CINVESTAV, IPN.

Multi-step method to solve the Schrödinger equation

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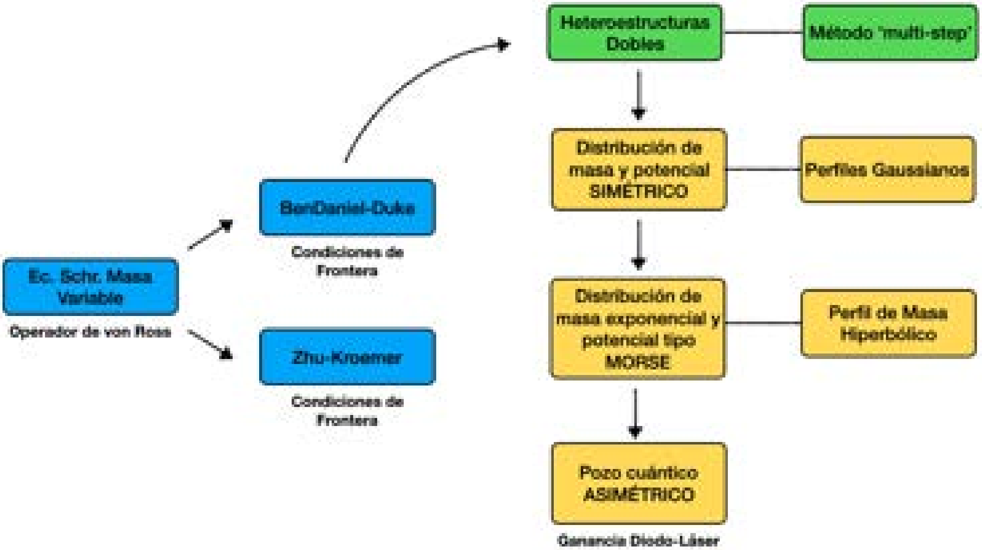
Content

Summary

- We consider particles with position-dependent effective mass in double heterostructures, subject to the action of different non-singular potentials whose dynamics are governed by the **Schrödinger equation**.
- The study in this quantum regime allows us to develop a numerical method to calculate the energy spectrum of these systems. When analytical results are obtained, the numerical results are consistent with them.
- Once this first objective has been achieved, our interest focuses on the study of particles whose dynamics are governed by the relativistic Dirac-Weyl type equations with Fermi speed dependent on the position and the **Dirac-type** equation with Fermi mass and velocity dependent on the position.

Summary


Heteroestructuras Dobles
Método 'multi-step'
Distribución de masa y potencial SIMÉTRICO
Perfiles Gaussianos
BenDaniel-Duke
Condiciones de Frontera
Ec. Schr. Masa Variable
Operador de von Roos
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Ganancia Diodo-Láser

Position-dependent mass

The time-independent Schrödinger equation in one dimension is the equation that models the dynamics of a particle of constant mass ($m = M_0$) subject to an electric potential ($V(z)$).

$$\left(\hat{H} - E\right)\psi(z) = \left(\hat{T} + V(z) - E\right)\psi(z) = 0$$

where $\hat{T}$ is the kinetic energy operator (KOE) and $\hat{H}$ is the total energy operator.

$$\hat{T} = \frac{1}{2M_0}\hat{p}^2; \qquad \hat{H} = \hat{T} + V(z).$$

$\hat{p} = -i\hbar\frac{d}{dz}$, is the moment operator.

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$\hat{p} = -i\hbar\frac{d}{dz}$, is the moment operator. Thus, the Schrödinger equation is explicitly stated as

$$\left(-\frac{\hbar^2}{2M_0}\frac{d^2}{dz^2} + V(z)\right)\psi(z) = E\psi(z)$$

Position-dependent mass

- When the mass depends on the position ($m = M_0 m(z)$), it becomes an operator that no longer commutes with the momentum operator ($\hat{p} = -i\hbar\frac{d}{dz}$).
- In such a circumstance, it is not trivial to assign the correct order of the operators (mass and momentum) that make up the kinetic energy operator (KEO).

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The operator that covers all the different proposals is due to O. von Ross [11]

$$T_{\mathrm{vR}}(\alpha, \beta) = \frac{1}{4}(m^{\alpha}\hat{p}m^{\beta}\hat{p}m^{\gamma} + m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha}). \tag{1}$$

where[1]

$$\hat{p} = -i\hbar\frac{d}{dz}; m = M_0 m(z), (M_0 = cte). \quad \alpha + \beta + \gamma = -1.$$

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Position-dependent mass

Then, the Schrödinger equation to solve is

$$\left(T_{\mathrm{vR}}(\alpha, \beta) + V(z) - E\right)\psi = 0 \tag{2}$$

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$$\left(-\frac{d}{dz}\frac{1}{m(z)}\frac{d}{dz} - \frac{1}{2}\left(\nu\frac{m''(z)}{m^2(z)} - \eta\frac{m'^2(z)}{m^3(z)}\right) + V(z) - E\right)\psi = 0. \tag{3}$$

where

$$\nu = -1-\beta, \quad \eta = -2(\beta+1)(\alpha+1) - 2\alpha^2.$$

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where

$$\nu=-1-\beta,\quad \eta=-2(\beta+1)(\alpha+1)-2\alpha^2.$$

In (3) we will make the variable changes $\psi(z)=m(z)^{1/4}\phi,\quad \rho=\int\sqrt{m(z)}dz$

