THE SHAPE EFFECTS ON THIN WIRES: DENSITY OF STATES

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Abstract

In a theoretical study three shapes of wire are considered, namely rectangular, square and circular cross-sectional wires under size quantization conditions. According to the effectively free electron model, Schroedingr equation is solved in the appropriate conditions. These solutions are imposed by the suitable boundary conditions in each case, and then the zeros of Bessel function are involved for calculating the density of states. Comparison is made among the three shapes under consideration. It was found that the density of states is shape-dependent.

Introduction :

The shape and dimensions of a sample are important in micro scale physics. When the size of the solid sample becomes of order of either the mean free path or the De-Brogle wavelength, two phenomena arise. They are either the classical [1] or quantum [2] size effects. Abdelraheem and Cottey [3] have studied the quantum size effects in wedge-shaped films. Their results give a different approaches from the usual slab. The singularity in the density of states in wedges is of a square root form which is different from the step-like singularity of a slab.

When we are interested in the surface and shape effects, the eigenvalues distribution is very important. The distribution of algin-frequencies for a finite volume of arbitrary shape and for the general boundary conditions on the surface has been investigated by Ballan and Bloch [4]. In the limit of wavelength small compared to any characteristic dimensions it was found that the eigenvalue distribution has an oscillating part. They [5] considered the shape of a slab as well as a sphere, and it was found that in the slab the density of states has θ-function singularity. For spherical shape it was found that the modulus of Fourier transform of the eigenvalue density oscillates with a characteristic length.

In this work we shall consider the distribution of the eigenvalues for three different shapes, namely a rectangular, square and circular thin wire and then a comparison among them is made. The motive for this is the investigation of the density of states because it represents a crucial point for all transport coefficients such as the longitudinal and transverse conductivity [6 & 7].

The model :

The electrons and/or holes in the sample are regarded as independent particles. These particles move in potential wells with flat bottoms and infinitely high walls and there masses are equal to the corresponding effective mass m* of the bulky sample.

Eigevalues and eigefunctions :

According to the model considered above, Schroedinger equation.

$$\nabla^2 \Psi + k^2 \Psi = 0 \qquad (1)$$

with

$$k^2 = 2\, m^* E/h^2 \qquad (2)$$

has for rectangular and square wires the solutions

$$\Psi(x) = A_1 e^{ik_x x} + B_1 e^{-ik_x x}\,, \qquad (3)$$

$$\Psi(y) = A_2 e^{ik_y y} + B_2 e^{-ik_y y}\,. \qquad (4)$$

and

$$\Psi(z) = A_3 e^{-ik_z z} + B_3 e^{-ik_z z}\,. \qquad (5)$$

where A_i and B_i (i =1,2 & 3) are costants to be determined and k_x, k_y and k_z are given such that

$$k_x^2 + k_y^2 + k_z^2 = k_E^2 \quad (6)$$

and for a cylindrical wire the cylindrical polar coordinates(r, θ, z) are more suitable to find solutions of equation (1)

$$\Psi(z) = C_1 e^{ik_z z} + D_1 e^{-ik_z z}, \quad (7)$$

$$\Psi(y) = C_2 e^{in\theta} + D_1 e^{in\theta} \quad (8)$$

and

$$R(r) = C_3 J_n(dr) + D_3 Y_n(dr) \quad (9)$$

where C_i and D_i (i= 1, 2, 3) are constnts, J_n (dr) and Y_n (dr) are Bessel functios of the first and second kind, respectivley, and n is their order, k is related to k_z and k_E by the equation.

