

Quantum Conductance in Nanoscale Conductor

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Abstract: The density of states (DOS) plays a very central role to determine how well something conducts, basically material conducts if there are many (DOS) around the equilibrium chemical potential or Fermi Level. The aim of this paper is to adopt specific model of (DOS), because most physicist assume that they have the (DOS) without discussing the (DOS) itself. This paper emphasized on discussing the (DOS) itself for the purpose to show where it comes from and how it could be modeled. The model used depends on solid state physics, the very complicated subject, where the solid is considered as a very complicated object. It is quite important to explain specifically the energy model to give the (DOS) and relate it to the conductivity in diffusive conductors and then compare it to the Drude formula of conductivity to connect them up. Because of the nice feature of the ballistic conductance to describe the ballistic transport as well as the diffusive one, since both originate from the same viewpoint. Also, it is possible to express the ballistic conductance (G_B), in quantum form as;

$$G_B = Mq^2/h$$

Where, q is the electron charge, h is the Planck's constant, M is number of modes.

From the above expression of the ballistic conductance, the number of modes (M) can be expressed in either of the dimensions (1D, 2D, 3D) respectively as;

$$M = \text{integer} \left(1, \frac{2w}{\left(\frac{h}{p}\right)}, \frac{\pi A}{\left(\frac{h}{p}\right)^2} \right)$$

Key words:

Density of states, equilibrium chemical potential, Fermi level, solid state physics, the conductivity, diffusive conductors, Drude formula, ballistic conductance, the number of modes (M).

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I. Introduction

The basic idea for explaining what is the density of states (DOS), is by taking a hydrogen atom discrete levels spaced by few electron volts (eV), for large atoms and molecules energy levels get closer together, and for solids lots of energy levels are allowed to form a band. To discuss conductors made from hundreds of atoms, it is quite convenient to talk about the (DOS) to tell how many states there are, in a given range of energy. Therefore, (DOS) can be defined as the number of states per unit energy, given by the following relation;

$$(DOS) = n/qV \quad (1)$$

Where, (n) is the number of the states. (qV) is the energy in electron volts.

(DOS) can be measured by photoemission experiments to hit the solid by an ultraviolet beam of light to see how much energy is required to knockout an electron from the solid. That energy is given by;

$$E = h\nu \quad (2)$$

Where, (h) is the Planck's constant. (ν) is the light frequency.

The suggested theoretical model is based upon the idea of the energy momentum relation, $E(P)$. Generally, an electron could have any momentum that corresponds to have any energy, in this case it is not clear to calculate the (DOS), because it is continuum without end, but an electron within a finite size solid can be relied on in this argument. Since all the momenta are not allowed, therefore, the discrete values of momentum inside the solid could have allowed values of (energy levels). This set of discrete momenta can be translated into discrete set of energies, which in turn can be translated also into density of states (DOS), or into number of modes (M) as well. For that purpose, usually, people start from Schrodinger equation to see something that

takes into account the wave nature of the electron, but not trying to go deep in quantum mechanics, it can be done in an elementary way by using the idea of DeBroglie wave length, after discretizing the momentum.

II. The Model

A relatively simple model was suggested, based on the idea of Energy -Momentum relationship $E(P)$. Since 1930's it well known from solid state physics, electrons in solids behave as if they are in vacuum, but with different energy-momentum relationship or with different mass known as the effective mass.

The starting point with this model is $E(P)$, or $E(K)$ relations to be plotted as a function of the momentum(P), or (K), their curves may be similar to the curves of the density of states $D(E)$ as a function of energy . Although $E(P)$ and $D(E)$ are totally different, because momentum is a vector and can point in any direction, either the positive or the negative (P) sides of the curve, while the density of states is an scaler value representing the number of levels per unit energy, so they stay at the positive side of the curve.

In this model $E(P)$ relationship is assumed to be given from experiments or any other theory that the electrons are in the energy range of interest, and they behave as if they have a particular $E(P)$. To obtain the (DOS) from $E(P)$, a function $N(P)$ should be defined to tell how many states there for the electrons are possessing all possible momenta up to a maximum value of (P). $N(P)$ could be defined as;

$$N(P) = AP^\psi \quad (3)$$

Where, (ψ) is number dimensions of the conductor used.

