

Q1. This is a problem related to the crystal structure. (15%)

Supposing the atoms to be rigid spheres, (a) in a conventional cubic lattice, how many primitive cells are included for the simple cubic (*sc*), face-centered cubic (*fcc*), body-centered cubic (*bcc*) structures, respectively? (b) Graphene is a 2D material with a honeycomb structure as shown below, please draw two different unit cells and their corresponding unit cells in the reciprocal space?

(a) Primitive Cells in Cubic Lattice Structures:

1. Simple Cubic (sc) Structure:

- In a simple cubic lattice, each lattice point is only at the corners of the cube.
- Each corner is shared by eight neighboring unit cells.
- Therefore, each simple cubic unit cell contributes $1/8$ of its volume to the specific unit cell we are considering.
- The total contribution is 1.
- Hence, there is 1 primitive cell per simple cubic structure.

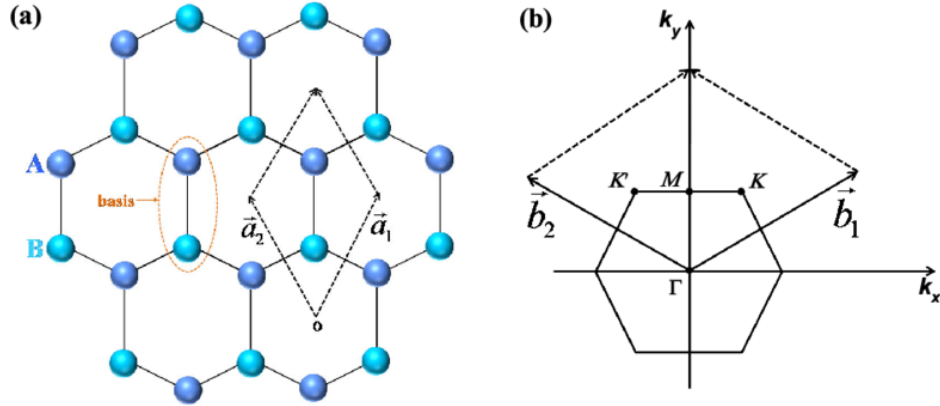
2. Face-Centered Cubic (fcc) Structure:

- In a face-centered cubic lattice, there is an additional lattice point at the center of each face in addition to the corner points.
- There are 6 faces, and each contributes $1/2$ of a lattice point to the specific unit cell we are considering (since the face is shared by two adjacent cubes).
- The corners are still shared by eight neighboring unit cells, contributing $1/8$ each.
- The total contribution is $\frac{6 \times 1}{2} + 8 \times \frac{1}{8} = 4$.
- Hence, there are 4 primitive cells per face-centered cubic structure.

3. Body-Centered Cubic (bcc) Structure:

- In a body-centered cubic lattice, there is an additional lattice point at the center of the cube in addition to the corner points.
- The corners are shared by eight neighboring unit cells, contributing $1/8$ each.
- The center point is not shared with any other unit cell.
- The total contribution is $8 \times \frac{1}{8} + 1 = 2$.
- Hence, there are 2 primitive cells per body-centered cubic structure.

(b) Graphene is a 2D material with a honeycomb structure: **two different unit cells** and their corresponding unit cells in the reciprocal space



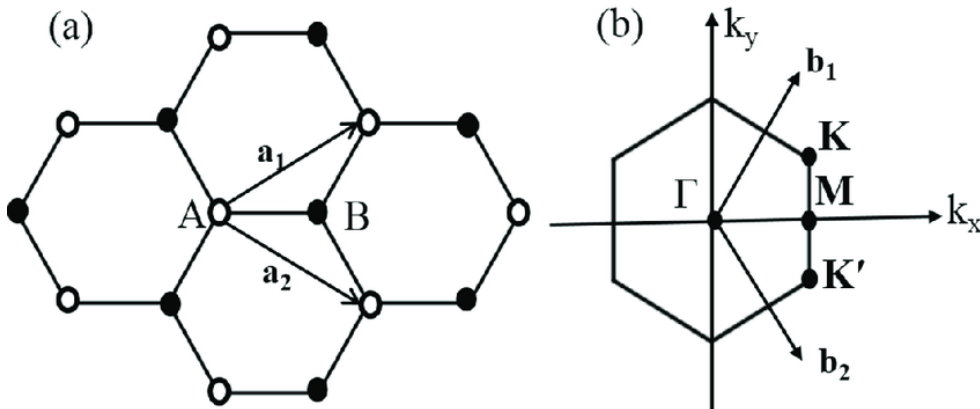
(a) The honeycomb crystal structure of graphene. The unit cell, rhombus, defined by vectors \vec{a}_1 and \vec{a}_2 containing two atoms belonging to sublattices A (blue) and B (cyan) are highlighted in light blue. (b) shows the graphene Brillouin zone in momentum space. The points K and K' denote the position of Dirac points while \vec{b}_1 and \vec{b}_2 represent the reciprocal lattice vectors

