).
\]  
(93)

In order to avoid too complicated notations, we used in equations (91)–(93) the same symbol as in equations (39)–(41) in the spirit of the definition (A.1) in the appendix; we hope that this ambiguity will not produce any confusions. Following exactly the same steps as for even states, we find (the index \(s\) is for sin, suggesting an odd state):
\[
p_s > = -\frac{1}{3}A_2^{s2}(1 - 2\pi^2\alpha_s^2 - \pi^4(3ag_s - 1)\alpha_s^4),
\]  
(94)
\[
g_s > = \frac{2}{27}A_2^6\left[1 - 3\pi^2\alpha_s^2 + 3\pi^4\left(1 - \frac{3}{2}ag_s\right)\alpha_s^4 - \pi^4\left(\frac{27}{2}g_s + \pi^2 + 9\pi^2ag_s\right)\alpha_s^6\right],
\]  
(95)
\[
K_s > = \frac{(1 - 3\pi^2\alpha_s^2 + 3\pi^4\left(1 - \frac{3}{2}ag_s\right)\alpha_s^4 - \pi^4\left(\frac{27}{2}g_s + \pi^2 + 9\pi^2ag_s\right)\alpha_s^6)}{|1 - 2\pi^2\alpha_s^2 - \pi^4(3ag_s - 1)\alpha_s^4|^{1/2}}.
\]  
(96)

If
\[
A_s > = P\sqrt{\frac{\beta}{\beta - 1}} > 1 \Leftrightarrow P > \sqrt{\frac{\beta - 1}{\beta}}
\]  
(97)
the power expansion for $K_\alpha$ is:

$$K_\alpha = 1 - \frac{27}{2} \pi^4 g_\alpha (\pi^2 a + 1) \alpha^6_\alpha + O(\alpha^8_\alpha)$$

(98)

and the physically convenient root has the form:

$$z(\beta > 1) = \pi^2 - \pi^2 \sqrt{g_\alpha (1 + \pi^2 a)} \alpha_\alpha + \frac{\pi^4}{2} a g_\alpha \alpha^2_\alpha + \pi^4 \sqrt{g_\alpha (1 + \pi^2 a)} \alpha^3_\alpha + \frac{\pi^6}{2} a g_\alpha \alpha^4_\alpha + \ldots.$$  

(99)

In terms of $p$ and $\beta$:

$$z(\beta > 1) = \pi^2 - \pi^2 \sqrt{1 + \pi^2 a} \frac{p}{\sqrt{\beta}} + \frac{\pi^4}{2} a \frac{p^2}{\beta} + \pi^4 \sqrt{1 + \pi^2 a} (\beta - 1) \left( \frac{p}{\sqrt{\beta}} \right)^3 + \frac{\pi^6}{2} a (\beta - 1) \frac{p^4}{\beta^2} + \ldots.$$  

(100)

3.3.2. The case $\beta < 1$. The exact eigenvalue equation for the first odd state, if $\beta < 1$, can be written as:

$$\sin \Phi_1 = \frac{1}{\sqrt{A^2_\zeta + \Phi_1^2}}, \ 0 < \Phi_1 < \pi.$$

(101)

With the algebraic approximation for $\sin \Phi_1/\Phi_1$, equation (87), it gives the following cubic equation in $z = \Phi_1^2$:

$$z^3 + (A^2_\zeta - 2\pi^2)z^2 + (-2\pi^2 A^2_\zeta + \pi^4 - \pi^4 a g_\alpha)z + \pi^4 A^2_\zeta - \pi^4 g_\alpha = 0.$$  

(102)

Following the same steps as before, we find:

$$z(\beta < 1) = \pi^2 - \pi^2 \sqrt{g_\alpha (1 + \pi^2 a)} \alpha_\alpha + \frac{\pi^4}{2} a g_\alpha \alpha^2_\alpha - \pi^4 \sqrt{g_\alpha (1 + \pi^2 a)} \alpha^3_\alpha - \frac{\pi^6}{2} a g_\alpha \alpha^4_\alpha + \ldots.$$  

(103)

For both cases—$\beta \leq 1$—in the limit of an infinitely deep well, $z(\beta \leq 1, \alpha_c = 0) = \pi^2$, $\Phi_1(\beta \leq 1, \alpha_c = 0) = \pi$, as requested, and the first correction to this value is negative. The expression of the root in terms of $p$ and $\beta$ is identical with (100).