(A) is a constant, it takes different forms depending on the number of dimensions (ψ).

The details of the constant (A) need not to be known for the time being to combine $E(P)$ with $N(P)$ to get $N(E)$, where $N(E)$ is the number of energy states up to a maximum energy value (E), whose derivative is the density of states.

Since $E(P)$ is known, (P) can be eliminated to get the number of the energy states $N(E)$ for an energy value less than some value (E), where the density of states $D(E)$ will be given by;

$$D(E) = \frac{dN(E)}{dE} \quad (4)$$

If the energy (E) is increased by (dE), extra states are added equal to the density of states $D(E)$. To discretize the momentum, (λ_D) can be related to momentum (P) by;

$$\lambda_D = \frac{h}{P} \quad (5)$$

Where, (λ_D) is DeBroglie wavelength.

(h) is the Planck's constant.

(P) is the momentum.

For one dimensional conductor of length (L), only the following momenta are allowed;

$$L = n \left(\frac{h}{P} \right) \quad (6)$$

The essence of this whole counting scheme, the way by which the states are counted, the length must be an integer (n) times the wavelength ($\lambda_D = \frac{h}{P}$) is called the period boundary conditions. Therefore, an electron can't have any momentum other than certain values of (P_n). The imposed condition is that an electron with certain wavelength to fit into a box of length (L).

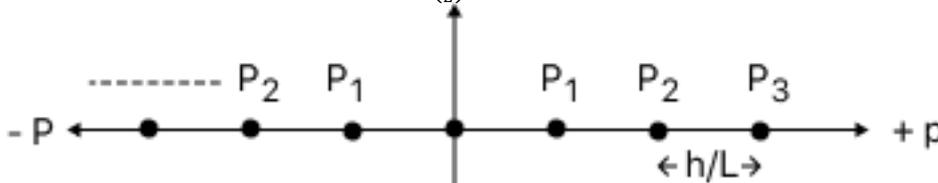
To turn equation (6) around gives the spacing between allowed values of momenta as discrete multiples of (h/L).

2.1 For one dimensional conductor (**1D**):

$$(P_n) = n \left(\frac{h}{L} \right) \quad (7)$$

So easily $N(P)$ can be found as;

$$N(P) = \frac{2P}{\left(\frac{h}{L}\right)} = \left(\frac{2L}{h}\right) P \quad (8)$$



The wave property of an electron possesses a wave number ($K = 2\pi/\lambda$), then;

$$P = \hbar K \quad (9)$$

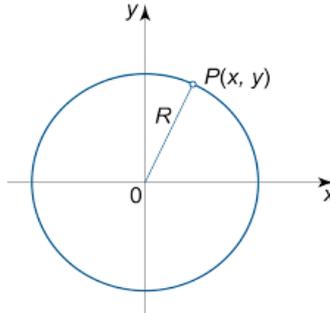
Where, \hbar is the reduced Planck's constant ($h/2\pi$).

Equation (9) gives the particle duality, therefore the momentum (p) and the wave number (K) are related by the reduced Planck's constant. (K) is not more than an equivalent form of the momentum,

$$K = \frac{P_n}{\hbar} = \frac{n \left(\frac{h}{L}\right)}{\hbar} = 2\pi n/L$$

2.2 For two-dimensional conductor (2D):

The total number of states $N(P)$ in this case with the momentum happened to be less than (P) is directly proportional to (P^2);



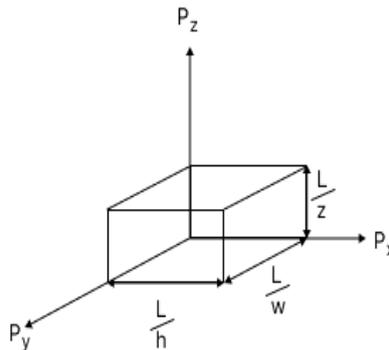
Because each state occupies an area $\left(\frac{h^2}{WL}\right)$, then;

$$N(P) = \frac{\pi P^2}{\left(\frac{h}{L}\right)\left(\frac{h}{W}\right)} = \left(\frac{\pi WL}{h^2}\right) P^2 \quad (10)$$

Where, (L) is the length in one direction, say (P_x).
 (W) is the length in the other direction, say (P_y).