If a is the distance between nearest neighbors, the primitive lattice vectors can be chosen

$$\vec{a}_1 = \frac{a}{2} (3, \sqrt{3}), \vec{a}_2 = \frac{a}{2} (3, -\sqrt{3}),$$

the reciprocal-lattice vectors are spanned by

$$\vec{b}_1 = \frac{2\pi}{3a} (1, \sqrt{3}), \vec{b}_2 = \frac{2\pi}{3a} (1, -\sqrt{3}).$$



(a) Honeycomb lattice structure of graphene. The unit cell consists of carbon atoms represented by A and B, a_1 and a_2 are the lattice vectors and (b) corresponding Brillouin zone of graphene at origin (Γ) with two Dirac points K and K' with the reciprocal lattice vectors

$$\vec{b}_1 = \frac{2\pi}{a} \left(\frac{\hat{x}}{\sqrt{3}} + \hat{y} \right) \text{ and } \vec{b}_2 = \frac{2\pi}{a} \left(\frac{\hat{x}}{\sqrt{3}} - \hat{y} \right)$$

Q2. This is a problem related to the lattice diffraction. (15%)

The space lattice of diamond is face-centered cubic. The primitive basis of the diamond structure has two identical atoms at coordinates (000) and (1/4 1/4 1/4) associated with each point of the fcc lattice. The basis consists of eight atoms if the cell is taken as the conventional cube. (a) Find the structure factor S of this basis. (b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd. (Notice that h, k, l may be written for v_1, v_2, v_3 and this is often done.)

There are two ways to derive the result. The first is the long proof that follows the suggestion to consider diamond as simple cubic with 8 atoms per cell. The second is the short proof that uses the fact that diamond is fcc with 2 atoms per cell.

Diamond described as simple cubic with 8 atoms/cell:

The diamond structure can be described as a simple cubic lattice with the eight point basis $(0, 0, 0), \frac{a}{2}(\hat{x} + \hat{y}), \frac{a}{2}(\hat{y} + \hat{z}), \frac{a}{2}(\hat{z} + \hat{x}), \frac{a}{4}(\hat{x} + \hat{y} + \hat{z}), \frac{a}{4}(-\hat{x} - \hat{y} + \hat{z}), \frac{a}{4}(\hat{x} - \hat{y} - \hat{z}), \frac{a}{4}(-\hat{x} + \hat{y} - \hat{z})$. (a)

The structure factor $S = \sum_j f_j e^{-i\vec{G} \cdot \vec{r}_j}$,

$$\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3 = \frac{2\pi}{a}(v_1 \hat{x} + v_2 \hat{y} + v_3 \hat{z})$$

and $f_j = f$ (all the atoms are the same).