Position-dependent mass

When replacing

$$\psi(z) = m(z)^{1/4}\phi, \quad \rho = \int \sqrt{m(z)}dz, \tag{4}$$

in (3), the function ϕ satisfies the Schrödinger equation with constant 'mass'

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Equation associated with (3)

$$-\frac{d^2\phi}{d\rho^2} + (\widetilde{V}(\rho) - E)\phi = 0, \tag{5}$$

$$\widetilde{V}(\rho) = V(z) + \frac{1}{2}\left(\eta + \frac{7}{8}\right)\frac{m'(z)^2}{m(z)^3} - \frac{1}{2}\left(\nu + \frac{1}{2}\right)\frac{m''(z)}{m(z)^2}. \tag{6}$$

$\nu = -1 - \beta, \quad \eta = -2(\beta + 1)(\alpha + 1) - 2\alpha^2$

Position-dependent mass

Recapitulating the ideas of this first part, we have the Schrödinger equation with position-dependent mass

$$(T_{\mathrm{vR}}(\alpha,\beta) + V(z) - E)\,\psi = 0$$

and this equation can be written as a Schrödinger type equation with constant mass and a effective potential $\widetilde{V}$ which depends on the parameters α and β, the mass profile M and the potential V

$$-\frac{d^2\phi}{d\rho^2} + (\widetilde{V}(\rho) - E)\phi = 0,$$

where

$$\widetilde{V}(\rho) = V(z) + \frac{1}{2}\left(\eta + \frac{7}{8}\right)\frac{m'(z)^2}{m(z)^3} - \frac{1}{2}\left(\nu + \frac{1}{2}\right)\frac{m''(z)}{m(z)^2}.$$

$$\nu = -1-\beta, \quad \eta = -2(\beta+1)(\alpha+1) - 2\alpha^2, \quad \psi(z) = m(z)^{1/4}\phi, \quad \rho = \int \sqrt{m(z)}dz.$$

Boundary conditions

Boundary conditions.
If there is an abrupt, finite change in potential and/or mass at point z_j, then the mass distribution m_j (m_{j+1}) and the wavefunction ψ_j (ψ_{j+1}) immediately to the left (right) of z_j must satisfy the pair of conditions depending on how we choose the values of α and β.

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If **we choose the BenDaniel-Duke OEC** ($\alpha = 0$, $\beta = -1$) we have the conditions [3, 1, 10, 9, 6]

$$\psi_j(z_j) = \psi_{j+1}(z_j), \qquad \frac{1}{m_j}\frac{d}{dz}\left(\psi_j(z)\right)_{z=z_j} = \frac{1}{m_{j+1}}\frac{d}{dz}\left(\psi_{j+1}(z)\right)_{z=z_j}. \tag{7}$$

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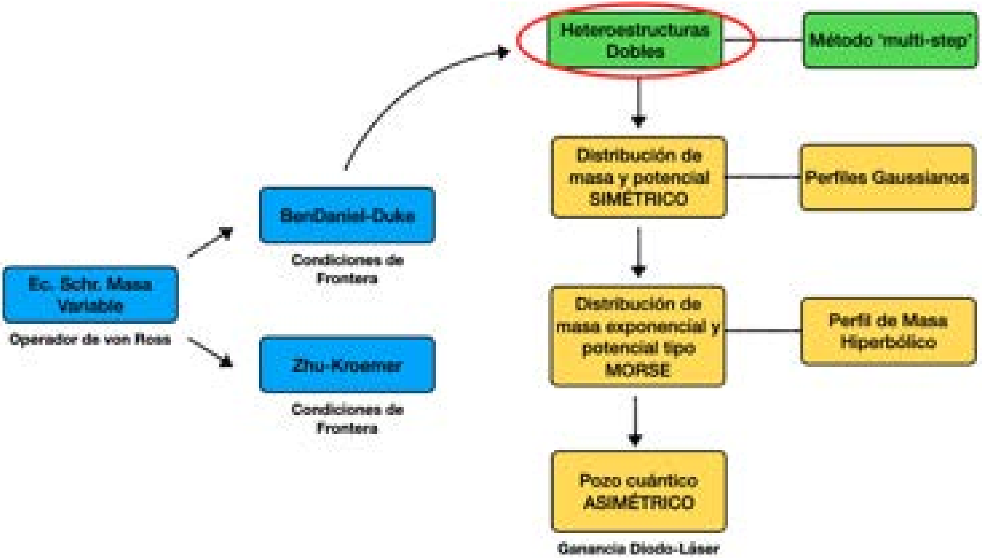
On the other hand, if **we choose the Zhu-Kroemer OEC** ($\alpha = -1/2$, $\beta = 0$), the pair of conditions is [3, 12, 5, 9, 4]

