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Transfer Matrix Algorithm: Energy Eigenvalue Calculation of an Arbitrary Potential Profile

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Abstract

The main objective of this article is to study transfer matrix algorithm, energy eigenvalue calculation. This article gives the idea that, in quantum mechanics, the transfer matrix algorithm is a method for calculating the energy eigenvalues of an arbitrary potential profile. The algorithm is based on the transfer formalism, which expresses the wave function of a particle in a potential as a product of matrices. The transfer matrix algorithm is particularly well suitedfor potentials that are piecewise constant, such as the potentials often used in quantum dot and quantum well devices.

The transfer matrix algorithm begins with the construction of the transfer.

Keywords:- Energy,Eigenvalues, potential profile, transfer matrix method.

Introduction:-

Eigen energy values of well known potential shapes, e.g. finite well, is easy to calculate because of the symmetry of the problem. In real world the potentials are, in general, not symmetric and cannot be solved without suitable approximation to simplify the problem. In this project, I will explore a transfer matrix algorithm to find the eigenvalues of a potential system with an arbitrary shape. In this method, the basic principle is the approximation of an arbitrary-shaped potential by a series of piece wise constant functions of known solution (Fig 1). Since the solution can easily be found in given piece of a potential, the total transfer matrix can be derived by a number of subsequent matrix multiplication of the corresponding potentials. From the total transfer matrix, energy eigenvalues can be extracted.

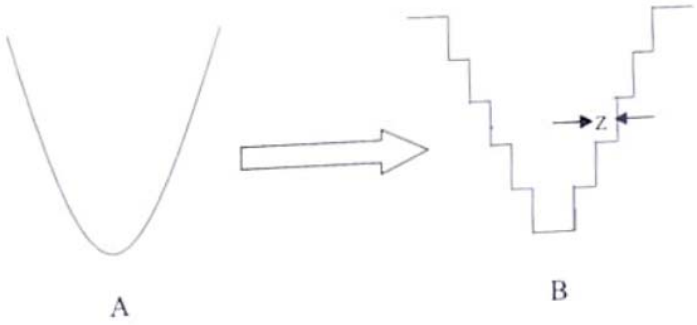

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Figure 1. Any arbitrary potential (A) can be approximated as a combination of piecewise linear potential (B) of known solution. Approximation becomes more realistic as thickness of the piece-wise potential "Z" becomes smaller.

To develop the theory of transfer matrix assume an arbitrary potential structure approximated as a set of piece-wise potentials, as shown in Figure 2. We can imagine that a wave incident on the structure from one side, with a given energy E. When the wave hits the surface, there will be some reflection and transmission. We can derive a matrix that relates the forward and the backward amplitudes, A_i and B_i just to the left of the *i"* interface to the forward and the backward amplitudes A_{i+1} and B_{i+1} just to the right of the*i"*interface (Figure 3). By multiplying those matrices together for all the layers, we can construct a single transfer matrix for the whole structure, which will enable us to analyze the entire multilayer structure. Each layer *i* will have a potential energy V_i, a thickness t_i and some effective material parameter m^i_{eff} (e.g.. this parameter could be electron mass in semiconductor). The position of the i^{th} interface relative to the position of the first interface in figure 2 can be written as

$$Z_l = \sum_{n=2}^{l} t_{n-1} \qquad (1)$$

In any given layer, if $E>V_i$, we will, in general, have a forward propagating wave (i.e. propagating to the right in Figure 2) of the form $A = A_0$, exp[$ik_i (z - z_i)$ and a backward propagating wave of the form $B = B_0$ exp[$-ik_i (z - z_i)$]. where A and B are complex numbers representing the amplitude of the forward and the backward waves, respectively.