$$k^2 = k_E^2 + k_z^2 \quad (10)$$

4. Bounary conditions :

For wires under consideration we choose the boundary conditions in such a way that: (i) For rectangular and square wire d,b << L_z so that the periodic boundry conditions are imposed on solutions (5) and the rigid boundary condition on equations (3) and (4). This produces under size quatization the eigenfunctions

$$\Psi_{plk_z} = (2/\Omega)^{1/2} e^{ik_z z} \sin(p\Pi y/b) \sin(l\Pi x/d) \quad (11)$$

where Ω , b and d are the length and the width of the wire, respectively, and

$$k_x = l\,\Pi/d, \qquad l = 1,2,3, ... \quad (11a)$$

$$k_y = p\,\Pi/b, \qquad p = 1,2,3, ... \quad (11b)$$

and

$$k_z = 2q\,\Pi/L_z, \qquad q = 0, \pm 1, \pm 2, \pm 3, ... \quad (11c)$$

This means that the eigenvalues k_x and k_y are distributed uniformly

$$(k_x)_{l+1} - (k_x)_l = \Pi/d$$

and

$$(k_y)_{p+1} - (k_y)_p = \Pi/b$$

The corresponding eigenvalues of these wave functions are

$$E_{plk} = \varepsilon_x 1^2 + \varepsilon_y p^2 + h^2 k^2_z / 2m^* \quad (12)$$

where

$$\varepsilon_x = \Pi^2 h^2 / 2m^* d^2 \text{ and } \varepsilon_y = \Pi^2 h^2 / 2m^* b^2 \quad (13)$$

(ii) For cylindrical wire $L_z >> R_0$ where R_0 is the wire radius. So that the periodic boundary conditioinis can be imposed on equation (7) and the rigid boundary conditiois on equation (8). This yeilds under size qantization the eigenstates

$$\Psi_{nmk} = [\Omega^{1/2} J^2_{n+1} (\alpha_{nm})]^{-1} e^{ik_z z} e^{in\theta} J_n (\frac{\alpha nm^r}{R}) \quad (14)$$

where $\Omega = \Pi R_0^2 L_z$ is the volume of the circular wire, and n = 0, 1,2, ... The integral [8].

$$\int_0^r r\, J^2_n (\alpha_{nm} r/R_0)\, dr = (R_0^2/2)\, J^2_{n+1} (\alpha_{nm})$$

has beeen used.

The corresponding eigenvalues of these wave-functions are

$$E_{nmk_z} = \varepsilon_0 \alpha^2_{nm} + h^2 k^2 /_z 2m^*. \quad (15)$$

where

$$\varepsilon_0 = h^2 / 2m^* R^2_0$$

with α_{nm} being the root of Bessel function of order n. From equations

(11) and (9) with the appropriate boundary conditions $k = \alpha_{nm} / R_0$, the distribution of the eigenvalues in k-space is not uniform because

$$\alpha_{nm} - \alpha_{nm+1} = \Pi \quad \text{only when } m >> n \qquad (16)$$

5. Density of states:

The density of states of rectangular and square wire of length 1_z can be obtained on the ground that k values in x and y direction are equantized due to the finite sizes b and d, but in z direction they are quasi-continous. Consequently, number of states N in such a wire has the form

$$N = \sum_{p,1} (1_z / 2\Pi)\ k_z \qquad (17)$$

where the sum is taken over the possible quantum numbers p and 1, and k_z can be obtained from equation (6) as

$$k_z = (k_E{}^2 - k_x{}^2 - k_y{}^2)^{1/2} \qquad (18)$$

The density of states D (E) [1] is defined as dn/dE and obtained by substituting equations (18), (11a) and (11b) into equation (17). Transformation from k-space into energy space is made by using equations (13). Then D (E) has the form

$$D_{rw}(E) = \frac{L_z \sqrt{2m^*}}{\Pi h} \sum_{1,p} (E - \varepsilon_x 1^2 - \varepsilon_y p^2)^{-1/2} \qquad (19)$$

Similar treatment of the density of states in a square wire results in the following equation.

$$D_{sw}(E) = \frac{L_z \sqrt{2m^*}}{\Pi h} \sum_{1,p} (E - \varepsilon_x (1^2 + p^2))^{-1/2} \qquad (20)$$

where the subscriptis rw and sw stands for rectangular and square wires, respectively.