$$\begin{aligned} S &= f(1 + e^{-i\vec{G} \cdot \frac{a}{2}(\hat{x} + \hat{y})} + e^{-i\vec{G} \cdot \frac{a}{2}(\hat{y} + \hat{z})} + e^{-i\vec{G} \cdot \frac{a}{2}(\hat{z} + \hat{x})} \\ &+ e^{-i\vec{G} \cdot \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})} + e^{-i\vec{G} \cdot \frac{a}{4}(-\hat{x} - \hat{y} + \hat{z})} + e^{-i\vec{G} \cdot \frac{a}{4}(\hat{x} - \hat{y} - \hat{z})} + e^{-i\vec{G} \cdot \frac{a}{4}(-\hat{x} + \hat{y} - \hat{z})}) \\ &= f(1 + e^{-i\pi(v_1 + v_2)} + e^{-i\pi(v_2 + v_3)} + e^{-i\pi(v_3 + v_1)} + e^{-i\frac{\pi}{2}(v_1 + v_2 + v_3)} \\ &+ e^{-i\frac{\pi}{2}(-v_1 - v_2 + v_3)} + e^{-i\frac{\pi}{2}(v_1 - v_2 - v_3)} + e^{-i\frac{\pi}{2}(-v_1 + v_2 - v_3)}) \\ &= f[(1 + e^{-i\pi(v_1 + v_2)} + e^{-i\pi(v_2 + v_3)} + e^{-i\pi(v_3 + v_1)}) \\ &+ e^{i\frac{\pi}{2}(v_1 + v_2 + v_3)}(1 + e^{i\pi(v_1 + v_2)} + e^{-i\pi(v_2 + v_3)} + e^{i\pi(v_3 + v_1)})] \end{aligned}$$

Since $e^{-i\pi v} = e^{-i\pi v} e^{i2\pi v} = e^{i\pi v}$ for $v = \text{integer}$,

$$S = f(1 + e^{-i\pi(v_1 + v_2)} + e^{-i\pi(v_2 + v_3)} + e^{-i\pi(v_3 + v_1)})(1 + e^{i\frac{\pi}{2}(v_1 + v_2 + v_3)})$$

(b)

So the zeros are

(i)

$$1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_3+v_1)} = 0$$

This means two of $e^{-i\pi(v_i+v_j)}$ are -1 and one is +1, i.e. two of $v_i + v_j$ are odd and one is even. It is possible only when two of v_1, v_2, v_3 are even and the remaining one is odd or two of v_1, v_2, v_3 are odd and the remaining one is even.

(ii)

$$1 + e^{i\frac{\pi}{2}(v_1+v_2+v_3)} = 0$$

$$\Rightarrow \frac{1}{2}(v_1 + v_2 + v_3) = \text{odd} \Rightarrow v_1 + v_2 + v_3 = 2 \times (\text{odd})$$

The allowed reflections are anything but (i) and (ii).

(1) All of v_1, v_2, v_3 are odd.

(2) All of v_1, v_2, v_3 are even. But if $v_1 + v_2 + v_3 = 2 \times (\text{odd})$, S still vanishes.

Thus $v_1 + v_2 + v_3$ needs to be $2 \times (\text{even})$. i.e. $v_1 + v_2 + v_3 = 4n$ when all of v_1, v_2, v_3 are even.

Diamond described as fcc with 2 atoms/cell:

The diamond structure can be described as a face centered cubic lattice with the basis $(0, 0, 0), \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$.

The reciprocal lattice is bcc with primitive vectors $\vec{b}_1 = \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z}), \vec{b}_2 = \frac{2\pi}{a}(+\hat{x} - \hat{y} + \hat{z}), \vec{b}_3 = \frac{2\pi}{a}(+\hat{x} + \hat{y} - \hat{z})$. The reciprocal lattice vectors are:

$$\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3 = \frac{2\pi}{a}[(-m_1 + m_2 + m_3)\hat{x} + (m_1 - m_2 + m_3)\hat{y} + (m_1 + m_2 - m_3)\hat{z}]$$

This can be written as

$$\vec{G} = \frac{2\pi}{a}[(v_1\hat{x} + v_2\hat{y} + v_3\hat{z})],$$

where the integers (v_1, v_2, v_3) are all odd or all even. The restriction to all odd or all even integers can be seen by considering a bcc lattice as a simple cubic lattice (the even integers) with body centers (the odd integers).

The structure factor $S = \sum_j f_j e^{-i\vec{G} \cdot \vec{r}_j}$ with $f_j = f$ since the two atoms are the same. Thus

$$S = f(1 + e^{-i\vec{G} \cdot \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})})$$

This is zero if $e^{-i\vec{G} \cdot \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})} = -1$, which means $\vec{G} \cdot \frac{a}{4}(\hat{x} + \hat{y} + \hat{z}) = (2n + 1)\pi$, i.e., an odd integer times π . Thus

$$\frac{\pi}{2}[v_1 + v_2 + v_3] = (2n + 1)\pi$$

or

$$v_1 + v_2 + v_3 = 4n + 2$$

where n is an integer. Since the v 's are all odd or all even, the only cases where $S = 0$ are they are even and do not sum to a multiple of 4.