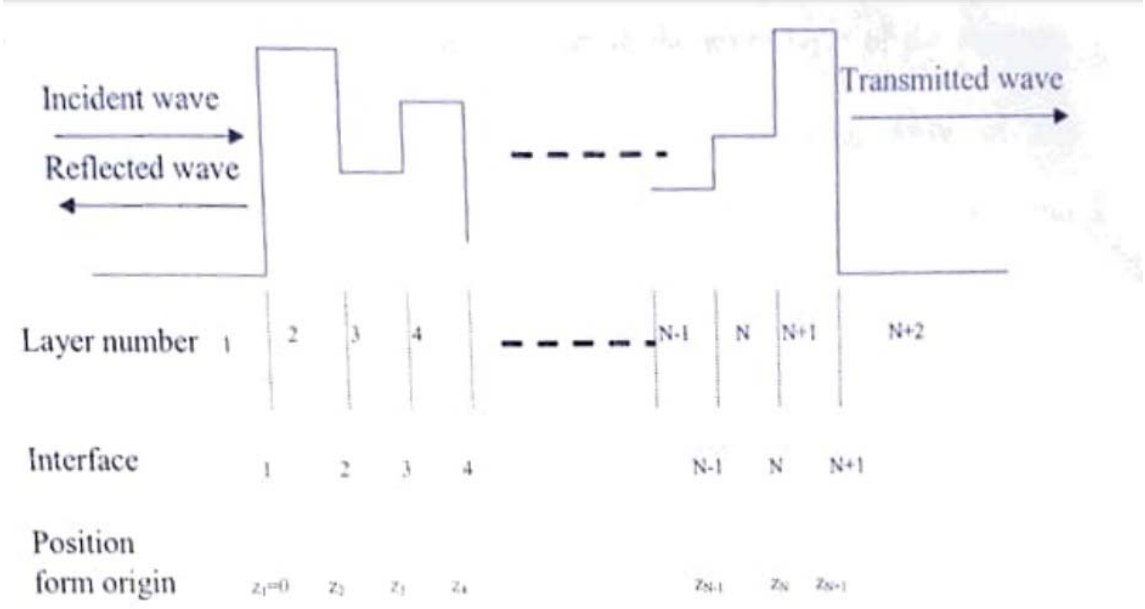

Figure 2. Schematic of the layered structure giving an arbitrary potential profile. The position of each layer interface and their distance from the origin are also depicted.

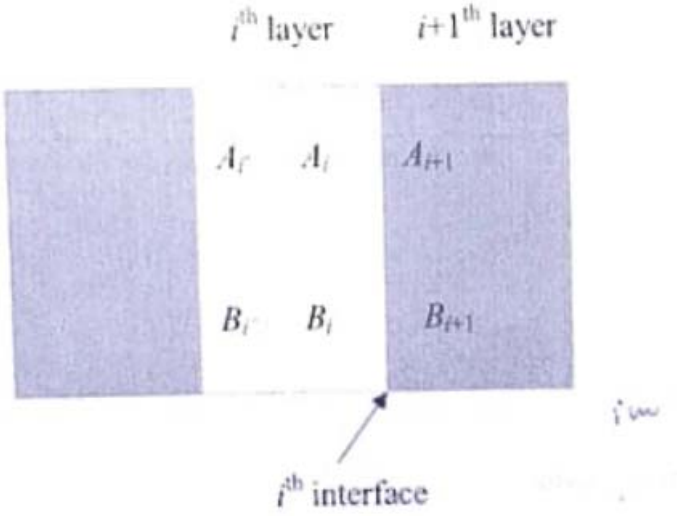

Figure 3. Constants *A* and *B* across the arbitrary i^{th} interface of two adjacent layers.

