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Semiconductor Quantum Wells with BenDaniel-Duke Boundary Conditions and Janus Nanorods

Victor Barsan

Additional information is available at the end of the chapter

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Abstract

The energy levels of bound states of an electron in a quantum well with BenDaniel-Duke boundary condition are studied. Analytic, explicit, simple, and accurate formulae have been obtained for the ground state and the first excited state. In our approach, the exact, transcendental eigenvalues equations were replaced with approximate, tractable, algebraic equations, using algebraic approximations for some trigonometric functions. Our method can be applied to both type I and type II semiconductors and easily extended to quantum dots. The same approach was used for the semi-quantitative analyze of two toy models of Janus nanorods.

Keywords: type I and type II semiconductors, BenDaniel-Duke boundary conditions, Janus nanorods, toy models

1. Introduction

In the last three decades, nanophysics became a domain of increasing interest and intense research, due to the huge number of new effects produced at nanoscale level, in quantum wells (QWs), quantum dots (QDs), Janus nanoparticles, etc. These new effects are fascinating from the perspective of both applied and theoretical physics. The semiconductors provide the largest area of challenging subjects, due to their applications in nanoelectronic devices, multifunctional catalysis, (bio-)chemical sensors, data storage, solar energy conversion, etc.

An attractive aspect of nanophysics is the fact that a quite large number of interesting problems can be approached using quite simple theoretical tools, sometimes at the level of one-particle quantum mechanics. In some cases, the properties of nanostructures like quantum

wells, quantum dots, or quantum rods can be explained by just solving the Schrodinger equation with simple potentials. For instance, the basic physical properties of a heterostructure consisting of a thin layer of a semiconductor A sandwiched between two somewhat larger semiconductors of identical composition, B can be obtained from the study of the movement of a particle with position-dependent mass (PDM) in a finite square well. This particle is, of course, a charge carrier in the semiconductor, and—in our case—will be an electron. 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.

But, simple as the theoretical tools needed for its investigation are, this problem of quantum mechanics involves two important issues: the position-dependent mass (PDM) quantum physics and semiconductor heterostructures. Let us shortly comment on these points.

The roots of the position-dependent effective mass concept are to be found in the pioneering works of Wannier (1937) and Slater (1949) (see Ref. 1 in [1]). 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 [2–4].

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 [5, 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 [5]. 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." ([5], 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 [7]), 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. When a transcendental equation mixes algebraic and trigonometric functions, it might be

possible to approximate the trigonometric functions with algebraic expression, and to transform, in this way, the exact transcendental equation into an approximate algebraic one. In its simplest form, for instance, in approximations like $\sin x \simeq x$, for $x \ll 1$, this “algebraization” is largely used. But what is really interesting is to use algebraic approximations of the trigonometric functions valid on their whole domain of definition, as de Alcantara Bonfin and Griffiths proposed in a recent paper [8]; such analytical approximations have been studied and extended by other authors [9].

In this chapter, we shall obtain approximate analytical results for the energy of electronic bound states in quantum wells and in simple models of Janus semiconductor nanorods. As the concept of Janus nanoparticle is less popular than the concept of QWs or QDs, we shall give here some short explanations.

Their name derives from the Roman god Janus: his head had two opposite faces. A Janus nanodot can be a sphere composed of two semispheres of different materials. A Janus nanorod can be a nanorod having the left half and the right half made of different materials. Due to their intrinsic duality, the opposite parts of Janus particles can be functionalized differently [10]. Janus particles with an electron-donor and -acceptor side may be used in photovoltaics. As the Janus nanoparticles have lower symmetry than their homogenous counterparts, their theoretical description is more difficult. In this chapter, we shall propose toy models for semiconductor Janus nanorods.

The structure of this chapter is the following. We shall firstly formulate the basic theory for the quantum mechanical problem of a quantum well, composed of a thin semiconductor sandwiched between two massive ones. This heterojunction can be modeled by a quantum well (QW), essentially a finite square well, with BenDaniel-Duke boundary conditions. Such a problem was recently discussed by several authors, like Singh et al. [11, 12], who replaced the trigonometric functions entering in the transcendental equations for the bound states energy by the first few terms of their series expansion; in this way, the equations become simple, tractable algebraic ones. Our approach is different, being based on a more sophisticated “algebraization” of trigonometric functions, as proposed by de Alcantara Bonfin and Griffiths [8]. We shall obtain explicit formulas (series expansions) for the ground state energy and for the first excited state, very accurate if the well is not too shallow. Our results can be applied to both type I and type II semiconductors.

In the last part of our chapter, we shall study two toy models for semiconductor Janus nanorods; for the simplest one, we shall obtain analytical expressions for some energy eigenvalues of electronic bound states.