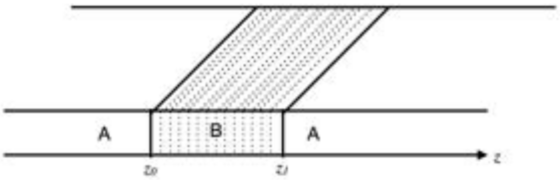
$$\frac{\psi_j(z_j)}{\sqrt{m_j}} = \frac{\psi_{j+1}(z_j)}{\sqrt{m_{j+1}}}, \qquad \frac{1}{\sqrt{m_j}}\frac{d}{dz}\left(\psi_j(z)\right)_{z=z_j} = \frac{1}{\sqrt{m_{j+1}}}\frac{d}{dz}\left(\psi_{j+1}(z)\right)_{z=z_j}. \tag{8}$$

Double heterostructures



Double heterostructure model

For the double heterostructure model we are going to assume that we have an arrangement like the one in the figure. In this intermediate region, we have a type B semiconductor and outside a type A semiconductor.



Graphic representation of a double heterostructure.

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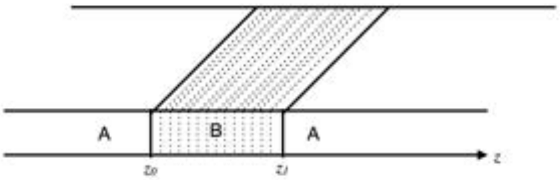
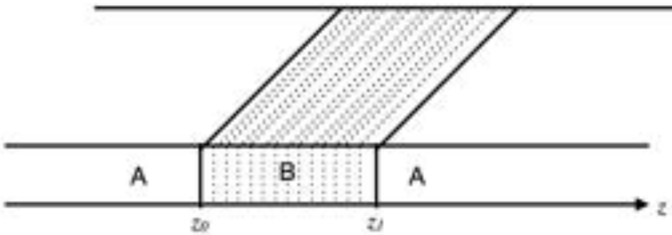


Graphic representation of a double heterostructure.

- In the intermediate region, a smooth dependence on the position of the effective mass of a particle subject to a smooth potential also occurs; outside this region, the behavior of both profiles is constant.

Modelo de heteroestructura doble



$$V(z) = \begin{cases} V_0 \\ V_{\text{in}}(z) \\ V_2 \end{cases} , \quad m(z) = \begin{cases} m_0 & ; \quad z < z_0, \\ m_{\text{in}}(z) & ; \quad z_0 \leq z < z_1, \\ m_2 & ; \quad z_1 \leq z, \end{cases}$$

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In the intermediate region the particle obeys the equation (2)

$$\left(-\frac{d}{dz}\frac{1}{m_{\text{in}}(z)}\frac{d}{dz} - \frac{1}{2}\left(\nu\frac{m''_{\text{in}}(z)}{m_{\text{in}}(z)^2} - \eta\frac{m'_{\text{in}}(z)^2}{m_{\text{in}}(z)^3}\right) + V_{\text{in}}(z) - E\right)\psi_{\text{in}} = 0, \tag{10}$$

and in the other regions, behavior is governed by the equations

$$\left(-\frac{1}{m_{0,2}}\frac{d^2}{dz^2} + V_{0,2} - E\right)\psi_{0,2}(z) = 0. \tag{11}$$

Double heterostructures

$$V(z) = \begin{cases} V_0 \\ V_{\text{in}}(z) \\ V_2 \end{cases} \quad , \quad m(z) = \begin{cases} m_0 & ; \quad z < z_0, \\ m_{\text{in}}(z) & ; \quad z_0 \leq z < z_1, \\ m_2 & ; \quad z_1 \leq z, \end{cases} \tag{12}$$

The complete solution, in the case of bound states, is written as

$$\psi_0(z) = Oe^{\eta_0 z} \qquad ; \quad z < z_0, \tag{13}$$

$$\psi_{\text{in}}(z) = P\psi^1_{\text{in}}(z) + Q\psi^2_{\text{in}}(z) \quad ; \quad z_0 \leq z < z_1, \tag{14}$$

$$\psi_1(z) = Se^{-\eta_2 z} \qquad ; \quad z_1 \leq z. \tag{15}$$

$\eta_{0,2} = \sqrt{m_{0,2}(V_{0,2} - E)}$ y O,P, Q, S They are normalization constants.

Double heterostructures

To these solutions we apply the **BenDaniel-Duke** boundary conditions ($\alpha = 0$, $\beta = -1$)[3, 1, 10, 9, 6]

$$\psi_j(z_j) = \psi_{j+1}(z_j), \qquad \frac{1}{m_j}\frac{d}{dz}\left(\psi_j(z)\right)_{z=z_j} = \frac{1}{m_{j+1}}\frac{d}{dz}\left(\psi_{j+1}(z)\right)_{z=z_j}. \tag{16}$$