The density of statesof cylindrical wire (cw) can be obtained from equation (15) by the same procedure as used in obtaining equations (19) and (20) in the form

$$D_{cw}(E) = \frac{L_z \sqrt{2m^*}}{\Pi h} \sum_{nm} (E - \alpha_{nm} \varepsilon_0)^{-1/2} \quad (21)$$

6. Discussion and calculations :

The one-dimensional density of states D_{rw} and D_{sw} involve summatin over values of the quantum numbers l, p. Values of ε_x and ε_y can be obtained from equation (13). For the ground state the calculations are done using equations (19) and (20). The results are shwon in Figs. (1) and (2).

Calculations of the density of states from equation (20) need the computation of Bessel functions and their roots α_{nm}. A computer program for such calculations is set up and, as mentiond earlier, the distribution of states in k space is not uniform and according to equation (16) we have to compute all terms of the summation in equation (20) up till the uniformity in the eigenvalues is achieved. The reuslts of these calculations are shown in Fig. (3). To make a comparison among the different shapes under consideraton, Fig. (4) summarizes the results for ech in the ground state (p = 0 for rectangular or square wire and n = 0 for cylindrical one).

7. Conclusion :

From this study it is obvious that the density of states is shape dependent and they reach their least value when the symmetry in the shape is low (rectangular wire) and the maximum value in the case of the high summetry (cylindricla wire).