The vectors which do not satisfy this condition are "allowed" reflections. Clearly this includes all cases where the v 's are all odd and the case where $v_1 + v_2 + v_3 = 4n$.

Q3. This is a problem related to the free electron model. (20%)

We consider the low-lying free electron bands of both *sc* and *bcc* lattices. For convenience, choose units such that $\hbar^2/2m = 1$. Show several low-lying bands in this empty lattice approximation with their energies E as a function of k in both the [100] and [110] directions in the first zone.

Empty Lattice Approximation

Actual band structures are usually exhibited as plots of energy versus wavevector in the first Brillouin zone. When wavevectors happen to be given outside the first zone, they are carried back into the first zone by subtracting a suitable reciprocal lattice vector.

When band energies are approximated fairly well by free electron energies $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2/2m$, it is advisable to start a calculation by carrying the free electron energies back into the first zone.

We look for a \mathbf{G} such that a \mathbf{k}' in the first zone satisfies

$$\mathbf{k}' + \mathbf{G} = \mathbf{k} , \quad \text{Reduced zone scheme}$$

where \mathbf{k} is unrestricted and is the true free electron wavevector in the empty lattice.

If we drop the prime on \mathbf{k}' as unnecessary baggage, the free electron energy can always be written as

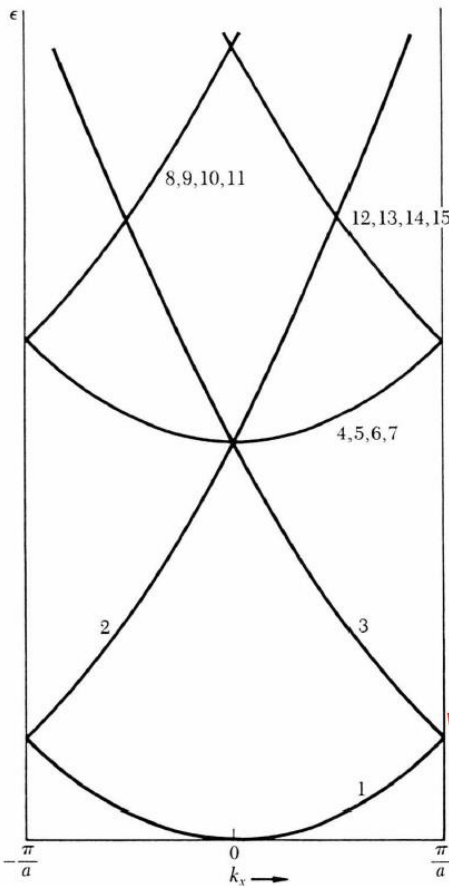
$$\begin{aligned} \epsilon(k_x, k_y, k_z) &= (\hbar^2/2m)(\mathbf{k} + \mathbf{G})^2 \\ &= (\hbar^2/2m) [(k_x + G_x)^2 + (k_y + G_y)^2 + (k_z + G_z)^2] , \end{aligned}$$

with \mathbf{k} in the first zone and \mathbf{G} allowed to run over the appropriate reciprocal lattice points.

Free electron bands for a simple cubic lattice in [100]

We consider as an example the low-lying free electron bands of a simple cubic lattice. Suppose we want to exhibit the energy as a function of \mathbf{k} in the [100] direction. For convenience, choose units such that $\hbar^2/2m = 1$. We show several low-lying bands in this empty lattice approximation with their energies $\epsilon(000)$ at $\mathbf{k} = 0$ and $\epsilon(k_x, 00)$ along the k_x axis in the first zone:

Band	$Ga/2\pi$	$\epsilon(000)$	$\epsilon(k_x, 00)$
1	000	0	k_x^2
2,3	$100, \bar{1}00$	$(2\pi/a)^2$	$(k_x \pm 2\pi/a)^2$
4,5,6,7	$010, 0\bar{1}0, 001, 00\bar{1}$	$(2\pi/a)^2$	$k_x^2 + (2\pi/a)^2$
8,9,10,11	$\bar{1}10, \bar{1}01, \bar{1}\bar{1}0, \bar{1}0\bar{1}$	$2(2\pi/a)^2$	$(k_x + 2\pi/a)^2 + (2\pi/a)^2$
12,13,14,15	$\bar{1}10, \bar{1}01, \bar{1}\bar{1}0, \bar{1}0\bar{1}$	$2(2\pi/a)^2$	$(k_x - 2\pi/a)^2 + (2\pi/a)^2$
16,17,18,19	$011, 0\bar{1}1, 01\bar{1}, 0\bar{1}\bar{1}$	$2(2\pi/a)^2$	$k_x^2 + 2(2\pi/a)^2$

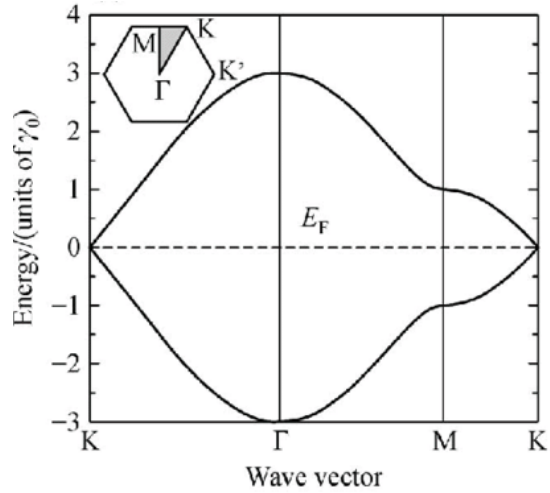
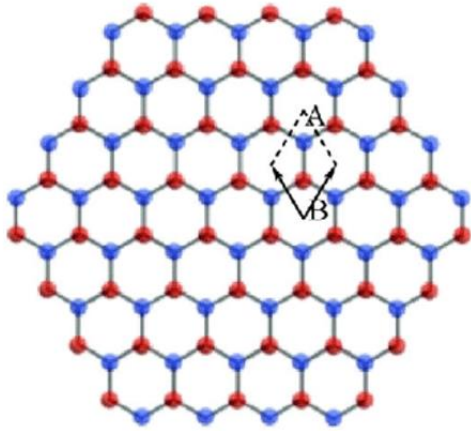


Reduced zone scheme

Figure 8 Low-lying free electron energy bands of the empty sc lattice, as transformed to the first Brillouin zone and plotted vs. $(k_x, 00)$. The free electron energy is $\hbar^2(\mathbf{k} + \mathbf{G})^2/2m$, where the \mathbf{G} 's are given in the second column of the table. The bold curves are in the first Brillouin zone, with $-\pi/a \leq k_x \leq \pi/a$. Energy bands drawn in this way are said to be in the reduced zone scheme.

Q4. This is a problem related to the Fermi surface. (15%)

Brillouin zones of two-dimensional layer materials. A two-dimensional material in the form of a honeycomb (as shown below) has two conduction electrons per atom. In the almost free electron approximation, sketch carefully the electron and hole energy surfaces. For the electrons choose a zone scheme such that the Fermi surface is shown as closed.



Honeycomb lattice structure of graphene consisting of two atoms (A and B) and Phonon spectra of graphene. The low energy band structure exhibits zero energy gap at the Dirac point.

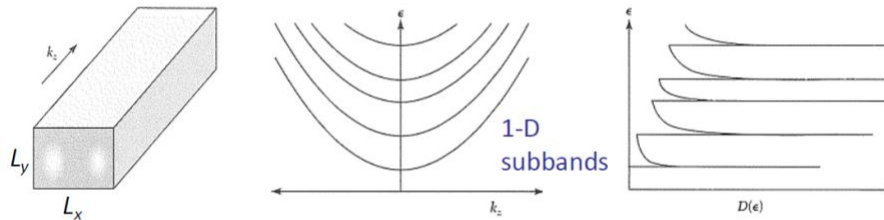
Q5. This is a problem related to the transport phenomena. (15%)

a) Calculate the density of states $D(E)$ for both the one- and two-dimensional conductor. Sketch the density of states as function of the electron energy E for a sequence of subbands.

b) Taking a one-dimensional conducting wire, which scattering processes are possible in electron transport if only a single subband is occupied? What is different if a second subband is occupied so that the Fermi-level intersects two subbands?