Double heterostructures

Using the **condition BD-D** at point z_0 and z_1, we obtain the following system of equations

$$Ore^{\eta_0 z_0} = P\psi_{\rm in}^1(z_0) + Q\psi_{\rm in}^2(z_0) = -P\chi_{11} - Q\chi_{12}, \tag{17}$$

$$Se^{-\eta_2 z_1} = P\psi_{\rm in}^1(z_1) + Q\psi_{\rm in}^2(z_1) = -P\chi_{21} - Q\chi_{22}, \tag{18}$$

where

$$\chi_{1i} = -\frac{m_0}{\eta_0}\frac{(\psi_{\rm in}^i(z))'|_{z=z_0}}{m_{\rm in}(z_0)}, \quad \chi_{2i} = \frac{m_2}{\eta_2}\frac{(\psi_{\rm in}^i(z))'|_{z=z_1}}{m_{\rm in}(z_1)}; \quad i = 1, 2. \tag{19}$$

Double heterostructures

Thus, we have a homogeneous system of linear equations that can be written in matrix form as

$$\mathbf{X}\begin{pmatrix} P \\ Q \end{pmatrix} = \begin{pmatrix} \psi^1_{\text{in}}(z_0) + \chi_{11} & \psi^2_{\text{in}}(z_0) + \chi_{12} \\ \psi^1_{\text{in}}(z_1) + \chi_{21} & \psi^2_{\text{in}}(z_1) + \chi_{22} \end{pmatrix}\begin{pmatrix} P \\ Q \end{pmatrix} = 0. \tag{20}$$

For the non-trivial solution of (20) the determinant of X must be zero

$$|\mathbf{X}| = 0. \tag{21}$$

This is a transcendental equation that, as will be seen in the examples, allows us to calculate the energies of the bound states, $E^{\text{BD-D}}$.

Double heterostructures

When the **condition (general) Z-K** [4] is applied to the solution (13-15) at points z_0 and z_1 , we arrive at the same system of equations for P and Q but with the changes

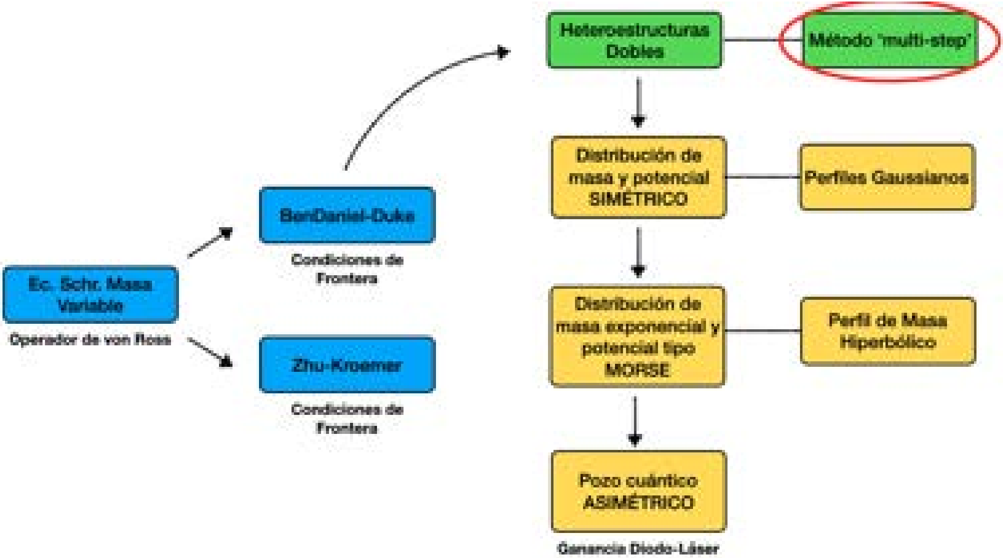
$$\chi_{ji} \to \hat{\chi}_{ji} \quad ; \quad j, i = 1, 2. \tag{22}$$

where

$$\hat{\chi}_{1i} = -\frac{\sqrt{m_{\text{in}}(z_0)}}{\eta_0} \left(\frac{\psi^i_{\text{in}}(z)}{\sqrt{m_{\text{in}}(z)}} \right)'_{z=z_0} , \quad \hat{\chi}_{2i} = \frac{\sqrt{m_{\text{in}}(z_1)}}{\eta_2} \left(\frac{\psi^i_{\text{in}}(z)}{\sqrt{m_{\text{in}}(z)}} \right)'_{z=z_1} \quad ; \quad i = 1, 2. \tag{23}$$

With these changes and the transcendental equation (21), we obtain the energy spectrum $E^{\text{Z-K}}$

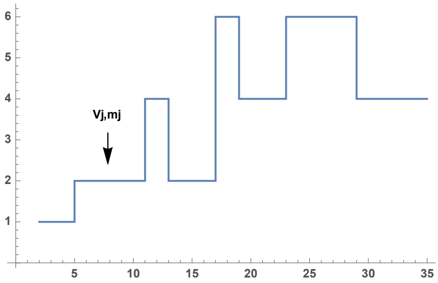
Método Multi-Step



Multi-Step Method

We consider a potential and a position-dependent effective mass distribution given by

$$V(z) = \begin{cases} V_0 \\ V_1 \\ V_2 \\ . \\ V_j \\ . \\ V_n \end{cases}, \quad m(z) = \begin{cases} m_0; & z < z_0, \\ m_1; & z_0 \leq z < z_1, \\ m_2; & z_1 \leq z < z_2, \\ . \\ m_j; & z_{j-1} \leq z < z_j, \\ . \\ m_n; & z_{n-1} \leq z. \end{cases}$$



These equations define the value of the potential V_j, the effective mass m_j and the solutions ψ_j in each j-th region $(j = 0, 1, 2, \ldots n)$ of one-dimensional space.

