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Propagation of ballistic electrons at imaginary wavenubmers through periodic structures

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Abstract

This article presents a theoretical and numerical discussion of the propagation of ballistic electrons through a periodic structure. It is known that, the propagation of electromagnetic waves through a metamaterial characterized by ε and μ is not allowed when ε and μ are different in signs. In analogy our structure acts as a metamaterial for the propagation of ballistic electrons. In particular, we have shown that the transmission of ballistic electrons is possible through the structure when the wave number is imaginary. The main parameters of each layer are given and the required equations for the ballistic electron propagation are presented. Transfer matrix method is used to find out the characteristics of the transmitted powers of the structure. In the numerical results, the mentioned powers and the phase time for ballistic electrons are computed and illustrated as a function of the layer thickness, the electron effective mass, the region energy, and the number of periods.

Keywords:
Ballistic electrons, imaginary wavenumber, propagation, quantum theory, Schrödinger equation, transmission.

1. Introduction:

There is an analogous between electromagnetic waves in classical theory and ballistic electrons in quantum theory, this can be seen as follows. Electromagnetic radiation consists of electromagnetic waves which are synchronized oscillations of electric and magnetic fields E and B, respectively. The oscillations of the two fields are perpendicular to each other and perpendicular to the direction of energy and wave propagation [1, 2]. The interaction of the electromagnetic radiations with the a matter is governed by the electric permittivity ε and the magnetic permeability μ of that medium. For a given expression of the electric field E of the electromagnetic waves Maxwell's equation can be used to calculate the corresponding magnetic field B of that waves [3, 4].

According to quantum theory for ballistic electrons, we have the charge carrier effective mass m, the potential energy V, and the energy E of propagating charge carriers. Moreover, the propagation of the ballistic electrons can be described by the Schrödinger wave equation and its plane wave solution ψ and its x first derivative [5, 6]. Due to the quantum-optical analogies, the parameters m and E − V for ballistic electrons correspond to the constants ε and μ of light propagation. The solution of the plane wave ψ and its first derivative correspond to the E and B fields in the electromagnetic wave propagation. In addition, the wave number k = [2m(E − V)]1/2/ħ for ballistic electron propagation correspond to the wave vector k = (ω/c)n, in electromagnetic wave propagation, where n = ± (εμ)1/2 is the refractive index of the medium [7].

Metamaterials (or left-handed materials) are man-made composites that possess, in a certain frequency region, negative real parts of both the permittivity and permeability [8, 9]. These materials have several peculiar characteristics such as negative refractive index, negative refraction and antiparallel orientation of the wave vector $\vec{k}$ and the pointing vector $\vec{S}$ [10, 11]. Left-handed materials have ability to amplify evanescent waves and used for construction of a perfect lens [12, 13]. Other different electrodynamic properties compared with regular materials are observed, including reversal of the Doppler effect, reversal of the Cerenkov radiation and reversal of convergence and divergence in convex and concave lenses etc.[14, 15]. As reported in [16, 17], in optical theory, the transmission is zero and all incident radiations are being reflected when ε and μ are different in signs which makes the refractive index imaginary. To observe the transmission of radiations, the refractive index n of a material must be real (positive or negative). This means that, electromagnetic waves can propagate in a medium when ε and μ are both positive as in regular media or both negative as in metamaterials.

D Dragoman et al [18] have studied ballistic electron propagation in periodic structures containing mono- and few –layer graphene regions and/or semiconducting stripes. D Dragman et al [19] have shown a metamaterial for ballistic electrons, which consists of a quantum barrier formed in a semiconductor with negative effective electron mass. H Huang et al [20] have demonstrated the consequence of negative effective mass density in acoustic metamaterials. W Kuehn et al [21] have investigated theoretically coherent ballistic motion of electrons in a periodic potential. Y Zhang et al [22] have demonstrated experimentally total negative refraction in real crystals for ballistic electrons and light.