Electronic Structure of 1-D Systems

Consider a quasi one-dimensional wire with a diameter of the order of the Fermi-wavelength λ_F and a length $L_z \ll l_e, l_\phi$. Electron transport through the wire is called ballistic in that case since an electron passes from one end to the other without being scattered at all.

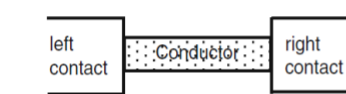


For free electrons the energy in the subbands is

$$E_i = \varepsilon_i(k_x, k_y) + \frac{\hbar^2 k_z^2}{2m^*}, \quad \psi(x, y, z) = \psi_{i,j}(x, y) e^{ik_z z} \quad i, j = \text{quantum numbers in the cross section}$$

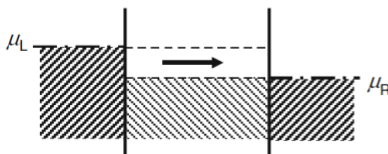
Thus, the energy bands represent a sequence of parabolas, each of which describes one transport channel shown in the above figure.

Electrical Transport in 1-D



The difference between the chemical potentials is given by the voltage U between the contacts,

$$\mu_L - \mu_R = eU.$$



Only the electron states between μ_L and μ_R contribute to the current flow from left to right. The current in one subband i is then

$$I_i = e \int_{\mu_R}^{\mu_L} D_i^{(1)}(E) v_i(E) dE$$

Since $D^{(1)}(E) = \frac{1}{\pi \partial E / \partial k_z}$ and $v_i(E) = \frac{1}{\hbar} \frac{\partial E_i}{\partial k_z} \rightarrow I_i = \frac{2e^2}{h} U.$

The universal conductance is $G_0 = \frac{2e^2}{h} = 7.74809 \times 10^{-5} \Omega^{-1} = 1/(129064 \Omega).$

If more than one channel fits into the conductor then each channel contributes $2e^2/h$ to the total conductance. The conductance quantum reduces to half the value e^2/h if the spin-degeneracy is lifted by a strong magnetic field.

a) Density of States (DOS) Calculation and Sketch:

For a one-dimensional band:

$$k \propto \sqrt{E(k) - E_0}, \text{ and } dk \propto \frac{dE}{\sqrt{E(k) - E_0}},$$

yielding

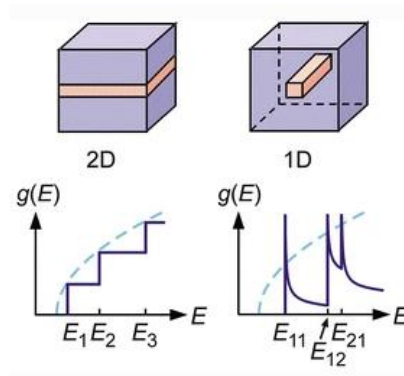
$$g_{1D}(E) \propto \frac{1}{\sqrt{E(k) - E_0}}. \quad (61)$$

The proportionality factor is $\sqrt{m^* / (2\pi^2 \hbar^2)}$; hence, $g_{1D}(E)$ is expressed in units of $m^{-1} \times J^{-1}$ or $cm^{-1} \times eV^{-1}$.

In a *two-dimensional band*, all states of equal energy between E and $E + dE$ lie in a ring of radius $k_r \propto \sqrt{E(\mathbf{k}) - E_0}$ and thickness dk as illustrated in Fig. 36b; for their number $dN \propto k_r dk$ applies. Since $E(\mathbf{k}) - E_0 \propto k_r^2$ we obtain a constant density of states

$$g_{2D}(E) \propto \theta(E - E_0), \quad (62)$$

$\theta(E - E_0)$ being the unit step function (i.e., 0 for $E < E_0$ and 1 for $E \geq E_0$). The factor is $m^*/(\pi \hbar^2)$, yielding $g_{2D}(E)$ in units of $cm^{-2} \times eV^{-1}$.