2. Basic theory

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

$$V(x) = \begin{cases} 0, & |x| \leq L/2 \\ V_0 > 0, & |x| > L/2 \end{cases} \quad (1)$$

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:

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

So, the Schrodinger equation for bound states is:

$$H\psi(x) = \left[-\frac{\hbar^2}{2} \frac{d}{dx} \left(\frac{1}{m(x)} \frac{d}{dx} \right) + V(x) \right] \psi_n(x) = E_n \psi_n(x) \quad (3)$$

Its physically acceptable solutions, that is, the wave functions, have to satisfy two conditions: (1) the continuity of the wave function and (2) 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 [6], defined by the Eq. (2), and takes the form:

$$\frac{1}{m_i} \frac{d\psi_{in}(x < L/2)}{dx} \Big|_{x \rightarrow L/2} = \frac{1}{m_o} \frac{d\psi_{out}(x > L/2)}{dx} \Big|_{x \rightarrow L/2} \quad (4)$$

Eq. (4) is known as the BenDaniel-Duke boundary condition. The notations ψ_{in} , ψ_{out} were used here to make more visible the physical content of this special boundary condition, and will not be maintained in the rest of the chapter.

The n th bound state has a unique energy, E_n , but two wave vectors, one inside the well, $k_{in,n}$, and another one outside, $k_{out,n}$:

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

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:

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

$$\psi_{2n}(x < 0) = \psi_{2n}(-x) \quad (7)$$

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

$$\begin{aligned}\psi_{2n+1}(x, 0 < x \leq L/2) &= A_{2n+1} \sin k_{in,2n+1}x \\ \psi_{2n+1}(x, x > L/2) &= B_{2n+1,s} \exp(-k_{out,2n+1}x)\end{aligned}\quad (8)$$

$$\psi_{2n+1}(x < 0) = -\psi_{2n+1}(-x) \quad (9)$$

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

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

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

So, the wave function outside the well is:

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

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

The wave functions are normalized if:

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

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

These results generalize the formula (24) in [11] and the Eqs. (25.3e, o) in [13].

It is convenient to use the potential strength P (introduced by Pitkanen [14], who actually used α , instead of P)

$$P = \sqrt{\frac{L^2}{2\hbar^2} m_i V} \quad (16)$$

and to define also ε_n , β , and X as:

$$\varepsilon_n = \frac{E_n}{V} \quad (17)$$

$$\beta = \frac{m_i}{m_0} \quad (18)$$

$$\Phi_n = k_{in,n} \frac{L}{2} \quad (19)$$

P , ε_n , β , and Φ_n are dimensionless quantities; Φ_n will be sometimes called dimensionless wave vector.

It is easy to see that:

$$k_{in,n} \frac{L}{2} = P\sqrt{\varepsilon_n} \quad (20)$$

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

$$k_{in,n}^2 + \beta k_{out,n}^2 = \frac{1}{(pL/2)^2} \quad (22)$$

Let us mention that, if the mass is position-independent, that is, if $m_i = m_o$, the eigenvalue equations are (see for instance [5], p. 3, Eqs. (15) and (16)):

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

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

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

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

$$\tan \frac{k_{in,2n+1}L}{2} = -\frac{k_{in,2n+1}}{k_{out,2n+1}}, \text{ odd states} \quad (26)$$

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

$$\Phi_{2n} \tan \Phi_{2n} = \frac{\sqrt{\beta}}{p} \sqrt{1 - p^2 \Phi_{2n}^2}, \quad n = 0, 1, \dots \text{even states} \quad (27)$$

$$\Phi_{2n+1} \cot \Phi_{2n+1} = -\frac{\sqrt{\beta}}{p} \sqrt{1 - p^2 \Phi_{2n+1}^2}, \quad n = 0, 1, \dots \text{odd states} \quad (28)$$

or, equivalently:

$$\frac{\cos \Phi_{2n}}{\Phi_{2n}} = (-1)^n \frac{p}{\sqrt{\beta + (1 - \beta)p^2 \Phi_{2n}^2}}, \quad n = 0, 1, \dots \text{even states} \quad (29)$$

$$\frac{\sin \Phi_{2n+1}}{\Phi_{2n+1}} = (-1)^n \frac{p}{\sqrt{\beta + (1 - \beta)p^2 \Phi_{2n+1}^2}}, \quad n = 0, 1, \dots \text{ odd states} \quad (30)$$

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 ($p \ll 1$) [15] and in the general case [8, 9, 16, 17].

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

In this chapter, we shall obtain precise analytical approximations for the energy of the first two states, that is, 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 formulae are both simple and accurate. In the limit $\beta \rightarrow 1$, we shall obtain the result of de Alcantara Bonfim and Griffiths, Eq. (17) of [8].