2.3 For three-dimensional conductor (3D):

Instead of an area as shown in the previous case, there will be a volume of a sphere this time, hence $N(P)$ is directly proportional to (P^3);



Because each state occupies a volume of $\left(\frac{h^3}{WLZ}\right)$, then;

$$N(P) = \frac{\frac{4\pi P^3}{3}}{\left(\frac{h}{Z}\right)\left(\frac{h}{L}\right)\left(\frac{h}{W}\right)} = \left(\frac{4\pi ZWL}{3h^3}\right) P^3 = \left(\frac{4\pi AL}{3h^3}\right) P^3 \quad (11)$$

Where, ($WZ = A$) is cross sectional area of each state.

To collect all these relations together in single expression for $N(P)$ in the three cases (1D, 2D, & 3D) respectively;

$$N(P) = (P/h)^\psi \left(2L, \pi WL, \frac{4\pi AL}{3}\right) \quad (12)$$

Therefore, equation (12) is an equivalent to equation (3), where (ψ) is the number of dimensions, and all the bracketed factors stand for the constant (A), which goes in front of the general relation of equation (3) depending on the size of the conductor under consideration.

Using the periodic boundary conditions, the rule of counting the states $N(P)$ is given by equation (12) above. This rule does not include any energy momentum relation $E(P)$, it is just based on the idea of discretization of momentum using DeBroglie wavelength to fit in a box.

The model can be completed by introducing a very useful relation independent of any specific $E(P)$ relation, valid for all types of $E(P)$ relations. This relation can be arrived to by differentiating $N(P)$ with respect to (P) ;

$$\begin{aligned} \frac{dN(P)}{dP} &= \frac{\psi}{h^\psi} (P)^{(\psi-1)} \left(2L, \pi WL, \frac{4\pi AL}{3} \right) \\ &= \frac{dN(E)}{dE} \cdot \frac{dE}{dP} = D(E) \cdot v \end{aligned}$$

Multiply both sides by (P) ;

$$P \frac{dN(P)}{dP} = P \cdot D(E) \cdot v$$

Therefore;

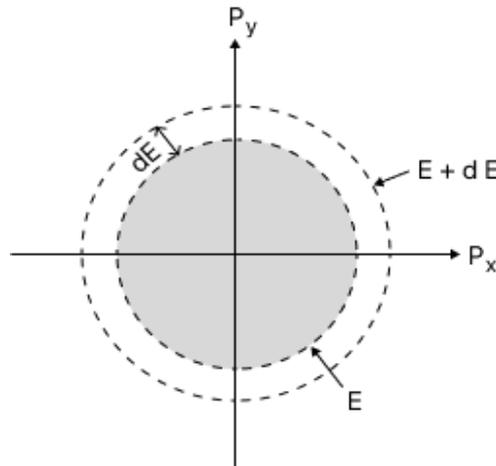
$$\psi \cdot N(P) = P \cdot D(E) \cdot v \quad (13)$$

Equation (13) is the required basic relation independent of $E(P)$, despite that, $\left(\frac{dE(P)}{dP}\right)$ is representing the velocity (v) without any assumption how $E(P)$ looks like.

III. Computations and Results

The rule of counting the states $N(P)$ obtained from the model simply by fitting only the corresponding momentum into a box using DeBroglie wavelength, making no use of any energy momentum relation. By coupling $N(P)$ with the energy momentum relation $E(P)$, the number of states $N(E)$ allowed in the energy range happened to be less than energy value (E) can be found. $E(P)$ in general, could have many complicated forms of relations, and by eliminating (P) , $N(E)$ will be given. The derivative of $N(E)$ with respect to (E) gives the density of states $D(E)$.

Assume an isotropic momentum, i.e. energy is the same for any momentum in all directions. In figure below the shaded area corresponds to certain energy values less than (E) .