Electronic density of states $g(E)$ in isotropic semiconductors (red), clad by barriers (blue) in 2D quantum well and 1D quantum wire. The dashed curve represents the 3D case drawn for reference.

b) Scattering Processes in Electron Transport:

Single Subband Occupied:

If only a single subband is occupied, the scattering processes are typically limited to intraband scattering. This means that electrons within the same subband can scatter due to various mechanisms, such as impurity scattering, phonon scattering, or electron-electron scattering. However, there is no scattering between electrons in different subbands because only one subband is occupied.

Fermi-Level Intersects Two Subbands:

When the Fermi level intersects two subbands, the scattering processes become more diverse. In addition to intraband scattering within each subband, there can be interband scattering between electrons in different subbands. This opens up new possibilities for scattering mechanisms.

For example:

- Electrons in one subband may scatter into the other subband due to impurities or defects.
- Phonon scattering may involve transitions between different subbands.

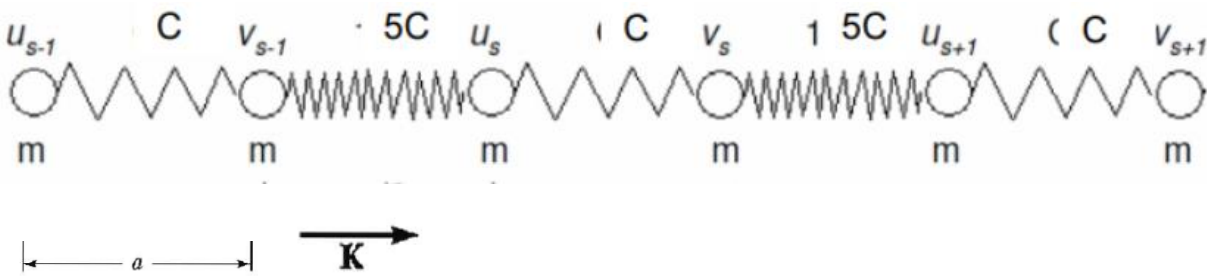
The presence of multiple subbands provides additional channels for electron scattering, impacting the overall transport properties of the system. The Fermi level now serves as a boundary between occupied and unoccupied subbands, and scattering processes can involve transitions across this boundary.

In summary, the key difference is the availability of interband scattering processes when multiple subbands are occupied, expanding the range of possible scattering mechanisms in the electron transport.

Q6. This is a problem related to the crystal vibration. (20%)

Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately C and $5C$. Let the atomic mass m be equal and the nearest-neighbor separation be a .

- Find $\omega(K)$ at the zone center and boundary of the 1st Brillouin zone.
- Sketch the dispersion relation.
- If the Raman spectroscopy is applied to measure the system's phonon dispersion, what will the spectrum look like and briefly interpret the data.



Each site has bond with force constant C on one side and $5C$ on the other side.

The equations of motion assuming that each plane interacts only with its nearest-neighbor planes.

$$M \frac{d^2 u_s}{dt^2} = C_1(v_s - u_s) + C_2(v_{s-1} - u_s) \quad M \frac{d^2 v_s}{dt^2} = C_1(u_s - v_s) + C_2(u_{s+1} - v_s)$$

We expect the solution in the form $u_s = u e^{i(sKa - \omega t)}$ \Rightarrow $\frac{d^2 u_s}{dt^2} = -\omega^2 u_s$. We also have $u_{s+1} = u_s e^{iKa}$
 $v_s = v e^{i(sKa - \omega t)}$ $\frac{d^2 v_s}{dt^2} = -\omega^2 v_s$ $v_{s-1} = v_s e^{-iKa}$

Substituting these into above equations gives: $-\omega^2 M u_s = (C_1 + C_2 e^{-iKa}) v_s - (C_1 + C_2) u_s$

$$-\omega^2 M v_s = (C_1 + C_2 e^{iKa}) u_s - (C_1 + C_2) v_s$$

In a matrix form: $\begin{bmatrix} -\omega^2 M + (C_1 + C_2) & -(C_1 + C_2 e^{-iKa}) \\ -(C_1 + C_2 e^{iKa}) & -\omega^2 M + (C_1 + C_2) \end{bmatrix} \begin{bmatrix} u_s \\ v_s \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

$$\Rightarrow \begin{vmatrix} -\omega^2 M + (C_1 + C_2) & -(C_1 + C_2 e^{-iKa}) \\ -(C_1 + C_2 e^{iKa}) & -\omega^2 M + (C_1 + C_2) \end{vmatrix} = 0 \quad (*)$$

$$*K = 0 \Rightarrow (*) \Leftrightarrow \left[-\omega^2 M + (C_1 + C_2) \right]^2 - (C_1 + C_2)^2 = 0$$

$$\Leftrightarrow (\varpi^2 M)^2 - 2(C_1 + C_2)\varpi^2 M = 0$$

$\Rightarrow \varpi^2 = 0; \frac{2(C_1 + C_2)}{M}$ which are the acoustical and optical branch, respectively.