3. Approximate analytical solutions for eigenvalue equations

3.1. The first even state (the ground state)

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

$$\frac{\cos \Phi_0}{\Phi_0} = \frac{p}{\sqrt{\beta + (1 - \beta)p^2 \Phi_0^2}}, \quad 0 < x < \frac{\pi}{2} \quad (31)$$

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

3.1.1. The case $\beta > 1$

It is useful to introduce the new parameters $\gamma_>$, $g_>$, $A_>^2$:

$$\gamma_> = \beta - 1, \quad g_> = \frac{1}{\gamma_>}, \quad A_>^2 = \frac{p^2 \beta}{\beta - 1} = p^2 \beta g_> \quad (32)$$

because the eigenvalue equation can be written in a simpler form:

$$\frac{\cos \Phi_0}{\Phi_0} = \frac{1}{\sqrt{\gamma_> \sqrt{A_>^2 - \Phi_0^2}}}, \quad 0 < \Phi_0 < \frac{\pi}{2} \quad (33)$$

In the most physically interesting cases, P is quite large (the wells are quite deep), and according to (32), $A_>$ is even larger, so it is more convenient to use A instead of P as “large parameter”.

We shall replace the exact, transcendental Eq. (31) with an approximate, algebraic equation, using one of the formulae proposed in [8] for $\cos x$, namely:

$$\cos x \simeq f(x, c) = \frac{1 - \left(\frac{2x}{\pi}\right)^2}{\sqrt{1 + cx^2}} \quad (34)$$

The precision of this approximation on various subintervals of $(0, 1)$ depends on the exact value of c , with $0.18 \lesssim c \lesssim 0.23$; in our numerical evaluation, we shall use the value $c = 0.22$. For a detailed discussion on this issue, see [18].

The algebraic approximation of the eigenvalue equation, we get with (34) is:

$$\frac{1}{\Phi_0} \frac{1 - \left(\frac{2\Phi_0}{\pi}\right)^2}{\sqrt{1 + c\Phi_0^2}} = \frac{1}{\sqrt{\gamma_{>}} \sqrt{A_{>}^2 - \Phi_0^2}} \quad (35)$$

with

$$\Phi_0^2 = z \quad (36)$$

(35) can be written as:

$$z^3 + \left(\frac{1}{16}\pi^4 c g_{>} - A_{>}^2 - \frac{1}{2}\pi^2\right)z^2 + \frac{\pi^2}{2} \left(\frac{\pi^2}{8} g_{>} + A_{>}^2 + \frac{1}{8}\pi^2\right)z - \frac{1}{16}\pi^4 A_{>}^2 = 0 \quad (37)$$

Following the approach outlined in [19] and applied to this problem in [18], introducing the notation:

$$C = \frac{\pi^2}{2} c \quad (38)$$

and considering that the well is not too shallow:

$$A_{>}^2 \gg 1$$

we obtain for the physically interesting root the expression:

$$\begin{aligned} z(\beta > 1) = & \frac{\pi^2}{4} - \frac{\pi^3}{8} \sqrt{\left(1 + \frac{C}{2}\right)(\sqrt{g_{>}}\alpha_{>})} + \frac{\pi^4}{32}(1 + C)(\sqrt{g_{>}}\alpha_{>})^2 \\ & + \frac{\pi^5}{32} \left(1 + \frac{Cg_{>}}{2}\right) \sqrt{\left(1 + \frac{C}{2}\right)\sqrt{g_{>}}\alpha_{>}^3} + \frac{\pi^6}{128} g_{>}(1 + C) \left(1 + \frac{Cg_{>}}{2}\right) \alpha_{>}^4 + \dots \end{aligned} \quad (39)$$

If the depth of the well increases indefinitely, $\alpha_{>} \rightarrow 0$ and $z_1 \rightarrow \pi^2/4$, $\Phi_0 \rightarrow \pi/2$, 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 $\sqrt{g_{>}}\alpha_{>}$ in the previous formula is negative.

It is useful to write (39) in terms of more physical parameters, p and β . In order to do this, let us notice that:

$$g_{>} \alpha_{>}^2 = \frac{p^2}{\beta}, \quad \alpha_{>}^2 = \frac{\beta - 1}{\beta} p^2 \quad (40)$$

so Eq. (39) takes the form:

$$\begin{aligned} z(\beta > 1) = & \frac{\pi^2}{4} - \frac{\pi^3}{8} \sqrt{\left(1 + \frac{C}{2}\right)} \frac{p}{\beta^{1/2}} + \frac{\pi^4}{32} (1 + C) \frac{p^2}{\beta} \\ & + \frac{\pi^5}{32} \sqrt{1 + \frac{C}{2}} \left(\beta - 1 + \frac{C}{2}\right) \frac{p^3}{\beta^{3/2}} + \frac{\pi^6}{128} \left(\beta - 1 + \frac{C}{2}\right) (1 + C) \frac{p^4}{\beta^2} + \dots \end{aligned} \quad (41)$$

and:

$$z(\beta = 1) = \frac{\pi^2}{4} - \frac{\pi^3}{8} \sqrt{\left(1 + \frac{C}{2}\right)} p + \frac{\pi^4}{32} (1 + C) p^2 + \frac{\pi^5}{32} \sqrt{1 + \frac{C}{2}} \frac{C}{2} p^3 + \frac{\pi^6}{128} \frac{C}{2} (1 + C) p^4 + \dots \quad (42)$$

It is a simple exercise to check that the first three terms of the previous formula coincides with the first three terms of the power series given by Eq. (17) of [8].