In this case

$$K_i = \sqrt{\frac{2m^i_{eff}(E-V_i)}{h^2}} \quad (2)$$

Where m^i_{eff} is the effective material parameter in the given layer of the structure Similarly, if $E < V_i$, we will have a forward decaying wave of the form $A = A_0$, $\exp[-k_i (z - z_i)]$, and a backward decaying wave of the form $B = B_0 \exp[k_i (z - z_i)]$, where

$$\kappa_i = \sqrt{\frac{2m^i_{eff}(V_i-E)}{h^2}} \quad (3)$$

One can notice that, $K_i = i\kappa_i\,(kappa)$; hence, for the mathematical simplicity, we can define the wave vector only by Eq. (2). Where*k* can be imaginary or real, depending on the imposed condition. Hence in any given layer, the wave function can be written as

$$\zeta(z) = A_i e^{ik_i(z-z_i)} + B_i e^{-ik_i(z-z_i)} \quad (4)$$

Boundary condition: If the effective material parameter of the two adjacent layers were the same across the interface, we would simply match the value and the derivative of the wave function at the interface as

$$\zeta^i|_{z=z_i} = \zeta^{i+1}|_{z=z_i+1} and \frac{\partial \zeta^i}{\partial z}|_{z=z_i} = \frac{\partial \zeta^{i+1}}{\partial z}|_{z=z_i+1} \quad (5)$$

This simple condition is not correct for the potential structure where the effective material parameter is different across the potential. The correct boundary conditions should be

$$\zeta^i|_{z=z_i} = \zeta^{i+1}|_{z=z_i+1} and \frac{1}{m^i_{eff}}\frac{\partial \zeta^i}{\partial z}|_{z=z_i} = \frac{1}{m^{i+1}_{eff}}\frac{\partial \zeta^{i+1}}{\partial z}|_{z=z_i+1} \quad (6)$$

Here, m^i_{eff} is the effective material parameter in the i^{th} layer. Using Eqs. (4) and (6), the transfer matrix can be found to relate the complex constants *A* and *B* of the i^{th} and the

$(i+1)^{th}$ layers. The first boundary condition defines the continuity of the wave function, ζ at the i^{th} interface, as shown schematically in Figure 3 and gives

$$\zeta = A_i + B_i = A_{i'+1} + B_{i'+1} \quad (7)$$

and the second boundary condition defines the continuity of $(1/m^i_{eff})d\zeta/dz$ across the i^{th} interface and gives

$$A_i - B_i = \Delta_i (A_{i'+1} - B_{i'+1}) \quad (8)$$

Where,

$$\Delta_i = \frac{k_{i+1} m^i_{eff}}{k_i m^{i+1}_{eff}} \quad (9)$$

Solving Eqs. (7) and (8) gives

$$A_i = A_{i'+1}\left(\frac{1+\Delta_i}{2}\right) + B_{i'+1}\left(\frac{1-\Delta_i}{2}\right), \quad (10)$$

And

$$B_i = A_{i'+1}\left(\frac{1-\Delta_i}{2}\right) + B_{i'+1}\left(\frac{1+\Delta_i}{2}\right) \quad (11)$$

which can be written in the matrix form as

$$[A_i B_i] = D_i \left[A_{i'+1} B_{i'+1}\right] \quad (12)$$

Where

$$D_i = \begin{vmatrix} \frac{1+\Delta_i}{2} & \frac{1-\Delta_i}{2} \\ \frac{1-\Delta_i}{2} & \frac{1+\Delta_i}{2} \end{vmatrix} \quad (13)$$

For the propagation in a given layer, i, whose layer thickness is t_i, *we have*

$$A_{i'} = A_i exp\,(-ik_i t_i)$$
$$B_{i'} = B_i exp\,(ik_i t_i) \quad (14)$$

Which again can be written in matrix form as

$$\begin{bmatrix} A_{i'} \\ B_{i'} \end{bmatrix} = P_i \begin{bmatrix} A_i \\ B_i \end{bmatrix} \quad (15)$$

With

$$P_i = \begin{vmatrix} \exp(-ik_i t_i) & 0 \\ 0 & \exp(ik_i t_i) \end{vmatrix} \quad (16)$$