In this study, we demonstrate the theoretical and analytical investigations of the propagation of ballistic electrons and electromagnetic waves through periodic structures. In optical theory the propagation of electromagnetic waves is not allowed and evanescent waves are formed when ε and μ of the structure are different in signs. In our work we show that, the propagation of ballistic electrons is possible and significant transmission is observed when one of the m and E – V parameters is negative and when the structure behave like metamaterial with both m and E – V negative. The plane wave solution of the Schrödinger equation and its first derivative are determined in each region. The boundary conditions are imposed at each interface to obtain the transmission coefficients by a transfer matrix method [23, 24, 25]. In the numerical analysis, the mentioned coefficients and the phase time for ballistic electrons in the metamaterial propagation regime are calculated as a function of the energy of the electron, the conduction band potential energy, the effective mass of the electron, the number of periods, and the thickness of each layer.

2. Theory:

Consider a periodic structure consisting of N periods bounded by two different media labeled by in and out as shown in Fig 1. Each period has two layers characterized by thicknesses d1and d2, electron effective masses m1 and m2, potential energies V1 and V2 as shown in the figure. A ballistic electrons incident on the plane x = 0 with normal incidence to the normal to the boundary, for simplicity.

According to quantum mechanics the ballistic electrons have wavelike properties described by the Schrödinger wave equation [26],

$$-\frac{\hbar^2}{2m_\ell}\frac{d^2\psi_\ell}{dx^2}+(V_\ell-E)\psi_\ell=0 \qquad (1)$$

Where ψ_ℓ is the plane wave solution in each region takes the form [26],

$$\psi_\ell = A_\ell e^{ik_\ell x} + B_\ell e^{-ik_\ell x} \qquad (2)$$

Where A_ℓ and B_ℓ are the amplitude of forward and backward traveling waves (ℓ = 1, 2, 3 … represents the region order) , $k_\ell = \sqrt{2m_\ell(E - V_\ell)}/\hbar$ is the wave number inside the corresponding material. Due to our

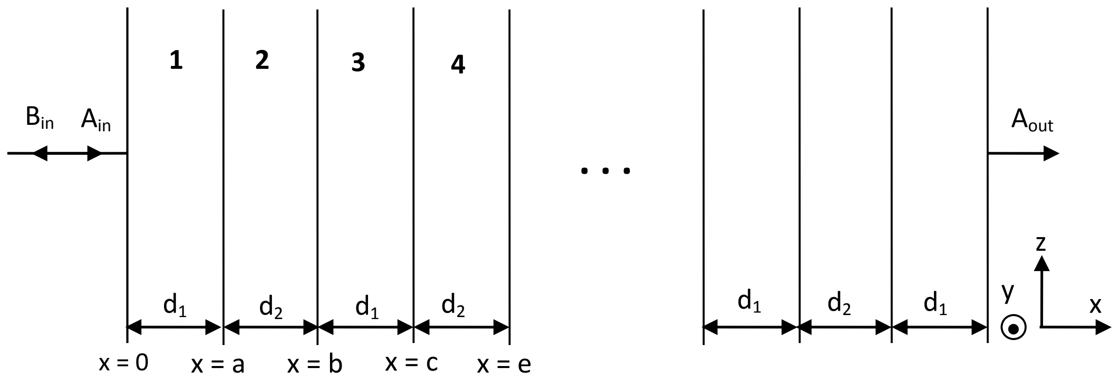

Figure 1: Schematic representation of a periodic structure of N periods embedded between two different media.

description of metamaterials given above, the ballistic electrons exist in metamaterials when both m_ℓ and $(E - V_\ell)$ have negative values.

The x derivative of ψ_ℓ normalized to the electron effective mass,

$$\frac{1}{m_\ell}\frac{d\psi_\ell}{dx} = iA_\ell P_\ell e^{ik_{\ell x} x} - iB_\ell P_\ell e^{-ik_{\ell x} x} \qquad (3)$$

where

$$P_\ell = \frac{k_\ell}{m_\ell} \qquad (4)$$

Matching the boundary conditions for ψ_ℓ and its x derivative at the interface x = 0 yields,

$A_{in} + B_{in} = A_1 + B_1$ (5)

$A_{in}P_{in} - B_{in}P_{in} = A_1P_1 - B_1P_1$ (6)

These two equations can be written in a matrix form,

$$\begin{pmatrix} 1 & 1 \\ P_{in} & -P_{in} \end{pmatrix}\begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ P_1 & -P_1 \end{pmatrix}\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \qquad (7)$$