The relative errors of the formulas (60), (74), (99), with respect to the exact roots of the corresponding algebraic equations, are very small—of about $10^{-4}$ to $10^{-6}$ for physically interesting values of the parameters $p$, $\beta$, $a$, $c$. The order of magnitude of the errors introduced by the algebraization of transcendental equations of the eigenvalues can be visualized in figures 2 and 3. In other words, the main contribution to the errors of our results is given by the approximation of trigonometric functions with algebraic ones, not by the approximation of the exact formulas of the roots of cubic equations with the low order terms of their series expansions. As already mentioned, one of the physical motivations of the calculation of the energy of bound states in heterostructures is to explain their
photoluminescence properties. In several cases (see for instance [20]), the authors use Barker’s formula for the energy levels in a square well [19]. Much more precise analytical expressions for these energy are available in the literature [10, 11], for the case of constant mass; in this paper, we propose similar formulas, considering the case of PDM.

3.4. Higher order states

In the previous subsections, we analysed the ground state \( (n=0) \) and the first excited state \( (n=1) \) of a square well, with BenDaniel–Duke boundary conditions. For \( n \geq 2 \), the de Alcantara-Bonfim formula (34) can be extended to larger arguments:

\[
\cos \Phi \approx \frac{1 - 4(\Phi - 2n\pi)^2/\pi^2}{\sqrt{1 + c(\Phi - 2n\pi)^2}}, \quad 2n\pi < \Phi < 2n\pi + \frac{\pi}{2}
\]

but the eigenvalue equation, obtained in this way, is a sextic equation (which cannot be reduced to a cubic equation in \( \Phi^2 \)), so cannot be solved. We meet similar difficulties if we try to use the eigenvalue equation in terms of the tan function, replaced by the approximate expression [11]:

\[
\text{Figure 4.} \text{ The plot of } \Phi_0^2 \text{ (a) and } \Phi_1^2 \text{ (b), which are proportional to the energies } E_0, E_1, \text{ as functions of the inverse potential strength } p.
\]
\[ \tan \Phi \simeq \frac{0.45\Phi (\Phi - n\pi)}{2\Phi (2n - 1)\pi}, \quad n\pi < \Phi < n\pi + \frac{\pi}{2}. \]  

(105)

Even the ‘parabolic approximation’ for \((\cos \Phi/\Phi)^2\) or \((\sin \Phi/\Phi)^2\), in the sense used in [16], gives a quartic equation for the dimensionless wave vector. Even if a quartic equation can be reduced to a cubic and a quadratic equation, the results are quite complicated. So the only practically acceptable approximations are the series expansions of the previous ‘algebraizations’ of \(\cos \Phi\), \(\tan \Phi\), in terms of \(\Phi/2n\pi \sim 1/4n\), \(n \geq 2\). So, the errors of such approximation, which keeps only the first order term, will be about \((1/4n)^2\), \(n \gg 2\).

3.5. Graphical illustration of our main results

In order to illustrate graphically some of our results, let us notice that, using equations (16)–(21), we can write the following relation for the energy:

\[ \frac{m_i L^2}{2\hbar^2} E_n = \Phi_n^2 = z_n(p). \]

(106)

where \(z_n\) is the root of the cubic equations obtained after the algebraization of the transcendental eigenvalue equations for the ground state \((n = 0)\) and for the first excited state \((n = 1)\). According to the equations (74) and (100), for a deep well, the root \(z\) (for simplicity, we dropped the index of \(z\)) can be approximated with a quartic potential in \(p\), the inverse of the potential strength \(P\). Let us mention that, if we replace in the definition of \(P\), equation (16), \(m_i\) with the free electron mass, we choose the length of the well \(L = 10\) nm and we express the potential \(V_0\) in electronvolts, we get:

\[ P = 25.616\sqrt{V_0}, \quad p = 3.903 \times 10^{-2} \frac{1}{\sqrt{V_0}}. \]

(107)

Consequently, in this example, the well can be considered as ‘deep’, and the energy, given by (106), is actually a function of the depth of the well, \(V_0\).