Multi-Step Method

Regardless of the values of α and β the solutions in each interval will be

$$\psi_j(z) = A_j e^{ik_j z} + B_j e^{-ik_j z}; \quad k_j = \sqrt{m_j(E - V_j)}. \tag{24}$$

These solutions must satisfy at points z_j some of the conditions (16) u (8). From the coefficients A_j and B_j we obtain **reflection coefficient** R_c through the reflection amplitude $R = \frac{B_0}{A_0}$. The reflection (transmission) coefficients $R_c = |R|^2$ ($T_c = |T|^2$), satisfy $R_c + T_c =$1.

Boundary conditions

If we apply the boundary conditions to the functions ψ_j at a point z_j

$$\psi_j(z) = A_j e^{ik_j z} + B_j e^{-ik_j z}, \quad \psi_{j+1}(z) = A_{j+1} e^{ik_{j+1} z} + B_{j+1} e^{-ik_{j+1} z}$$

then

$$\frac{B_j}{A_j} = \frac{r_{j,j+1} + \frac{B_{j+1}}{A_{j+1}} e^{-2ik_{j+1} z_j}}{1 + r_{j,j+1} \frac{B_{j+1}}{A_{j+1}} e^{-2ik_{j+1} z_j}} e^{2ik_j z_j}, \tag{25}$$

where

$$r_{j,j+1} = \frac{k_j \mu_j - k_{j+1} \rho_j}{k_j \mu_j + k_{j+1} \rho_j}. \tag{26}$$

R for a single interfaces ($n = 1$)

For a single interface, we have two functions

$$\psi_0(z) = A_0 e^{ik_0 z} + B_0 e^{-ik_0 z}; \quad \psi_1(z) = A_1 e^{ik_1 z} + B_1 e^{-ik_1 z}$$

with $B_1 = 0$ and $z_0 = 0$, so

$$\left(\frac{B_j}{A_j} = \frac{r_{j,j+1} + \frac{B_{j+1}}{A_{j+1}} e^{-2ik_{j+1} z_j}}{1 + r_{j,j+1} \frac{B_{j+1}}{A_{j+1}} e^{-2ik_{j+1} z_j}} e^{2ik_j z_j} \right)$$

$$R = \frac{B_0}{A_0} = r_{01} = \frac{k_0 \mu_0 - k_1 \rho_0}{k_0 \mu_0 + k_1 \rho_0} \tag{27}$$

R for two single interfaces ($n = 2$)

In this case, we have three functions

$$\psi_0(z) = A_0 e^{ik_0 z} + B_0 e^{-ik_0 z}, \quad \psi_1(z) = A_1 e^{ik_1 z} + B_1 e^{-ik_1 z}, \quad \psi_2(z) = A_2 e^{ik_2 z}$$

$(B_2 = 0)$. Using equation (25) for the coefficients of the three functions, we have the relationships

$$\frac{B_0}{A_0} = \frac{r_{01} + \frac{B_1}{A_1} e^{-2ik_1 z_0}}{1 + r_{01} \frac{B_1}{A_1} e^{-2ik_1 z_0}} e^{2ik_0 z_0}, \quad \frac{B_1}{A_1} = \frac{r_{12} + \frac{B_2}{A_2} e^{-2ik_2 z_1}}{1 + r_{12} \frac{B_2}{A_2} e^{-2ik_2 z_1}} e^{2ik_1 z_1} = r_{12} e^{2ik_1 z_1}. \quad (28)$$

Thus, the reflection coefficient is

$$\frac{B_0}{A_0} = \frac{r_{01} + r_{12} e^{2ik_1 w_1}}{1 + r_{01} r_{12} e^{2ik_1 w_1}} \quad (29)$$

where we define $w_1 = z_1 - z_0$ and $z_0 = 0$.

R for n interfaces

The recursive formula, using the **condition BD-D**, for the reflection amplitude of the system described by Eq. (24) is [2]

$$
\begin{aligned}
R = r_{012\ldots n} = \frac{B_0}{A_0} = \frac{r_{01} + r_{12\ldots n} e^{2ik_1 w_1}}{1 + r_{01} r_{12\ldots n} e^{2ik_1 w_1}}, \\
r_{12\ldots n} &= \frac{r_{12} + r_{23\ldots n} e^{2ik_2 w_2}}{1 + r_{12} r_{23\ldots n} e^{2ik_2 w_2}}, \\
&\vdots \\
r_{n-1,n} &= \frac{\hat{k}_{n-1} - \hat{k}_n}{\hat{k}_{n-1} + \hat{k}_n},
\end{aligned}
\tag{30}
$$

where the quantities have been defined

$$
w_j = z_j - z_{j-1}, \quad r_{lj} = \frac{\hat{k}_l - \hat{k}_j}{\hat{k}_l + \hat{k}_j}; \quad \hat{k}_j = \frac{k_j}{m_j}.
$$

[2] The reflection (transmission) coefficients $R_c = |R|^2$ ($T_c = |T|^2$), satisfy $R_c + T_c = 1$.