This equation can be rewritten as,

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+\frac{P_{in}}{P_1} & 1-\frac{P_{in}}{P_1} \\ 1-\frac{P_{in}}{P_1} & 1+\frac{P_{in}}{P_1} \end{pmatrix}\begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} \qquad (8)$$

or

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = m_1\begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} \qquad (9)$$

where

$$m_1 = \frac{1}{2}\begin{pmatrix} 1+\frac{P_{in}}{P_1} & 1-\frac{P_{in}}{P_1} \\ 1-\frac{P_{in}}{P_1} & 1+\frac{P_{in}}{P_1} \end{pmatrix} \qquad (10)$$

Following the same procedure at the interface x = a, where a = d1 we have,

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = m_2\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \qquad (11)$$

where

$$m_2 = \frac{1}{2}\begin{pmatrix} \left(1+\frac{P_1}{P_2}\right)e^{-ik_{2x}d_1+ik_{1x}d_1} & \left(1-\frac{P_1}{P_2}\right)e^{-ik_{2x}d_1-ik_{1x}d_1} \\ \left(1-\frac{P_1}{P_2}\right)e^{ik_{2x}d_1+ik_{1x}d_1} & \left(1+\frac{P_1}{P_2}\right)e^{ik_{2x}d_1-ik_{1x}d_1} \end{pmatrix} \qquad (12)$$

Substitute about the matrix $\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$ from eq 9 into eq 11,

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = m_2 m_1\begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} \qquad (13)$$

With the interface x = b, where b = d1 + d2,

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = m_3\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} \qquad (14)$$

where

$$m_3 = \frac{1}{2}\begin{pmatrix} \left(1+\frac{P_2}{P_3}\right)e^{-ik_{3x}(d_1+d_2)+ik_{2x}(d_1+d_2)} & \left(1-\frac{P_2}{P_3}\right)e^{-ik_{3x}(d_1+d_2)-ik_{2x}(d_1+d_2)} \\ \left(1-\frac{P_2}{P_3}\right)e^{ik_{3x}(d_1+d_2)+ik_{2x}(d_1+d_2)} & \left(1+\frac{P_2}{P_3}\right)e^{ik_{3x}(d_1+d_2)-ik_{2x}(d_1+d_2)} \end{pmatrix} \qquad (15)$$

Substitute about the matrix $\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$ from eq 13 into eq 14,

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = m_3 m_2 m_1 \begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} \qquad (16)$$

With the interface x = c, where c = 2d1 + d2,

$$\begin{pmatrix} A_4 \\ B_4 \end{pmatrix} = m_4 \begin{pmatrix} A_3 \\ B_3 \end{pmatrix} \qquad (17)$$

To find the matrix m4, in eq 5 perform, d1→ 2d1 and modify the subscripts of k and P as 2→3, 3→4.

Substitute about the matrix $\begin{pmatrix} A_3 \\ B_3 \end{pmatrix}$ from eq 16 into eq 17,

$$\begin{pmatrix} A_4 \\ B_4 \end{pmatrix} = m_4 m_3 m_2 m_1 \begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} \qquad (18)$$

Still with the same procedure at all of the other interfaces yields,

$$\begin{pmatrix} A_{out} \\ B_{out} \end{pmatrix} = m_f m_{f-1} \ldots m_4 m_3 m_2 m_1 \begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} \qquad (19)$$

where the subscript f denotes for the final interface.

The product of 2 x 2 matrices is still 2 x 2 matrix, thus writing,

$$\begin{pmatrix} A_{out} \\ B_{out} \end{pmatrix} = M \begin{pmatrix} A_{in} \\ B_{in} \end{pmatrix} \qquad (20)$$

where

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = m_f m_{f-1} \ldots m_4 m_3 m_2 m_1 \qquad (21)$$

which is the transfer matrix that relates the amplitudes Ain and Bin in the incident medium to the amplitude Aout in the emerging medium (note that Bout = 0). Then,

Aout=M11Ain+M12Bin (22)

0 = M21Ain + M22Bin (23)