We shall plot our main results, i.e. the series expansions of the dimensionless wave vectors, \(\Phi_0^2\) and \(\Phi_1^2\), as functions of \(p\), on the range \(0 < p < 0.1\), when the conditions of convergence are satisfactorily fulfilled (figure 4). The energy is a monotonically increasing function of \(\beta\); its values, for \(\beta = 1\), are obtained from equations (29) and (30); they are approximated with algebraic equations using the formulas (34) and (87).

4. Discussion: applications to other nanostructures

Our calculations can be easily applied to type II heterointerfaces, when one of the effective mass of the charge carrier is negative: \(m_{in} m_{out} < 0\) ([6], chapter 3, equations (35) and (36)); a detailed description of such heterointerfaces can be found for instance in [6], p 66. So, instead of (23) and (24), the eigenvalue equations take the form:

\[ \tan \frac{k_{in,2nL}}{2} = -\frac{m_i}{|m_i|} \frac{k_{out,2n}}{k_{in,2n}}, \quad \text{even states}, \]

(108)

\[ \tan \frac{k_{in,2n+1L}}{2} = \frac{|m_i|}{m_i} \frac{k_{out,2n+1}}{k_{in,2n+1}} = \frac{1}{|\beta|} \frac{k_{out,2n+1}}{k_{in,2n+1}}, \quad \text{odd states} \]

(109)

and can be solved following exactly the same approach.
As already mentioned, the wave function in the Schrödinger equation (3) can be interpreted as an envelope function. This approximation works well when the materials constituting the heterostructures are perfectly lattice-matched and they crystallise in the same crystallographic structure (in most cases, the zinc blende structure). Its application is restricted to the vicinity of the high-symmetry points in the host’s Brillouin zone (Γ, X, L). Actually, most of the heterostructures’ energy levels relevant to actual devices are relatively close to a high symmetry point in the host’s Brillouin zone. A popular example is given by the lowest conduction states of GaAs–GaAlAs heterostructures with GaAs layer thickness is about 100Å or larger. A detailed description of the cases in which the envelope function model is successful is given in [6], p 68.

As there are some similarities between QWs and QDs, our results are also relevant for these devices. The simplest remark is that the eigenvalues equation for the first odd state in a QD is identical to that corresponding to the l = 0 state in a QD (see for instance [14], pr. 63). Also, the eigenvalue equations for the wave vectors of bound energy levels of a finite barrier rectangular shaped QD, equation (36) in [17], are quite similar to ours—(27) and (28), but somewhat more complicated. The ground state energy of electrons and holes in a core/shell QD is given by equation (21) of [18], an equation similar to ours, just mentioned previously. Such results are important, inter alia, for the interpretation of photoluminescence spectra and photon harvesting of QDs.

5. Conclusions

In this paper, we solved a simple problem: the Schrödinger equation for a square potential, with BenDaniel–Duke boundary conditions, paying special attention to approximate analytical expressions of energy eigenvalues. All the results are obtained with mathematics accessible to an undergraduate student. This simple exercise can facilitate student’s understanding of more complex and profound issues, like PDM, envelope function or types I and II semiconductor heterojunctions. Also, it valorizes the simplest way of solving the cubic equation, a subject usually avoided at undergraduate level. Our approach can be extended to QDs of various architectures and can be used for explanation of photoabsorbtion spectra and photon harvesting.

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Appendix. The real roots of a cubic equation

We shall outline here some basic aspects concerning the cubic equation [21]. Although it was solved more than five centuries ago—in circa 1500 by Scipione del Ferro, the most convenient form of the solutions, obtained using hypergeometric functions, became popular quite late [22]. Our intention is to give here a short and practical guide for obtaining the real roots of a cubic equation.

Let us consider its general form:

\[ z^3 + a_2z^2 + a_1z + a_0 = 0. \]  

(A.1)
With a change of variable:
\[
z = x - \frac{1}{3}a_2
\]  
(A.2)

it can be put in the ‘depressed form’:
\[
x^3 + p_c x = q_c,
\]  
(A.3)

where:
\[
p_c = \frac{3a_1 - a_3^2}{3}, \quad q_c = \frac{9a_1a_2 - 27a_0 - 2a_3^3}{27}.
\]  
(A.4)

The standard notations for these quantities is \(p, q\). In order to avoid the confusion with the inverse of the potential strength, \(p\), we used the symbol \(p_c\) (the index \(c\) is for ‘cubic’).