R para n interfaces

If the **condition Z-K** is considered, the recursive character of the formula (30) is maintained but the quantity $r_{n-1,n}$ changes to

$$r_{n-1,n} = \frac{k_{n-1} - k_n}{k_{n-1} + k_n}. \tag{31}$$

Discretization of smooth profiles

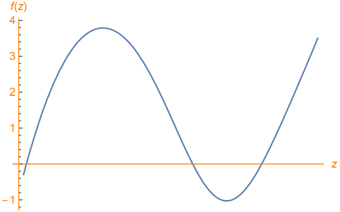


Figura: (a) Arbitrary smooth function $f(z)$

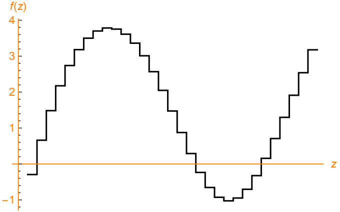
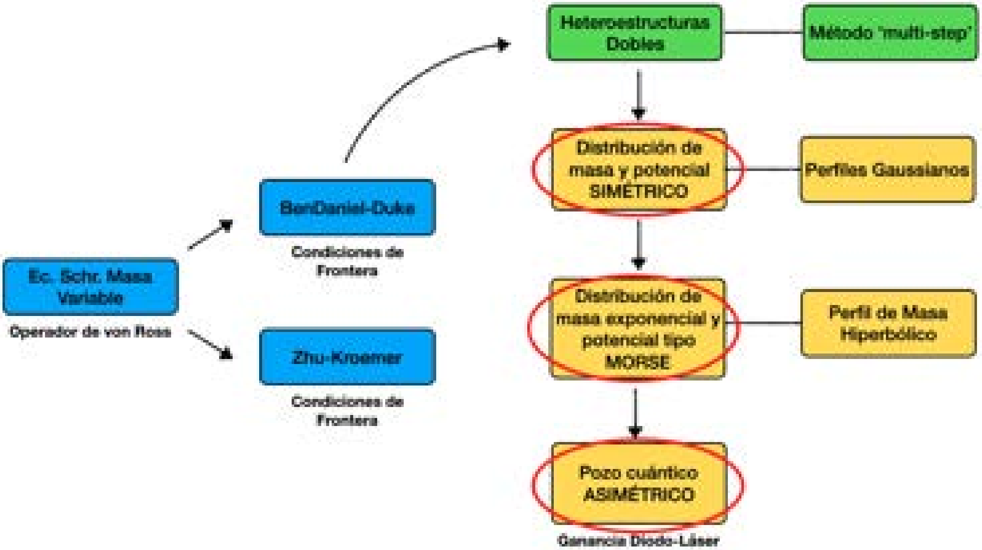


Figura: (b) Discrete representation of $f(z)$

Given an arbitrary smooth function $f(t)$ of mass or potential (a) it can be discretized through a succession of constant finite steps (b) given by Eq (24).

The poles of the coefficient R_c are approximations to the eigenvalues of the smooth problem.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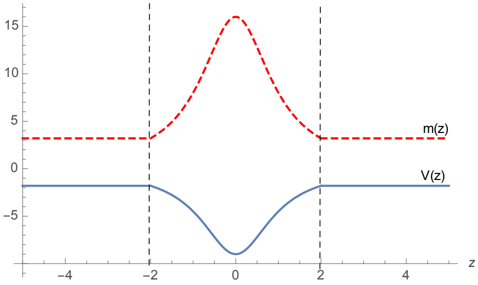
Symmetrical mass and potential distributions

We consider the **symmetric** model given by the following potential and mass distribution

$$V(z) = \begin{cases} V_0 \\ V_{\text{in}}(z) = -\frac{\mu^2}{1+z^2} \\ V_2 \end{cases}, \quad m(z) = \begin{cases} m_0 & ; \quad z < z_0 < 0, \\ m_{\text{in}}(z) = \frac{\sigma^2}{1+z^2} & ; \quad z_0 \leq z < z_1, \\ m_2 & ; \quad z_1 \leq z, \end{cases} \tag{32}$$

Graph shows the symmetric mass distribution and potential well of equation (36) as functions of z; $\sigma = 4, \mu = 3, z_0 = -2$. $z_1 = |z_0|$ and μ, σ are arbitrary real parameters. We define $V_{\text{in}}(z_0) = V_0 = V_2$ and $m_{\text{in}}(z_0) = m_0 = m_2$. Thus $V(z)$ and $m(z)$ are continuous.