If the momentum increased a little bit, correspondingly (E) will increase by an amount (dE), so we have slightly bigger circle, hence the number of states available are increased representing the density of states at that energy.

Generally, $E(P)$ can be described by:

$$E(P) = E_c + \beta P^\alpha \quad (14)$$

Where, (E_c) is the bottom end of the band, (E_c) varies with (P) in a certain way. (β) is an important constant, multiplied by (P^α) , depending on (α) , (β) varies with (P) in a certain way.

When parabolic bands are dealt with $\left(\alpha = 2, \beta = \frac{1}{2m}\right)$, but it is better to keep equation (14) in its general form for the purpose of other $E(P)$ relations. From equation (14), the momentum (P) is given as;

$$P = \left(\frac{E(P) - E_c}{\beta} \right)^{\frac{1}{\alpha}} \quad (15)$$

Eliminate (P) by substituting equation (15) in equation (3) to get $N(E)$,

$$N(E) = A \left(\frac{E(P) - E_c}{\beta} \right)^{\frac{\psi}{\alpha}} \quad (16)$$

The general expression of the density of states $D(E)$, depends on the number of dimensions (ψ) and the factor (α) which describes how the $E(P)$ relation varies with the momentum.

$$D(E) = \left(\frac{\psi A}{\alpha}\right) \left(\frac{1}{\beta}\right)^{\frac{\psi}{\alpha}} (E(P) - E_c)^{\left(\frac{\psi}{\alpha}-1\right)} \quad (17)$$

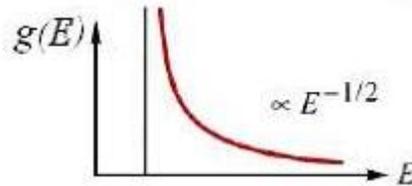
To apply these results for specific case, the most common one is the parabolic band, where ($\alpha = 2$):

3.1 For one dimensional conductor (**1D**):

($\alpha = 2, \psi = 1$), therefore;

$$D(E) \sim (E(P) - E_c)^{-\frac{1}{2}}$$

$D(E)$ can be represented by the following figure;

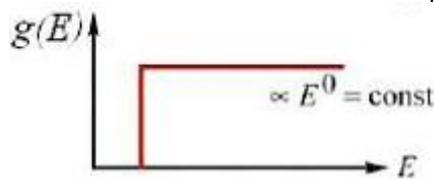


The figure has a singularity right near the band edge (E_c) with energy.

3.2 For two-dimensional conductor (**2D**):

($\alpha = 2, \psi = 2$), therefore;

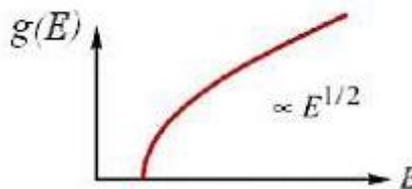
$$D(E) \sim (E(P) - E_c)^0 = \text{constant} = \left(\frac{\psi A}{\alpha \beta}\right)$$



3.3 For three-dimensional conductor (**3D**):

($\alpha = 2, \psi = 3$), therefore;

$$D(E) \sim (E(P) - E_c)^{\frac{1}{2}}$$



Comments

There are many popular materials such as the graphene where energy momentum relation $E(P)$, can take a linear relationship with (P);

$$E(P) = V_0 P^\alpha$$

$$P = \left(\frac{E}{V_0}\right)^{1/\alpha}$$

Where, ($\alpha = 1$) for graphene, so $E(P)$ can be combined with the rule of counting states $N(P)$ to obtain $N(E)$ by eliminating the momentum (P);

$$N(P) = AP^\psi$$

$$N(E) = A \left(\frac{E}{V_0}\right)^{\frac{\psi}{\alpha}}$$

$$D(E) = \frac{dN(E)}{dE} = \left(\frac{\psi A}{\alpha}\right) \left(\frac{1}{V_0}\right)^{\frac{\psi}{\alpha}} E^{\left(\frac{\psi}{\alpha}-1\right)}$$

Instead of the parabolic $E(P)$ relationship, it is linear now and all the above results will change to another shapes as follows;