If the parameter $A_{>}$ cannot be considered “large,” the exact expression of the root can be obtained using the standard approach [19]; they are elementary, but cumbersome, and will be not given here; the interested reader can find them in [18] .

3.1.2. The case $\beta < 1$

If $\beta < 1$, the eigenvalue equation for the dimensionless wave vector is:

$$\frac{\cos \Phi_0}{\Phi_0} = \frac{1}{\sqrt{\gamma_{<}} \sqrt{A_{<}^2 + \Phi_0^2}}, \quad 0 < \Phi_0 < \frac{\pi}{2} \quad (43)$$

with the following definitions for the parameters:

$$\gamma_{<} = 1 - \beta, \quad \frac{1}{\gamma_{<}} = g_{<}, \quad A_{<}^2 = \frac{P^2 \beta}{1 - \beta} = P^2 \beta \gamma_{<} \quad (44)$$

Using the de Alcantara Bonfim-Griffiths algebraization for $\cos x$ (34) [8], it gives an algebraic equation, which becomes, with the same substitution

$$\Phi_0^2 = z \quad (45)$$

a cubic equation:

$$z^3 + \left(A_{<}^2 - \frac{1}{2}\pi^2 - \frac{1}{16}\pi^4 c g_{<} \right) z^2 + \frac{\pi^2}{2} \left(\frac{1}{8}\pi^2 - A_{<}^2 - \frac{\pi^2}{8} g_{<} \right) z + \frac{1}{16}\pi^4 A_{<}^2 = 0, \quad \beta < 1 \quad (46)$$

Following the same steps as in the previous case, we find that the parameters $g_{>}$, $\alpha_{>}$ enter into the various expressions needed for obtaining the cubic roots only through the monoms $g_{>}\alpha_{>}^2$, $\alpha_{>}^2$ at various powers, and the roots of Eq. (46) can be obtained from the root (39) making the substitution:

$$g_{>} \rightarrow -g_{<}, \quad \alpha_{>}^2 \rightarrow -\alpha_{<}^2 \quad (47)$$

in Eq. (39). The final result, $z(\beta < 1)$, expressed in terms of p and β , has exactly the form (41).

3.2. The first odd state

3.2.1. The case $\beta > 1$

The exact eigenvalue equation for the first odd state, which is also the first excited state, can be written as:

$$\frac{\sin \Phi_1}{\Phi_1} = \frac{1}{\sqrt{\gamma_{>}} \sqrt{A_{>}^2 - \Phi_1^2}}, \quad \frac{\pi}{2} < \Phi_1 < \pi \quad (48)$$

As the shape of the function $\sin x/x$ on the interval $[0, \pi]$ is quite similar with the shape of $\cos x$ on the interval $[0, \pi/2]$, we can try an algebraization for $\sin x/x$ similar to that proposed by de Alcantara Bonfim and Griffiths for $\cos x$:

$$\frac{\sin \Phi_1}{\Phi_1} \simeq \frac{1 - (\Phi_1/\pi)^2}{\sqrt{1 + a\Phi_1^2}}, \quad 0 < \Phi_1 < \pi, \quad a \simeq 0.2 \quad (49)$$

A detailed discussion of the precision of this approximation is given in [18] (see Fig. 3 and Eq. (88)). Following, exactly the same steps as in the case of the ground state, we find that

$$z(\beta) = \pi^2 - \pi^2 \sqrt{(1 + \pi^2 a)} \frac{p}{\sqrt{\beta}} + \frac{\pi^4}{2} a \frac{p^2}{\beta} + \pi^4 \sqrt{(1 + \pi^2 a)} (\beta - 1) \left(\frac{p}{\sqrt{\beta}} \right)^3 + \frac{\pi^6}{2} a (\beta - 1) \frac{p^4}{\beta^2} + \dots \quad (50)$$

For $\beta < 1$, the expression of the root, in terms of β and p is identical with (50), written in terms of $g_{<}$, $g_{>}$, $\alpha_{<}$, $\alpha_{>}$, the formulae are different, see Eqs. (99) and (103) in [18].

For both cases— $\beta \lesssim 1$ —in the limit of an infinitely deep root, $z(\beta \lesssim 1, \alpha_{<} = 0) = \pi^2$, $\Phi_1(\beta \lesssim 1, \alpha_{<} = 0) = \pi$, as requested, and the first correction to this value is negative.

The relative errors of the formulas (39) and (50), with respect to the exact roots of the corresponding algebraic equations, are very small—of about $10^{-4} \dots 10^{-6}$ for physically interesting values

of the parameters p , β , a , c . 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 formulae 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 [15]. Much more precise analytical expressions for these energy are available in the literature [8, 9], for the case of constant mass; in this paper, we propose similar formulas, considering the case of position-dependent mass.

