Evaluation of density of electron states – A simple approach

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Abstract

The density of electron states in one, two and three dimension is evaluated by following a simple procedure which makes the significance of Fourier space apparent. Using this approach, the relativistic electron gas is also discussed. The approach is easily adaptable to an undergraduate physics course.

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1. Introduction

Density of states, D(E) = dn/dE, which is the number of energy states per unit energy at E, is an important quantity in many – particle systems , such as a gas or a solid. In terms of D(E),many physical quantities such as the number of particles or the total energy or any other quantity such as the specific heat may be obtained.

$$N = \int dE\, D(E) f(E) \qquad (1)$$

$$E = \int dE\, E\, D(E) f(E) \qquad (2)$$

where *f(E)* is the suitable distribution function for the many – particle system. For example, it is the Fermi –Dirac distribution function for a many electron system. Several text books on Solid State Physics [1] and Statistical Mechanics [2] contain detailed discussions on *D(E).*

At present there is considerable interest on the physics of low dimensional systems such as quantum wells (QW),quantum well wires (QWW), quantum dots (QD) and super lattices (SL).[3]. Fabrication, observation of novel properties and applications of these systems have revolutionized the semiconductor field. Several interesting properties exhibited by these systems arise due to the peculiar nature of *D(E)* in different dimensions. Properties in between these dimensions (quasi two dimension, for example) may also be obtained. In general, the derivation of *D(E)* in different dimensions is different [3]. In the present work we give a unique, yet simple method of evaluation of the density of states in different dimensions.

2. Density of electron states.

A. Non relativistic case

We consider a non interacting electron system (a gas) to which Fermi – Dirac statistics is applicable. The conventional derivation for *D(E)* is as follows, for a 3D gas. At 0 K, we have

$$2 \times \frac{4}{3}\pi k_F^{\,3} \times \left(\frac{L}{2\pi}\right)^3 = N \qquad (3)$$

where $\frac{4}{3}\pi k_F^{\,3}$ is the volume of the Fermi sphere, $\left(\frac{L}{2\pi}\right)^3$ is the density of electron states obtained from periodic boundary conditions, N is the total number of electrons and the factor 2 arises due to spin degeneracy. The above result not only

gives, $k_F = (3\pi^2 N/V)^{1/3}$, $E_F = (\hbar^2 k_F^2)/2m$ and also shows that $D(E) \alpha E^{1/2}$. The density of states varies as the square root of energy at the Fermi energy. Usually, this is taken to be valid for all $E \leq E_F$.

The derivations is one and two dimensions are similar to the above. The results are

$$2 \cdot k_F \cdot \left(\frac{L}{2\pi}\right) = N \qquad \text{(1D)} \qquad (4)$$

and

$$2 \cdot \pi k_F^2 \cdot \left(\frac{L}{2\pi}\right)^2 = N \qquad \text{(2D)} \qquad (5)$$

Thus *D(E)* is proportional to $E^{1/2}$ in 3D, constant (independent of energy) in 2D and $E^{-1/2}$ in 1D.Thus the evaluation of D(E) requires the information available in momentum space. In the discussion presented above, the use of this information is indirect. To bring out the information in a more apparent manner we suggest writing $D(E) = \frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dN}$ and use $E = \frac{\hbar^2 k^2}{2m}$ for a free particle.The periodic boundary conditions on free particle energy eigen functions lead to $e^{ikx} = e^{ik(x+L)}$. This gives $e^{ikL} = e^{2\pi ni}$ where n is an integer. Q uantization follows and we get $k_n = \frac{2\pi n}{L}$, where *L* is the size of a box; many such huge boxes are assumed to fill the space.

In 1D, $\frac{dn}{dk} = \frac{L}{\pi}$ from the above expression for quantization of wave vectors, We multiply the above by 2 to take into account spin degeneracy. Hence

$$D(E) = \frac{L}{\pi}\frac{m}{\hbar^2 k} = \frac{L}{\pi}\frac{m}{\hbar^2}\frac{\hbar}{(2mE)^{\frac{1}{2}}} = \frac{L}{\pi}\left(\frac{m}{2\hbar^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}}.$$

Hence the density of states per unit length g(E) is $\left(\frac{m}{2\pi^2\hbar^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}}$.