Conductor size	ψ	α	Density of the state's relationship	Shape $D(E) \sim E$
1D	1	1	$D(E) \sim (E)^0 = \text{constant}$	Step function
2D	2	1	$D(E) \sim E$	Straight line
3D	3	1	$D(E) \sim (E)^2$	Parabola

The energy momentum relationship can be more complicated than that, it could have been in relativistic form, where energy is the square of some constant and some (P^2) ;

$$E(P) = (E_g^2 V_0^2 P^2)^{\frac{1}{2}}$$

In this case we can't use the relation;

$$D(E) = \left(\frac{\psi A}{\alpha}\right) \left(\frac{1}{\beta}\right)^{\frac{\psi}{\alpha}} (E(P) - E_c)^{\left(\frac{\psi}{\alpha}-1\right)}$$

Energy momentum relation $E(P)$ and $N(P)$ should be taken to find $N(E)$, then the derivative of $\left(\frac{dN(E)}{dE}\right)$, is taken to get $D(E)$.

The rule of counting the number of states $N(P)$, can be used to obtain an expression for the number of modes $M(E)$, at the same time the number of modes $M(E)$ can be related to the ballistic conductance (G_B) given by;

$$G_B = q^2 D \left(\frac{\bar{v}}{2L}\right)$$

Where, q is the electron charge. D is the density of states.

\bar{v} is the average velocity, L is the conductor (channel) length.

The average velocity (\bar{v}), involve some numerical factors depending on the number of dimensions.

$$G_B = \frac{q^2 DV}{2L} \left(1, \frac{2}{\pi}, \frac{1}{2}\right) \quad (18)$$

Where, (V) is the maximum velocity to be averaged according to number of dimensions.

The quantity $\left(\frac{\bar{v}}{2L}\right)$, is called the density of modes, defined as the number of modes $M(E)$ divided by the Planck's constant;

$$\left(\frac{\bar{v}}{2L} = \frac{M(E)}{h}\right)$$

The density of modes is the material property, which has special significance.

From equation (18) above the ballistic conductance can be expressed in quantum form as;

$$G_B = Mq^2/h$$

Then;

$$M(E) = h \frac{DV}{2L} \left(1, \frac{2}{\pi}, \frac{1}{2}\right) \quad (19)$$

If an expression for the density of states $D(E)$ is at hand, it can be multiplied by the velocity to find the number of modes $M(E)$, alternatively the general relation given by equation (13) can be introduced in the model, namely;

$$\psi \cdot N(P) = P \cdot D(E) \cdot v$$

Then,

$$D(E) \cdot v = \frac{\psi \cdot N(P)}{P}$$

Substitute in equation (19) above to get;

$$M(E) = \frac{\psi \cdot N(P)h}{2PL} \left(1, \frac{2}{\pi}, \frac{1}{2}\right)$$

Bring in $N(P)$ from equation (12), and with a little algebra and rearrangement;

$$M(E) = \left(\frac{P}{h}\right)^{(\psi-1)} (1, 2W, \pi A)$$

This result gives totally different interpretation if rewritten in a different way by taking the factor $\left(\frac{P}{h}\right)^{(\psi-1)}$ into the bracket

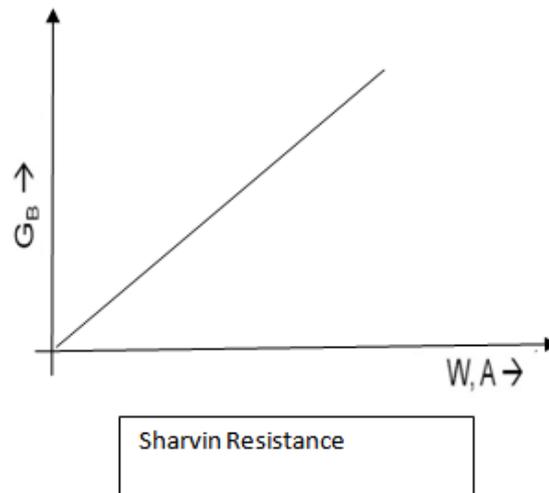
$$M(E) = \left(1, \frac{W}{\left(\frac{h}{2P}\right)}, \frac{\pi A}{4\left(\frac{h}{2P}\right)^2}\right)$$

$$M(E) = \left(1, \frac{W}{\left(\frac{\lambda}{2}\right)}, \frac{\pi A}{4\left(\frac{\lambda}{2}\right)^2}\right) \quad (20)$$