3.3. Higher-order states

In the previous subsections, we analyzed 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:

$$\cos \Phi \simeq \frac{1 - 4(\Phi - 2n\pi)^2/\pi^2}{\sqrt{1 + c(\Phi - 2n\pi)^2}}, \quad 2n\pi < \Phi < 2n\pi + \frac{\pi}{2} \quad (51)$$

but the eigenvalue equation, obtained in this way, is a sextic equation (which cannot be reduced to a cubic equation in Φ^2), so it cannot be solved. We meet similar difficulties if we try to use in the eigenvalue equation the algebraization of \tan (see later on, Eq. (73) and (74) of the present paper). Even the "parabolic approximation" for $(\cos x/x)^2$ or $(\sin x/x)^2$, in the sense used in [16], gives a quartic equation for the dimensionless wave vector. Its roots are given by complicated, but still elementary formulas.

3.4. Graphical illustration of our main results

In order to illustrate graphically some of our results, let us notice that, using Eqs. (17)–(22), we can write the following relations for the energy:

$$\frac{m_i L^2}{2\hbar^2} E_n = \Phi_n^2 = z_n(p) \quad (52)$$

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 Eqs. (39) and (50), for a deep well, the root z can be approximated with a quartic polynomial in p , the inverse of the potential strength P . Let us mention that, if we replace in the definition of P , Eq. (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 electron volts, we get:

$$P = 25.616\sqrt{V_0}, \quad p = 3.9 \times 10^{-2} \frac{1}{\sqrt{V_0}} \quad (53)$$

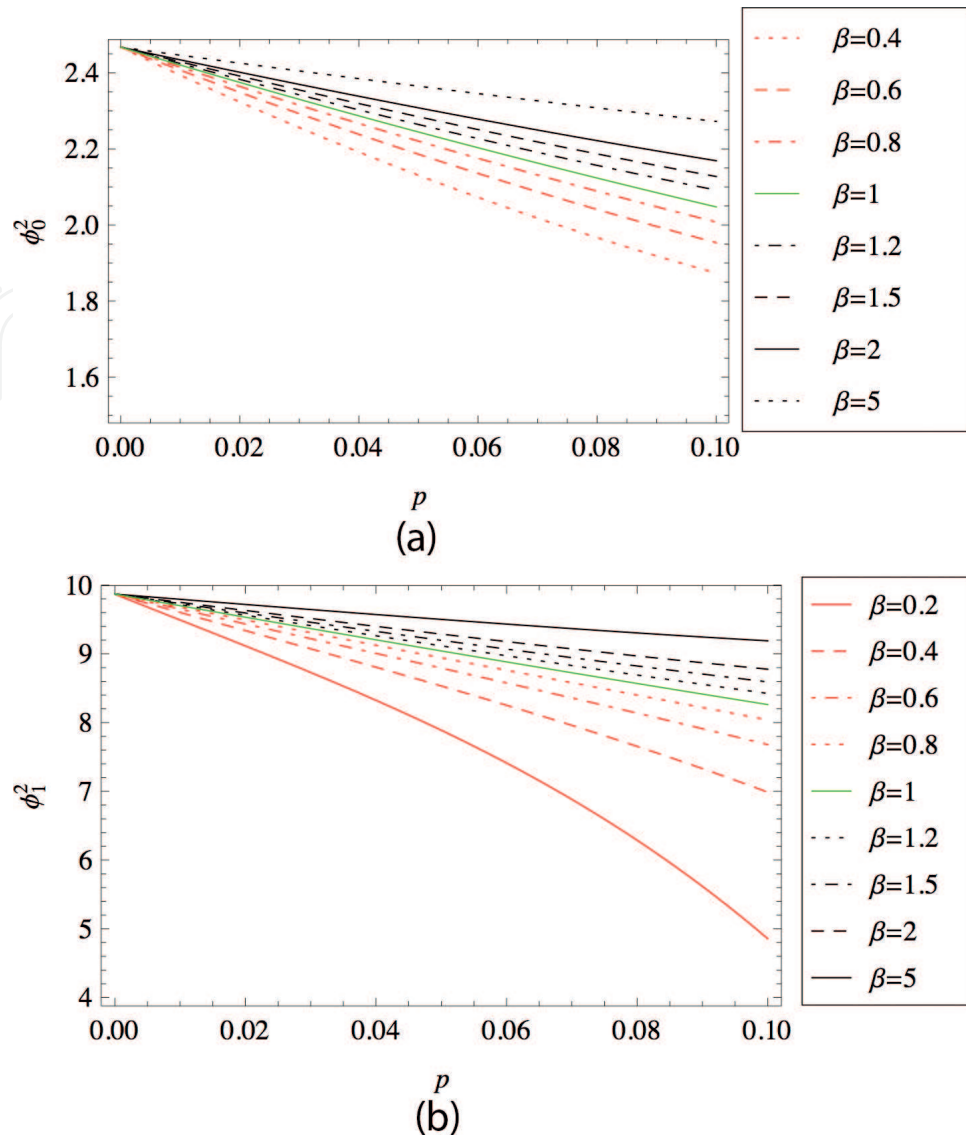


Figure 1. The plot of Φ_0^2 (a) and Φ_1^2 (b), which are proportional to the energies E_0 , E_1 , as functions of the inverse potential strength p .