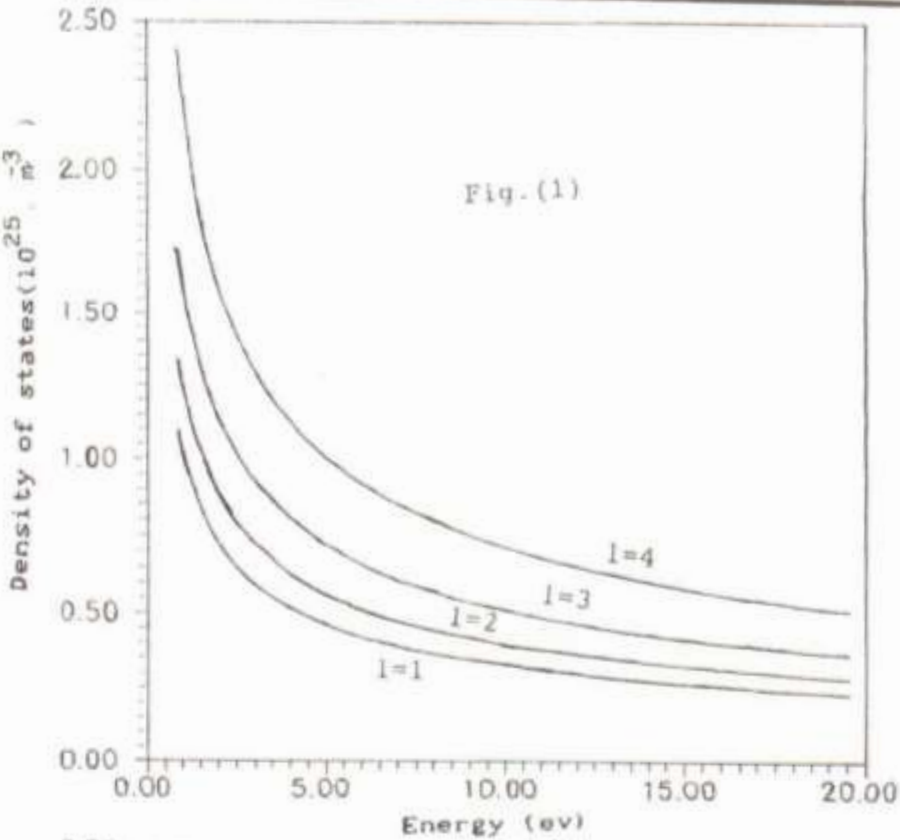
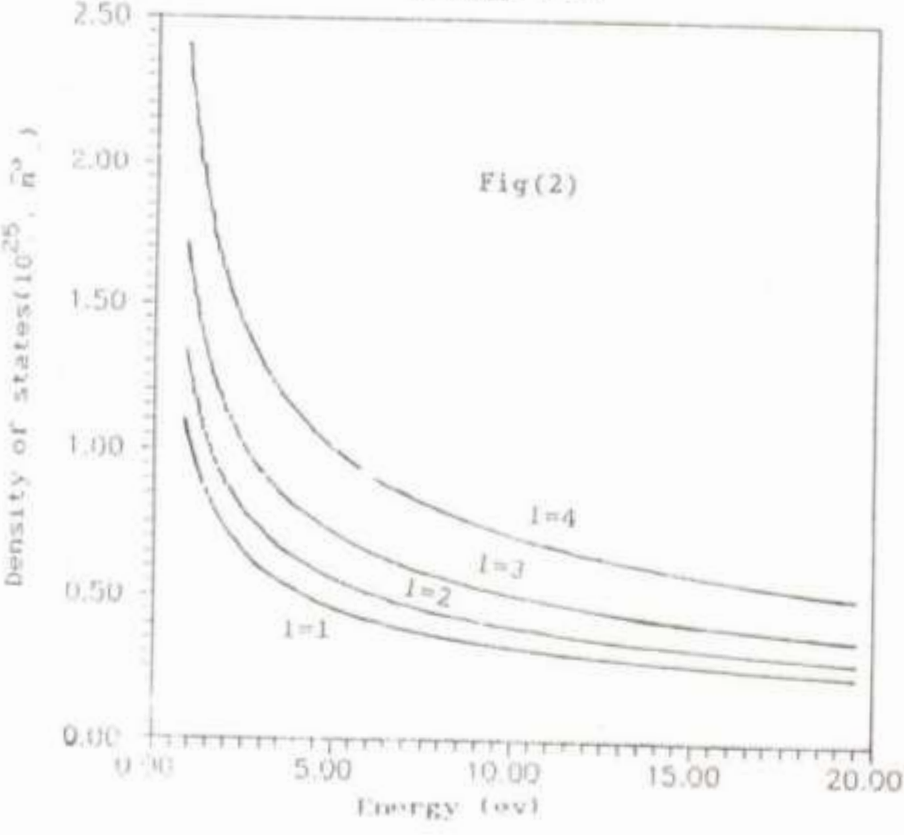
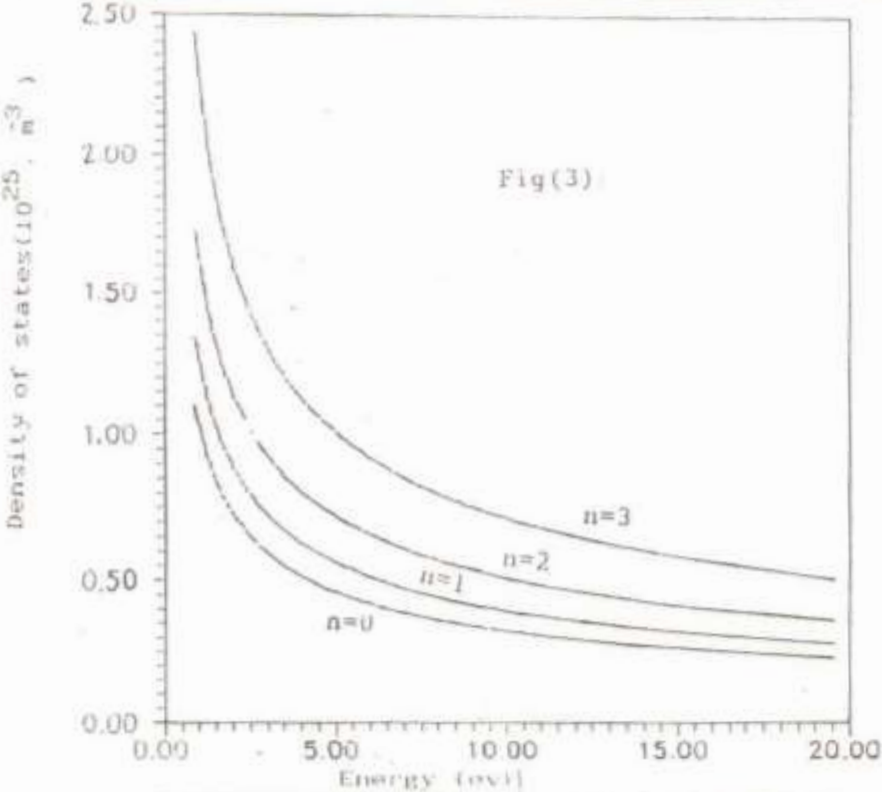
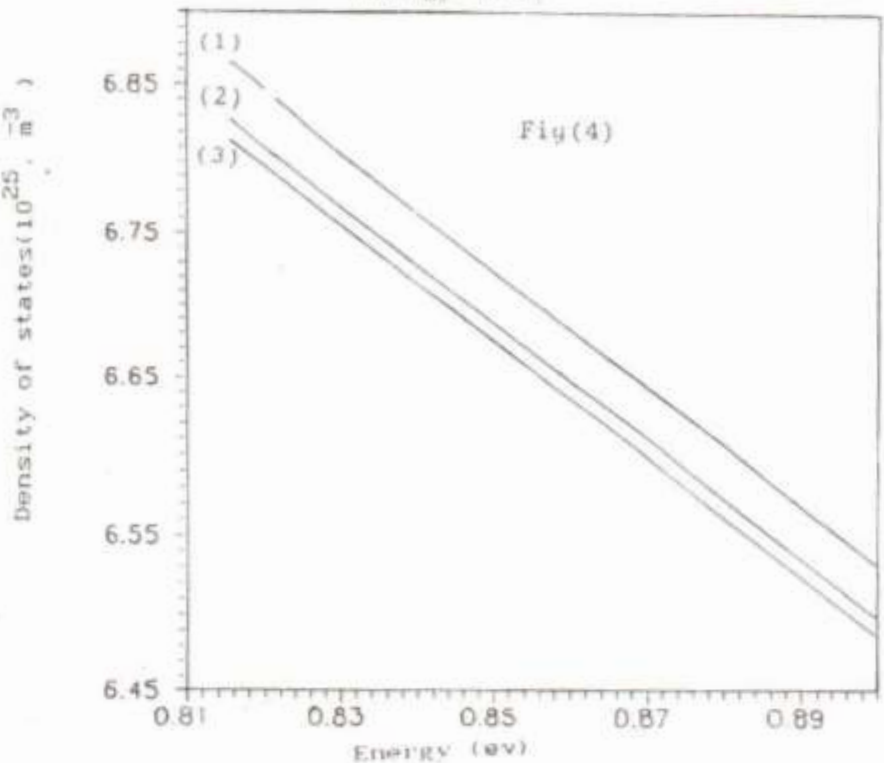


Fig.(1)
Density of states(10^{25} . m^{-3})
Energy (ev)
l=4
l=3
l=2
l=1


Fig(2)
Density of states(10^{25} . m^{-3})
Energy (ev)
l=4
l=3
l=2
l=1


2.50
2.00
1.50
1.00
0.50
0.00
Density of states(10^{25} , m^{-3})
Fig(3)
n=3
n=2
n=1
n=0
0.00
5.00
10.00
15.00
20.00
Energy (ev)


6.85
6.75
6.65
6.55
6.45
Density of states(10^{25} , m^{-3})
(1)
(2)
(3)
Fig(4)
0.81
0.83
0.85
0.87
0.89
Energy (ev)

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