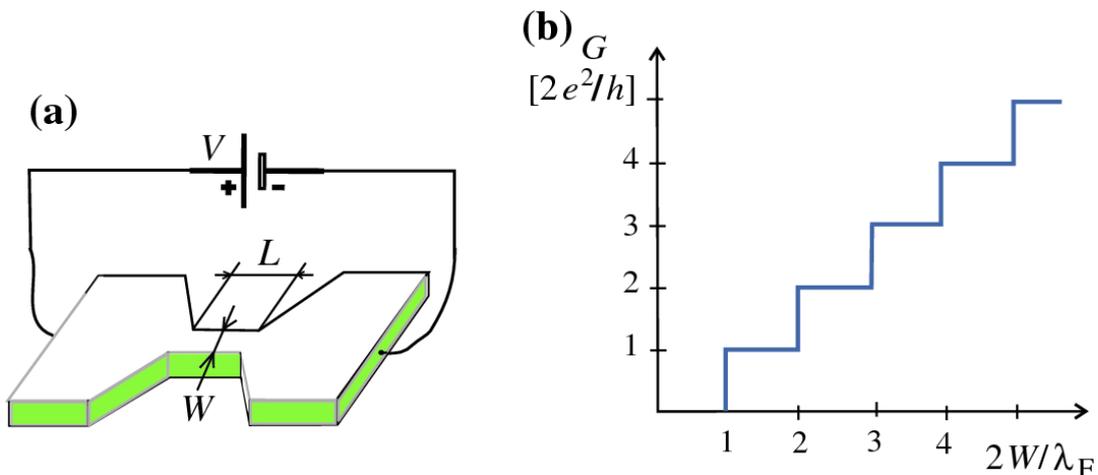
Therefore, the number of modes physically equal to (one) for (1D) conductor, (2D) conductor tells how many wavelengths of De-Broglie fit into the width, and (3D) conductor tells how many DeBroglie wavelengths fit in either direction of the cross-sectional area.

Note the word mode originates from the same idea of the electromagnetic wave guides when the transverse modes for electromagnetic wave guides need to be determined.

An important consequence of equation (20), if multiplied by the constant value $\left(\frac{q^2}{h}\right)$, gives the ballistic conductance (G_B). Since the number of modes $M(E)$, is directly proportional to the width (W), or the cross-sectional area (A) of the conductor, this has been observed in 1970's, and it is sometimes called Sharvin resistance;



In 1990 a very important development took place, that is in small devices with very small cross sections, where the number of modes in the order of ten to twenty thousands, it was observed that the ballistic conductance takes a quantized form rather than go linearly with (W , or A), it goes in steps (see figure below);



To understand the phenomena, $M(E)$ is not exactly equal to the bracketed quantities in equation (20), if any of the bracketed quantities happened to be a rational number, it should be a whole positive number, because the number of modes is given by how many states available in that width or cross sectional area, therefore the correct expression should be the integer part of either of them. When $M(E)$ is small and (G_B) is quantized, $M(E)$ should be an integer value of the quantities bracketed in equation (20);

$$M(E) = \text{integer} \left(1, \frac{W}{\left(\frac{\lambda}{2}\right)}, \frac{\pi A}{4 \left(\frac{\lambda}{2}\right)^2} \right)$$

But normally no care attention is given to that when $M(E)$ is large enough in the order of thousands and more, because it makes no difference if it is (1000 or 1001). Since this big number causes the steps to be

very close together, it needs to be averaged with $(-\partial f/\partial E)$ factor over an energy range (KT) . The steps smoothed out at higher temperatures; with low temperatures the phenomenon is very well established with conductors of small cross sections. This was first seen in semiconductors like $(GaAs)$, since then people see it in all kinds of materials even in hydrogen molecules.

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