Remembering, when we replacing

$$\psi(z) = m(z)^{1/4}\phi, \quad \rho = \int \sqrt{m(z)}dz, \tag{33}$$

in (3), the ϕ function satisfies the Schrödinger equation with 'constant mass'

Equation associated with (3)

$$-\frac{d^2\phi}{d\rho^2} + (\widetilde{V}(\rho) - E)\phi = 0, \tag{34}$$

$$\widetilde{V}(\rho) = V(z) + \frac{1}{2}\left(\eta + \frac{7}{8}\right)\frac{m'(z)^2}{m(z)^3} - \frac{1}{2}\left(\nu + \frac{1}{2}\right)\frac{m''(z)}{m(z)^2}. \tag{35}$$

$\nu = -1 - \beta, \quad \eta = -2(\beta + 1)(\alpha + 1) - 2\alpha^2$

Symmetrical mass and potential distributions

$$V(z) = \begin{cases} V_0 \\ V_{\text{in}}(z) = -\frac{\mu^2}{1+z^2} \\ V_2 \end{cases}, \quad m(z) = \begin{cases} m_0 & ; \quad z < z_0 < 0, \\ m_{\text{in}}(z) = \frac{\sigma^2}{1+z^2} & ; \quad z_0 \leq z < z_1, \\ m_2 & ; \quad z_1 \leq z, \end{cases} \tag{36}$$

(39) is the solution of the equation (modified Pöschl-Teller potential [2, 7])

$$\frac{d^2\phi}{d\rho^2} + \left(\kappa^2 + \frac{\lambda(\lambda-1)}{\sigma^2}\frac{1}{\cosh^2\frac{\rho}{\sigma}}\right)\phi = 0. \tag{37}$$

By solving the equation in complete one-dimensional space, with the condition that its solution vanishes at infinity, the energy spectrum ($\kappa^2 = E - \frac{1/4+2\eta-3\nu}{\sigma^2}$) is

$$\mathbf{E}_n = -\frac{(\lambda-1-n)^2}{\sigma^2} + \frac{1/4+2\eta-3\nu}{\sigma^2}; \quad n = 0, 1, 2\ldots, \lambda-1. \tag{38}$$

The solution is

$$\psi_{\rm in}(z) = \left(\frac{\sigma^2}{1+z^2}\right)^{1/4}(1+z^2)^{\lambda/2}\left\{P\,{}_2F_1\left(a,b,\frac{1}{2};-z^2\right)+Qz\,{}_2F_1\left(a+\frac{1}{2},b+\frac{1}{2},\frac{3}{2};-z^2\right)\right\}. \quad (39)$$

with

$$a = \frac{1}{2}(\lambda + i\kappa\sigma), \quad b = \frac{1}{2}(\lambda - i\kappa\sigma).$$

where

$$\kappa^2 = E - \frac{1/4 + 2\eta - 3\nu}{\sigma^2}, \quad \lambda(\lambda-1) = -(1/4 + 4\nu - 2\eta - \mu^2\sigma^2).$$

Symmetrical mass and potential distributions

$$\psi_{\text{in}}(z) = \left(\frac{\sigma^2}{1+z^2}\right)^{1/4} (1+z^2)^{\lambda/2} \left\{P \times {}_2F_1\left(a, b, \frac{1}{2}; -z^2\right) + Q \times z\,{}_2F_1\left(a+\frac{1}{2}, b+\frac{1}{2}, \frac{3}{2}; -z^2\right)\right\}.$$

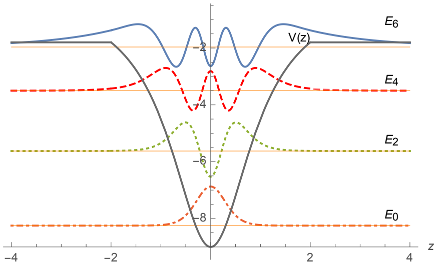


Figura: Even wavefunctions for energies $E_0 = -1.96428$, $E_2 = -3.5013$, $E_4 = -5.6250$ and $E_6 = 8.25$.

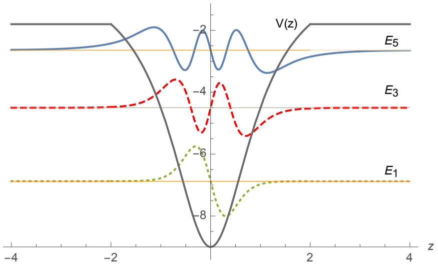


Figura: Odd wave functions for energies $E_1 = -2.63724$, $E_3 = -4.50009$ and $E_5 = -6.8750$.

Symmetrical well and mass

Heteroestructura doble (36) ($\sigma = 4, \mu = 3, z_0 = -2$)							
Condición BD-D							
	E_0	E_1	E_2	E_3	E_4	E_5	E_6
Ec. Transcendental , $E^{\text{BD-D}}$	-8.25	-6.875	-5.625	-4.50009	-3.5013	-2.63724	-1.96428
Polos de $R_c^{\text{BD-D}}$	-8.25	-6.875	-5.625	-4.50009	-3.5013	-2.63724	-1.96428
Ec. (38), $\mathbf{E}_n$	-8.25	-6.875	-5.625	-4.5	-3.5	-2.625	-1.875
Condición Z-K							
Ec. Transcendental , $E^{\text{Z-K}}$	-8.3099	-6.9297	-5.6745	-4.54428	-3.53899	-2.66042	-1.94466
Polos de $R_c^{\text{Z-K}}$	-8.3099	-6.9297	-5.6745	-4.54428	-3.53899	-2.66042	-1.94466
Ec. (38), $\mathbf{E}_n$	-8.3099	-6.9297	-5.6745	-4.54430	-3.539103	-2.65890	-1.90370

Values of the energies of the bound states of the symmetric potential well with symmetric position-dependent mass with parameters $\sigma = 4, \mu = 3, z_0 = -2$ using the BD-D and Z-K conditions .