Let

$$t = \frac{A_{out}}{A_{in}} = \frac{M_{11}M22 - M_{12}M_{21}}{M_{22}} \qquad (24)$$

and

$$r = \frac{B_{in}}{A_{in}} = -\frac{m_{21}}{m_{22}} \qquad (25)$$

The transmission and reflection coefficients T and R respectively, are defined as [6],

$$T = \frac{P_{out}}{P_{in}} |t|^2 \, , \quad R = |r|^2 \qquad (26)$$

To check the formation of evanescent waves we perform the following [6], The characteristic matrix of a period of tow layers with thicknesses d1, d2 inserted between the incident and the transmitted media is,

M=M1M2= $\begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$ (27)

where

$$M_1 = \begin{pmatrix} \cos(k_{1x}d_1) & -\sin(k_{1x}d_1)/P_1 \\ P_1 \sin(k_{1x}d_1) & \cos(k_1 d_1) \end{pmatrix} \quad (28)$$

and M2 is the same with 1→2.

The characteristic matrix of a period with thicknesses d = d1 + d2 inserted between the incident and the transmitted media is,

$$M = \begin{pmatrix} \cos(k_x d) & -\sin(k_x d\ )/P \\ P\sin(k_x d) & \cos(k_x d) \end{pmatrix} \quad (29)$$

where kx is the corresponding wavenumber. From 27 and 29 we have,

cos(kxd)=(m11+m22)/2 (30)

Wave propagation through the entire structure is allowed only if [6],

|cos(kxd)=(m11+m22)/2|≤1 (31)

3. Numerical Results

In this section, the phase kd given in eq 31 is calculated as a function of the energy of the electron for changing values of the potential energies constituted each period and then for changing values of the thicknesses of the layers. The transmission and reflection coefficients are calculated as a function of the electron energy for changing values of the number of periods and thicknesses of the layers. In the calculations, normal incidence is considered for simplicity. The electron effective mass in the layers of each period are considered to be m1 = .04mo, m2 = – .02mo, where mo is the free electron effective mass. The electron effective mass in the incident and transmitted media are selected to be min = mout = .03mo. The potential energy in the incident and transmitted media are assumed to be Vin = Vout = 0.

Figure 2 shows the phase kd as a function of the energy of the electrons for zero potential energy of the second layer constituted each period, V2 = 0 and for different values of the potential energy of the first layer, V1 = .2 eV, .4 eV, .7 eV (part a) and for different values of thicknesses of each period, d1 = d2 = 2 nm, 3 nm, 3.5 nm (part b). Through this figure we can show that, the verification of eq 31 is the main condition for the propagation to be possible through the structure. For example in figure 2a, for the line corresponds to V1 = .4 eV, eq 31 is valid in the E range .2 - .9 eV and hence the propagation is possible in this range. In the part of E range .2 - .4 eV, k1 and k2 are both imaginary, because m1 is positive, E – V1 is negative, m2 is negative, E – V2 is positive. In the part of E range .4 - .9 eV, k1 is real positive and k2 is imaginary, since both m1 and E – V1 are both positive, m2 is negative, E – V2 is positive. This in itself is contrary to the optical theory in which the spread of electromagnetic waves is not allowed when k is imaginary. The same illustration applies to the lines correspond to V1 = .2 eV and V1 = .7 eV in part a and to the three lines in part b of Fig 2.