We shall plot our main results, that is, the series expansions of the dimensionless wave vectors, Φ_0^2 and Φ_1^2 , as functions of p , on the range $0 < p < 0.1$, when the condition of convergence is satisfactorily fulfilled (**Figure 1**). The energy is a monotonically increasing function of β ; its values, for $\beta = 1$, are obtained from Eqs. (42) and (50).

3.5. Applications to other nanostructures

Our calculations can be easily applied to type II semiconductors heterostructures, when one of the effective mass of the charge carrier is negative: $m_i m_o < 0$ ([5], chapter 3, Eqs. (35) and (36)); a detailed description of such heterointerfaces can be found for instance in [5], p. 66. So, instead of (25) and (26), the eigenvalue equations take the form:

$$\tan \frac{k_{in,2n}L}{2} = -\frac{m_i}{|m_o|} \frac{k_{out,2n}}{k_{in,2n}} = -|\beta| \frac{k_{out,2n}}{k_{in,2n}}, \text{ even states} \quad (54)$$

$$\tan \frac{k_{in,2n+1}L}{2} = \frac{|m_o|}{m_i} \frac{k_{in,2n+1}}{k_{out,2n+1}} = \frac{1}{|\beta|} |\beta|, \text{ odd states} \quad (55)$$

and can be solved following exactly the same approach.

As already mentioned, the wave function in the Schrodinger Eq. (3) can be interpreted as an envelope function. This approximation works well when the materials constituting the heterostructures are perfectly lattice-matched and they crystallize in the same crystallographic structure (in the most cases, the zinc blend 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 closed to a symmetry

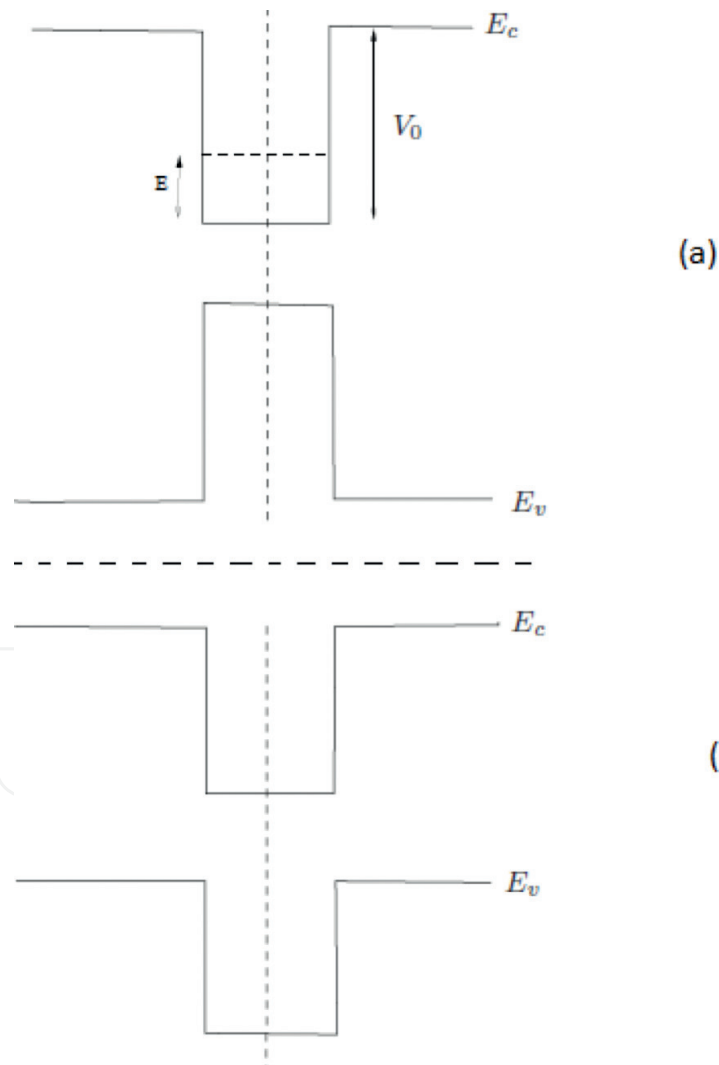


Figure 2. Schematic representation of the conduction band E_c and of the valence band E_v for type I (a) and type II (b) semiconductors.

point in the host's Brillouin zone. A popular example is given by the lowest conduction states of GaAs-GaAlAs heterostructures with GaAs layer (typically, its thickness is about 100 Å or larger). A detailed description of the cases in which the envelope function model is successful is given in [5], p. 66 (See **Figure 2**).

As there are some similarities between QWs and QDs, our results are also relevant for these devices. The simplest remark is that the eigenvalues equations for the first odd state in a QW are identical to that corresponding to the $l = 0$ state in a QD (see for instance [13], problem 63). Also, the eigenvalue equations for the wave vectors of the energy levels for a finite barrier rectangular shaped QD, Eq. (36) in [21], are quite similar to ours—(29) and (30), but somewhat more complicated. The ground state energy of electrons and holes in a core/shell QD is given by the Eq. (21) of [22], 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.