Combining Eqs. (12) and (15) we can have a transfer matrix equation combining the coefficients in the given i^{th} layer to the coefficients in the next $i+1^{th}$ layer as

$$\begin{pmatrix} A_l \\ B_l \end{pmatrix} = \tau_{l(l+1)} \begin{pmatrix} A_{l+1} \\ B_{l+1} \end{pmatrix}, \quad (17)$$

Where

$$\tau_{l(l+1)} = D_l P_l = \begin{pmatrix} 1 + \frac{m^l_{eff} k_{l+1}}{m^{l+1}_{eff} k_l} & 1 - \frac{m^l_{eff} k_{l+1}}{m^{l+1}_{eff} k_l} \\ 1 - \frac{m^l_{eff} k_{l+1}}{m^{l+1}_{eff} k_l} & 1 + \frac{m^l_{eff} k_{l+1}}{m^{l+1}_{eff} k_l} \end{pmatrix} \begin{bmatrix} e^{-ik_l + t_{l+1}} & 0 \\ 0 & e^{-ik_l + t_{l+1}} \end{bmatrix} \quad (18)$$

Here, t_i is the thickness of the i^{th} layer. For a large number of layers, as shown in Figure 2 for N+2 layers, the total transfer matrix can be written as the product of the transfer matrices across each layer

$$\begin{pmatrix} A^1 \\ B^1 \end{pmatrix} = \tau_{total} \begin{pmatrix} A^{l_{N+2}} \\ B^{l_{N+2}} \end{pmatrix} \quad (19)$$

Where

$$\tau_{total} = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix} = \tau_{12}\tau_{23}\tau_{34} \dots \dots = D_1 P_2 D_2 P_3 D_3 \dots \dots P_{N+1} D_{N+1} P_{N+2} \quad (20)$$

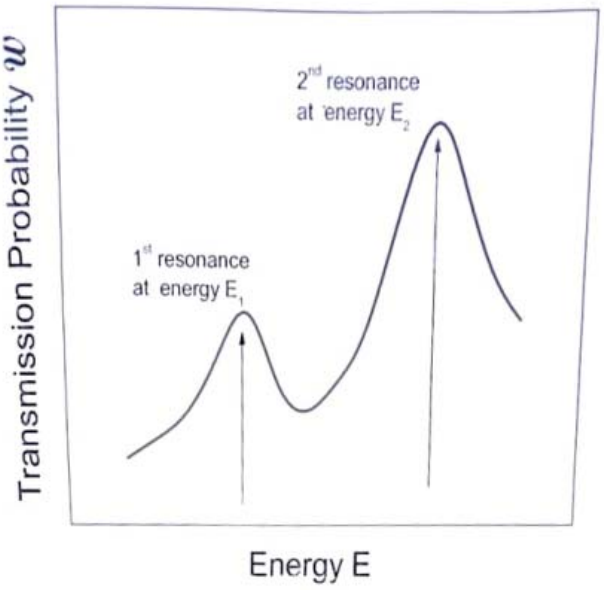

Figure 4. Schematic for the transmission probability *vs*. energy plot. The energy corresponding to the maximum transmission probability gives the corresponding energy level of the system.

We now require $A^1 = B^{iN+2} = 0$ for decaying solutions in the first and the last barriers, which corresponds to the resonant condition in the potential system and the corresponding energy would be the eigen energy of the system. Hence, the condition to find the eigen energy stales can be written as

$$w_{11}(E) = 0 \qquad (21)$$

Eq. (21) has to be solved numerically. At a given energy E, when the energy of the system matches the energy E of the wave impinged on the structure, a resonance occurs. During the resonance, the probability of transmission of the wave across the structure would be the maximum. The amplitude of the transmitted wave during the resonance is given as $1/w_{11}$. It is more convenient to work with a positive definite number, hence, the probability density of the transmitted wave, $W = |1/w_{11}|^2$ can be used to track the resonance. As shown schematically in Figure 4, the transmission probability can be found for all the possible expected energy range. During the resonance, W becomes maximum at certain energies $E=E1, E2....$, giving the first, second,... energy levels of the system.

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