In 2D, we write the quantization for k_x and k_y as

$k_x = \frac{2\pi}{L} n_x$ and $k_y = \frac{2\pi}{L} n_y$.

Therefore, $dk_x\, dk_y = \left(\frac{2\pi}{L}\right)^2 dn_x\, dn_y$.

In polar coordinates this becomes $2\pi k dk = \left(\frac{2\pi}{L}\right)^2 dn$.

Hence $\frac{dn}{dk} = 2\pi k\left(\frac{L}{2\pi}\right)^2 = \frac{4\pi kA}{4\pi^2} = \frac{k}{\pi}A$. The factor 2 is used for spin degeneracy. A is the area L^2. Hence $D(E) = (Am/\pi\hbar^2)$. So, density of states per unit area of the sample is $m/\pi\hbar^2$.

A similar procedure in 3D gives for the density of states per unit volume, $1/\pi^2\hbar^3(2m^3)^{1/2}E^{1/2}$.

These results are the same as those obtained earlier.

B. Relativistic Electron gas.

In the relativistic case we use $E^2 = c^2p^2 + m_0^2c^4$, where m_0 is the rest mass of the electron. In the extreme relativistic case $cp >> m_0c^2$, so $E = cp = c\hbar k$. This immediately leads to the following expressions for the density of states (per unit length in 1D, area in 2D and volume in 3D):

$$g(E) = \begin{cases} \frac{2}{c\hbar} & \text{in 1D} \\ \frac{1}{2\pi(c\hbar)^2} E & \text{in 2D} \\ \frac{1}{2\pi^2(c\hbar)^3} E^2 & \text{in 3D} \end{cases}$$

A comparison of the non relativistic and relativistic cases is provided in Table 1

3. Applications of relativistic case

It is interesting to note that the average energy of a 3D relativistic electron gas at 0 K is given by

$$\langle E\rangle_{3D,R} = \int_0^{EF} dE\; E\, D(E) f(E) \Big/ \int_0^{EF} dE\; D(E) f(E)$$

where *f(E)* is the Fermi –Dirac distribution function whose value is 1 at 0 K for $E \leq E_F$

We obtain $\langle E \rangle_{3D,R} = (3/4)E_F$ The result for the non relativistic case is $(3/5)E_F$.

As another application of the relativistic case, we obtain the Fermi energies in 1, 2 and 3 dimensions.

We obtain

$$n=\int_0^{EF} g(E)dE = \begin{cases} \frac{2}{c\,h} E_F & \text{in 1D} \\ \frac{1}{2\pi c^2 h^2} E_F^{\,2} & \text{in 2D} \\ \frac{1}{3\pi^2 c^3 h^3} E_F^{\,3} & \text{in 3D} \end{cases}$$

where n is the electron concentration.

Hence E_F is proportional to n (no. of electrons per unit length, in 1D), $n^{1/2}$ (electrons per area, in 2D) and $n^{1/3}$(electron concentration per volume, in 3D)

One can evaluate other properties like specific heat etc.

Conclusions:

We have provided a simple procedure to evaluate the density of electron states in different dimensions which brings out the significance of momentum space. Application to relativistic electron gas gives interesting results for Fermi energy and average energy. These results differ substantially from the corresponding expressions of the non relativistic case.

Table 1. Variation of physical quantities in 1D,2D and 3D : Relativistic & Non-Relativistic cases

Quantity	NR			R		
	1D	2D	3D	1D	2D	3D
g(E)	$E^{1/2}$	Constant	$E^{-1/2}$	Constant	E	E^2
E_F	n^2	n	$n^{2/3}$	n	$n^{1/2}$	$n^{1/3}$

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