4. The infinite square well with two semiconductor slabs

4.1. The symmetric case

Let us consider an infinite 1D square well, delimited by two rigid walls situated in $-L/2$, respectively $L/2$, containing two semiconductor slabs, of equal width, but of different materials. It is a toy model for a Janus nanorod, composed of two different semiconductors, with large work functions. We preferred to choose this particular case (equal width), in order to avoid too cumbersome mathematical calculations. The electron effective mass is position dependent, like in (2):

$$m(x) = \begin{cases} m_1, & -L/2 < x < 0 \\ m_2, & 0 < x < L/2 \end{cases} \quad (56)$$

with:

$$m_2 = \beta m_1 \quad (57)$$

We want to investigate how the energies of the electronic bound states will be affected, compared to the situation when in the infinite well there is only one slab, with effective electron mass m_1 or m_2 . As

$$E = \frac{\hbar^2 k_1^2}{2m_1} = \frac{\hbar^2 k_2^2}{2m_2} \quad (58)$$

we have, with (57):

$$k_2 = \sqrt{\beta} k, \quad k = k_1 \quad (59)$$

The electronic wave function is obtained solving the Schrodinger equation, as in the case of a finite well, studied in Section 2:

$$\psi(x) = \begin{cases} A_1 \sin(k_1 x + \varphi_1), & -L/2 < x < 0 \\ A_2 \sin(\sqrt{\beta} k_1 x + \varphi_2), & -L/2 < x < 0 \end{cases} \quad (60)$$

The boundary conditions for the wave function give:

$$\sin\left(-\frac{kL}{2} + \varphi_1\right) = 0 \quad (61)$$

$$\sin\left(\sqrt{\beta} \frac{kL}{2} + \varphi_2\right) = 0 \quad (62)$$

and the continuity in the origin:

$$A_1 \sin \varphi_1 = A_2 \sin \varphi_2 \quad (63)$$

The BenDaniel-Duke boundary condition means:

$$\frac{1}{m_1} \psi'(0_-) = \frac{1}{m_2} \psi'(0_+) \quad (64)$$

or:

$$\sqrt{\beta} A_1 \cos \varphi_1 = A_2 \cos \varphi_2 \quad (65)$$

Together with the orthonormality condition for the wave function, Eqs. (61)–(63) and (65) form a system of five equations for five quantities, k , φ_1 , φ_2 , A_1 , A_2 . As the amplitudes are not of primary interest, we can combine (64) and (65) to obtain:

$$\frac{1}{\sqrt{\beta}} \tan \varphi_1 = \tan \varphi_2 \quad (66)$$

Replacing in (66), the values of φ_1 , φ_2 obtained from (61) and (62):

$$\varphi_1 = n_1 \pi + \frac{kL}{2}, \quad \varphi_2 = n_2 \pi - \sqrt{\beta} \frac{kL}{2} \quad (67)$$

we get:

$$\tan \frac{kL}{2} = -\sqrt{\beta} \tan \sqrt{\beta} \frac{kL}{2} \quad (68)$$

With

$$\frac{kL}{2} = K \quad (69)$$

it can be written as:

$$\tan K + \sqrt{\beta} \tan \sqrt{\beta} K = 0 \quad (70)$$

If $\sqrt{\beta} = 1$, (67) gives:

$$2 \tan \frac{kL}{2} = n\pi \rightarrow k_n = \frac{n\pi}{L} \quad (71)$$

$$k_1 = \frac{\pi}{L} \rightarrow K_1 = \frac{\pi}{2} \quad (72)$$

so the solutions corresponding to the infinite well with an homogenous medium inside the walls.

Eq. (70) is a transcendental one, and its solutions cannot be expressed as a finite combination of elementary functions. A quite popular analytical approximation for the tangent function has been proposed by de Alcantara-Bonfim [8] and generalized by the present author [9]:

$$\tan x \simeq \frac{0.45\pi(x - n\pi)}{2x - (2n - 1)\pi}, \quad \left(n - \frac{1}{2}\right)\pi < x < n\pi \quad (73)$$

$$\tan x \simeq \frac{0.45\pi(x - n\pi)}{(2n + 1)\pi - 2x}, \quad n\pi < x < \left(n + \frac{1}{2}\right)\pi \quad (74)$$

In order to see how this approximation works, let us consider the first two roots of Eq. (68), if $\beta \lesssim 1$. For $\beta = 0.9$, we obtain (for instance, using the command FindRoot in Mathematica) $K_{1,exact} = 1.65804$ and $K_{2,exact} = 3.29797$, close to $\pi/2$, respectively π , that is, to the values corresponding to $\beta = 0$. We shall discuss the case of the second root of Eq. (70). As $K_{2,exact} = 3.29797 \in (\pi, \frac{3}{2}\pi)$ and $K_{2,exact}\sqrt{\beta} = 2.9682 \in (\frac{\pi}{2}, \pi)$, the two tangent functions appearing in Eq. (70) will be approximated by the two variants of Eqs. (73) and (74), the result being the following:

$$\frac{K - \pi}{3\pi - 2K} + \frac{\sqrt{\beta}(\sqrt{\beta}K - \pi)}{2\sqrt{\beta}K - \pi} = 0 \quad (75)$$

