PARTICLE IN A MULTI-STEP QUANTUM WELL

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Abstract. We developed the method of solving the Schrodinger equation for multi-step quantum well, with arbitrary step number. The solution very useful for modeling of semiconductor hetero-structures of varying composition.

1. Introduction

Semiconductor quantum structures - quantum wells, quantum wires, quantum dots are very important for modern electronics and optoelectronics. As in quantum structures additional parameters for controlling electrical and optical properties, such as size, shape and material distribution, appear. In the presented paper we investigate multistep quantum wells; particularly we find eigen functions and eigen values of particle (electron, hole) confined in it.

2. Theoretical framework

We model our physical potential with the following potential

$$V(x) = \begin{cases} V_N & |x| < L_N \\ V_{N-1} & L_N < |x| < L_{N-1} \\ \vdots & \\ V_2 & L_3 < |x| < L_2 \\ 0 & L_1 < |x| \end{cases} \tag{1}$$

where the depth and the width of each successive well is arbitrary

$$V_N < V_{N-1} < \ldots < V_1 < 0 \qquad \text{and} \qquad 0 < L_N < L_{N-1} < \ldots < L_1$$

If a particle is located in this potential and it's energy is $V_m < E < V_{m-1}$ then its wavefunction (odd and even) will be of this form:

$$\phi(x) = \begin{cases} Ae^{-\alpha_0 x} & x > L_1 \\ B_1 \cosh(\alpha_1 x) + C_1 \sinh(\alpha_1 x) & L_1 > x > L_2 \\ \vdots & \\ B_{m-1} \cosh(\alpha_{m-1} x) + C_{m-1} \sinh(\alpha_{m-1} x) & L_{m-1} > x > L_m \\ B_m \cos(a_m x) + C_m \sin(\alpha_m x) & L_m > x > L_{m-1} \\ \vdots & \\ B_{N-1} \cos(a_{N-1} x) + C_{N-1} \sin(\alpha_{N-1} x) & L_{N-1} > x > L_N \\ D \sin(\alpha_N x) \text{ or } D \cos(\alpha_N x) & L_N > x > 0 \end{cases} \tag{2}$$

expansion to x < 0 will have the same coefficients just with the different signs. Then these coefficients can be expressed as:

$$\begin{bmatrix} B_n \\ C_n \end{bmatrix} = T(n)^{-1}_{n,n} \left(\prod_{j=1}^{n-1} T(j)_{j+1,j} T(j)^{-1}_{j,j} \right) \Gamma \begin{bmatrix} A \\ 0 \end{bmatrix} \tag{3}$$

For the even case:

$$\begin{bmatrix} D \\ 0 \end{bmatrix} = T(N)^{-1}_{N,N} \left(\prod_{j=1}^{N-1} T(j)_{j+1,j} T(j)^{-1}_{j,j} \right) \Gamma \begin{bmatrix} A \\ 0 \end{bmatrix} \quad (4)$$

and for the odd case:

$$\begin{bmatrix} 0 \\ D \end{bmatrix} = T(N)^{-1}_{N,N} \left(\prod_{j=1}^{N-1} T(j)_{j+1,j} T(j)^{-1}_{j,j} \right) \Gamma \begin{bmatrix} A \\ 0 \end{bmatrix} \quad (5)$$

Here the terms $T(j)_{n,m}$ are some 2x2 matrices that depend on j,n,m. Equating the right hand side of the (4), (5) equating to 0 we obtain from the first component the energy spectrum for the odd wavefunction and from the second component - energy spectrum for the even wavefunction. However the equations are difficult to solve since the L's and V 's were taken arbitrary, nevertheless it may be possible to regularize the choice of those quantities in a way to get solvable equations for the energy spectrum

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