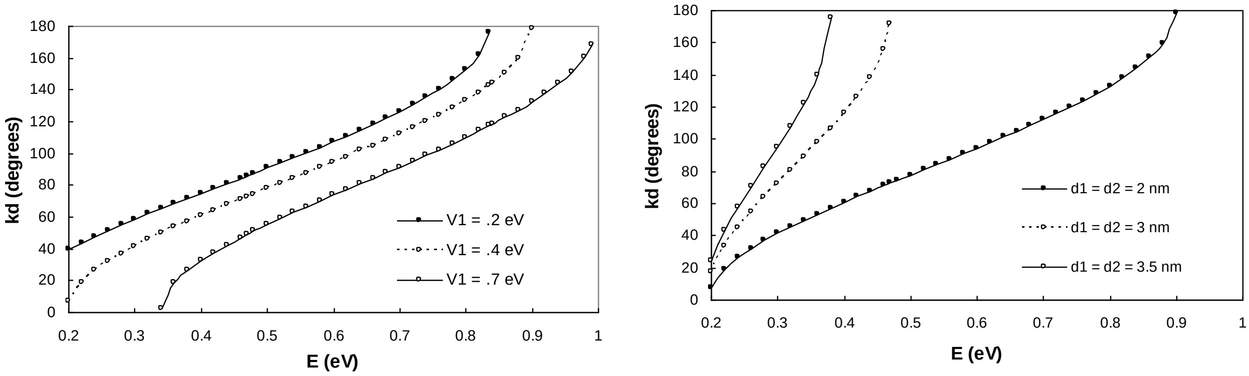

Figure 2: The phase kd as a function of the energy of the electrons for V2 = 0 and for (a) V1 = .2 eV, .4 eV, .7 eV, (b) d1 = d2 = 2 nm, 3 nm, 3.5 nm.

Figure 3 presents the transmission (a) and reflection (b) coefficients versus the energy of the electron at V1 = .4 eV, V2 = 0, for different values of the number of periods N = 5, 10 and for different values of thicknesses d1 = d2 = 2 nm, 3 nm. The energy of the electron is changed between .15 eV and .35 eV, because the simultaneously imaginary values of k1 and k2 can be realized in this range. As it can be seen from Fig 3a, the transmission is significant and has notice values in the mentioned range of the electron energy. This emphases that, the behavior of the propagation of ballistic electrons as described by quantum theory is different from the behavior of the propagation of electromagnetic wave as described by optical theory.

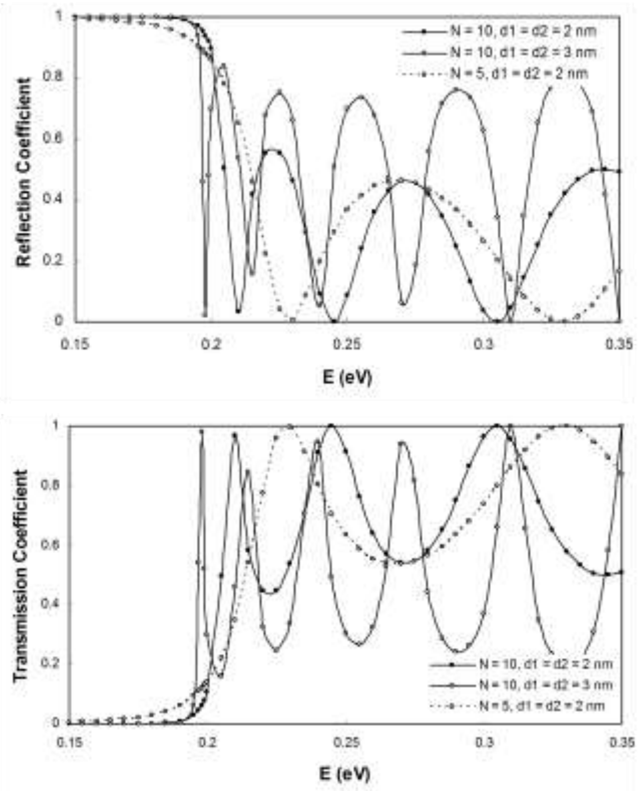

Figure 3: The transmission (a) and reflection (b) coefficients versus the energy of the electron for V1 = .4 eV, V2 = 0, N = 5, 10, d1 = d2 = 2 nm.

4. Conclusions

In this work, the propagation of ballistic electrons through a layered structure is studied in details with the emphases on the imaginary wave numbers. First of all, the structure is described and its main parameters are defined. Then the required equations for the solution of the Schrödinger equation and its first derivative, the propagation constant, and the phase constant are provided. Later, the boundary conditions are applied and the transfer matrix method is used to obtain the transmission and reflection coefficients in the closed form. Finally, the phase constant and the mentioned coefficients as a function of electron energy, the potential energy of the layers, the thicknesses of the layers, and the number of periods are studied numerically to observe the behavior of the structure when the propagation constant is imaginary. As it can be seen from the theoretical and numerical results, if the wave number is imaginary, the propagation of the charge carrier through the structure is possible and the transmission is observable which is contrary to the classical theory in optics.

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