With a scale transformation:
\[
x = \sqrt[3]{\frac{4|p_c|}{3}} y
\]  
(A.5)

the depressed equation (A.3) can be written in a form appropriate for comparison with triple-angle formulae for trigonometric or hyperbolic functions:
\[
4y^3 + 3\sigma_p y = K,
\]  
(A.6)

where
\[
K = \frac{1}{2} q_c \left( \frac{3}{|p_c|} \right)^{3/2}
\]  
(A.7)

and \(\sigma_p\) is the signum function:
\[
\sigma_{p<0} = -1, \quad \sigma_{p>0} = +1.
\]  
(A.8)

If \(p_c > 0\), the equation:
\[
4y^3 + 3y = K
\]  
(A.9)

has one real root:
\[
y = \sinh \left( \frac{1}{3} \sinh^{-1} K \right).
\]  
(A.10)

If \(p_c < 0\) and \(|K| \geq 1\), the equation
\[
4y^3 - 3y = K, \quad |K| \geq 1
\]  
(A.11)

has only one real root:
\[
y(K \geq 1) = \cosh \left( \frac{1}{3} \cosh^{-1} K \right)
\]  
(A.12)

or
\[
y(K \leq -1) = -\cosh \left( \frac{1}{3} \cosh^{-1} |K| \right).
\]  
(A.13)

If \(p_c < 0\) and \(|K| \leq 1\), the equation
\[
4y^3 - 3y = K, \quad |K| \leq 1
\]  
(A.14)
has three real roots:

\[ y_1 = \sin \left( \frac{1}{3} \arcsin K - \frac{\pi}{3} \right) \] \hspace{1cm} (A.15)

\[ y_2 = \sin \left( \frac{1}{3} \arcsin K + \frac{\pi}{3} \right) \] \hspace{1cm} (A.16)

\[ y_3 = -\sin \left( \frac{1}{3} \arcsin K \right) \] \hspace{1cm} (A.17)

Finally, the roots of the general equation (A.1) are:

\[ z = x - \frac{1}{3} a_2 = \sqrt[3]{\frac{4|p_1|}{3}} y - \frac{1}{3} a_2. \] \hspace{1cm} (A.18)

So, the algorithm to be followed in order to solve the cubic equation is the following:

(1) we calculate \( p_1 \), \( q_1 \) and determine their sign;

(2a) if \( p_1 > 0 \), the equation (A.9) has only one real root, equation (A.10);

(2b) if \( p_1 < 0 \), we check if \( |K| \) is \( \leq 1 \);

(2b.1) if \( |K| > 1 \), the equation (A.1) has only one real root, given by equation (A.12) or equation (A.13), according to the sign of \( K \);

(2b.2) if \( |K| < 1 \), the equation (A.1) has three real roots, given by equations (A.15)–(A.17).

Using elementary trigonometric identities, the equations (A.15)–(A.17) can be put in the more elegant form:

\[ t_k = \cos \left( \frac{1}{3} \arccos K - \frac{2\pi k}{3} \right). \] \hspace{1cm} (A.19)

It is easy to check that:

\[ t_0 = y_2, \ t_1 = y_3, \ t_2 = y_1. \] \hspace{1cm} (A.20)

The case of multiple roots will be discussed separately. If we make Viete’s substitution:

\[ x = w - \frac{R}{3w} \] \hspace{1cm} (A.21)

in the depressed equation, we get a quadratic equation in \( w^3 \):

\[ (w^3)^2 - q_1 w^3 - \frac{1}{27}p_1^3 = 0 \] \hspace{1cm} (A.22)

with the roots:

\[ w^3 = \frac{1}{2} q_1 \pm \sqrt[3]{-\frac{1}{4} q_1^2 + \frac{1}{27} p_1^3} = R \pm \sqrt{R^2 + Q^3}. \] \hspace{1cm} (A.23)

The existence of a multiple root corresponds to the condition:

\[ \frac{1}{4} q_1^2 = -\frac{1}{27} p_1^3 \] \hspace{1cm} (A.24)

this means that:

\[ p_1 < 0, \ K^2 = 1. \] \hspace{1cm} (A.25)

The value of the multiple (double) root is obtained putting \( w^3 = (q_1/2)^{1/3} \) in Viete’s substitution equation (A.21).
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