Finally, a potential function and a position-dependent mass function are analyzed, both modeled by a pair of asymmetric parabolic wells given by the equations

$$V(z) = V0 \begin{cases} 1 \\ f(z) \\ g(z) \\ 1 \end{cases}, \quad m(z) = \begin{cases} m_0 & ; \quad z < b \\ m_1 + (m_0 - m_1) f(z) & ; \quad b \leq z < c, \\ m_1 + (m_0 - m_1) g(z) & ; \quad c \leq z < d, \\ m_0 & ; \quad d \leq z. \end{cases} \tag{40}$$

where

$$f(z) = \frac{(z - (c+a)/2)^2}{((c-a)/2)^2}, \quad g(z) = \frac{(z - (d+c)/2)^2}{((d-c)/2)^2}.$$

Graph showing the asymmetric parabolic quantum well as a function of z; $V_0 = 0.3$ eV, $a = 9.4$ nm, $b = 11$ nm, $c = 25$ nm, $d = 31$ nm, $m_1 = 0.0665 m_e$ and $m_0 = 0.0960 m_e$ (m_e= rest electron mass)

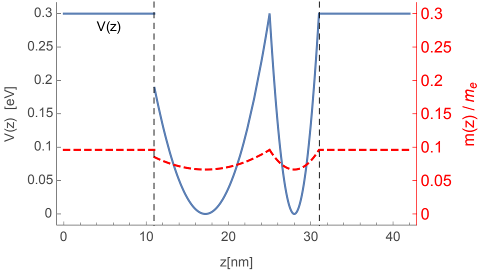
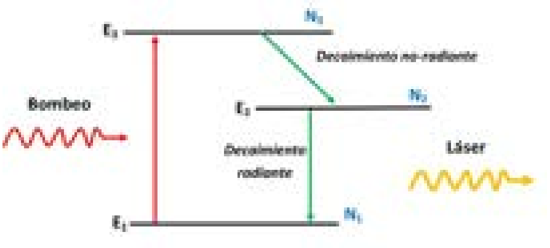


Table D

Double heterostructure (40) ($V_0 = 0.3$ eV, $a = 9.4$ nm, $b = 11$ nm, $c = 25$ nm, $d = 31$ nm, $m_1 = 0.0665\ m_e$, and $m_0 = 0.0960\ m_e$; $[E_n] =$ meV.)				
	E_1	E_2	E_3	$\overline{D}\,\%$
Ref [8]	50.527710	117.369463	156.513093	
Poles of $R_c^{\text{BD-D}}$	50.5284	117.34107	156.51738	0.009 %
Poles of $R_c^{\text{Z-K}}$	54.1197	130.65338	160.38424	6.974 %
Energy values (meV) for the first three bound states with constant mass $m^* = m_1 = 0.0665\ m_e$				
R_c poles	44.3005	109.30502	134.58205	

This example cannot be solved analytically (we couldn't). The energies of the bound states were obtained **numerically** in [8] using functions of the **orthonormalized basis** of the infinite square potential, here we obtained them by the **multi-step** method and compared them with those reported in [8].

Double asymmetric parabolic quantum well



Observation: The emission frequency ω and the *gain* of the laser are theoretically different depending on the initial choice of the ambiguity parameters α and β of the kinetic energy operator and not due only to the geometry of the system.

When using the BD-D condition, the difference between $|E_3 - E_2| = 39.17631$ eV, with the Z-K condition we have $|E_3 - E_2| = 29.730844$ eV, while the difference $|E_3 - E_1|$, which is the excitation energy needed for the electron to change from the ground state to the second excited state, essentially remains the same in both cases (105.98898 eV; 106.264524 eV)

Conclusions

- The energy spectrum (number of bound states and energy values) is sensitive to the mass profile used and in some cases the use of one boundary condition or another significantly influences the energy value.

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- The examples studied show that the average percentage difference between the spectrum obtained using the BD-D condition and that obtained using the Z-K condition increases when the rate of change in the mass profile tends to be large.

Conclusions

- The energy spectrum (number of bound states and energy values) is sensitive to the mass profile used and in some cases the use of one boundary condition or another significantly influences the energy value.
- The examples studied show that the average percentage difference between the spectrum obtained using the BD-D condition and that obtained using the Z-K condition increases when the rate of change in the mass profile tends to be large.
- The multi-step method can be used as a useful tool to solve the Schrödinger equation.

Conclusions

- Our methodology allows us to calculate the energy spectrum of double heterostructures for any ambiguity condition, as well as for potentials and masses that can be approximated by the equation (24).

Conclusions

- Our methodology allows us to calculate the energy spectrum of double heterostructures for any ambiguity condition, as well as for potentials and masses that can be approximated by the equation (24).
- We have shown quantitatively that the *gain* of the semiconductor laser diodes discussed in the reference [8] is strongly affected by the model ambiguity hypothesis. This evidences the emergent, and not “first principles”, character of the Schrödinger equation with position-dependent effective mass as discussed in the introduction of the thesis.

Thank you

Thank you!

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