So, K can be obtained as a root of a second order equation, namely:

$$K(\beta) = \frac{\pi - 3\beta + 1 + \sqrt{9\beta^2 - 24\beta^{\frac{3}{2}} + 26\beta - 8\beta^{1/2} + 1}}{4\beta^{1/2}(1 - \beta^{1/2})} \quad (76)$$

We find that $K(\beta = 0.9) = K_{2,approx} = 3.2987$, so quite close to the exact value, the error being:

$$\frac{K_{2,exact} - K_{2,approx}}{K_{2,exact}} = \frac{3.29797 - 3.2987}{3.29797} = -2.2135 \times 10^{-4} \quad (77)$$

However, due to the rapid variation of the tangent functions near its singularities, this approximation method must be used with utmost care, as it can easily give unacceptable results (this is the case of the first root, for $\beta = 0.9$).

4.2. The asymmetric case

Let us consider now the case of a rectangular infinite asymmetric well, with the potential:

$$V(x) = \begin{cases} \infty, & x < -L/2 \\ 0, & -L/2 < x < 0 \\ V_0, & 0 < x < L/2 \\ \infty, & x > L/2 \end{cases} \quad (78)$$

with $V_0 > 0$, containing, as in the previous example, two semiconductor slabs. It is also a toy model of a Janus nanorod, somewhat more realistic than that discussed in Section 4.1. We also chose a particular geometry (the same width for each slab) to avoid irrelevant mathematical complications. For an electronic bound state of energy $E > V_0$, the wave vectors (and the electronic effective masses) are different in different slabs, according to the relations:

$$E = \frac{\hbar^2 k_1^2}{2m_1}; \quad E - V_0 = \frac{\hbar^2 k_2^2}{2m_2}, \quad m_2 = \beta m_1 \quad (79)$$

Defining the wave vector k_0 by:

$$V_0 = \frac{\hbar^2 k_0^2}{2m_1} \quad (80)$$

noticing that:

$$k_2^2 = \beta(k_1^2 - k_0^2) \quad (81)$$

and following exactly the same steps as in the symmetric case, we obtain the following eigenvalue equation:

$$\frac{1}{K_1} \tan K_1 + \frac{\sqrt{\beta}}{\sqrt{K_1^2 - K_0^2}} \tan \sqrt{\beta(K_1^2 - K_0^2)} = 0 \quad (82)$$

with the notations:

$$K_1 = \frac{k_1 L}{2}, \quad K_2 = \frac{k_2 L}{2}, \quad K_0 = \frac{k_0 L}{2} \quad (83)$$

If $0 < E < V_0$, k_2 (and, evidently, K_2) become imaginary, and $\tan K_2 \rightarrow -i \tanh K_2$. The Eq. (82) and its hyperbolic counterpart are much complicated than (68); even if there are some methods of obtaining approximate analytical solutions, they will be not discussed here. The case of a finite asymmetric well, with two different semiconductor slices, can be studied following exactly the same approach, but now the complications are even more serious, as the wave function extends outside the wells.

5. Conclusions

In this chapter, we obtained approximate analytical solutions for the eigenvalue equation of the first two bound states in a semiconductor quantum well, in a particular case of position-dependent mass of the charge carrier—in fact, the simplest one, corresponding to BenDaniel-Duke boundary conditions. This position dependence can be characterized by β , the ratio of the mass inside, to the mass outside the well. Actually, we obtained quite simple expressions for the dimensionless wave vector, in terms of the potential strength and of β . Even if we solved this problem in terms of one-particle quantum mechanics, obtaining the wave function and the eigenvalues of the bound states, our results can be directly applied in the theory of envelope functions in the conduction band at heterointerfaces. Our approach is based on the “algebraization” of trigonometric functions present in the transcendental eigenvalue equations; in this way, they are transformed in tractable algebraic equations.

We also proposed two models for a semiconductor Janus nanorod—a system, which was not yet treated analytically.

Our results can be easily extended to more realistic (e.g., linear) position dependence of the mass carrier and to other nanosystems. For instance, the eigenvalue equations for the wave vectors of bound energy levels of a finite barrier rectangular-shaped quantum dot, Eq. (36) in [21], are quite similar to ours—(22), (23), but somewhat more complicated. The ground state energy of electrons and holes in a core/shell quantum dot is given by Eq. (21) of [22], an equation similar to ours, just mentioned previously. Such results are important, inter alia, for the interpretation of photoluminescence spectra of heterojunctions.

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Author details

Victor Barsan

Address all correspondence to: vbarsan@theory.nipne.ro

National Institute for Physics and Nuclear Engineering, Bucharest-Magurele, Romania

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