Now, chose $C_1 = C$ and $C_2 = 5C$. The solutions are

$$\varpi_1 = 0 \text{ and } \varpi_2 = \sqrt{12C/M}$$

The zero-frequency mode at $k = 0$ is called the Goldstone mode.

$$*K = \frac{\pi}{a} \Rightarrow (*) \Leftrightarrow (\varpi^2 M)^2 - 2(C_1 + C_2)\varpi^2 M + (C_1 + C_2)^2 - (C_1 - C_2)^2 = 0$$

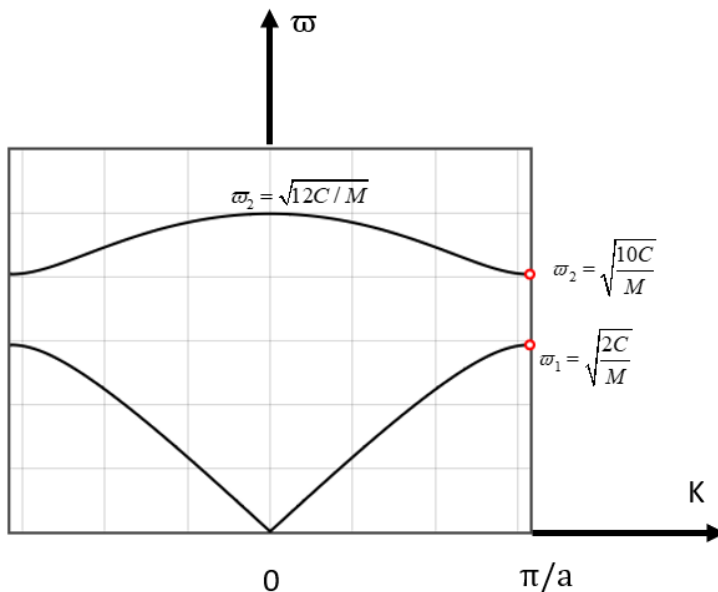
$$\Leftrightarrow (\varpi^2 M)^2 - 2(C_1 + C_2)\varpi^2 M + 4C_1 C_2 = 0 \Leftrightarrow (\varpi^2 M - 2C_1)(\varpi^2 M - 2C_2) = 0 \Rightarrow \varpi^2 = \frac{2C_1}{M}; \frac{2C_2}{M}$$

Now, chose $C_1 = C$ and $C_2 = 5C$. The solutions are

$$\varpi_1 = \sqrt{\frac{2C}{M}} \text{ and } \varpi_2 = \sqrt{\frac{10C}{M}}$$

b) Sketch the dispersion relation:

The dispersion relation can be sketched as a plot of $\omega(K)$ versus K .



c) Raman Spectroscopy:

In Raman spectroscopy, the scattered light intensity is measured as a function of frequency. The Raman spectrum will show peaks corresponding to the vibrational modes of the crystal.

For the given problem, the spectrum is expected to have peaks at frequencies corresponding to the $\omega(K)$ values calculated earlier. Specifically, there will be a peak at $\omega(0)=0$ (due to the zone center mode) and a peak at $\omega(\pi/a)=2Cm\omega(a\pi)=2mC$

(due to the boundary of the 1st Brillouin zone mode).

Interpretation:

- The peak at $\omega(0)=0$ represents a mode with no displacement at the zone center, which could correspond to a long-wavelength acoustic mode.
- The peak at $\omega(\pi/a)$ represents a mode with a displacement at the boundary of the Brillouin zone, likely a short-wavelength optical mode.

The presence of these peaks in the Raman spectrum provides information about the vibrational properties of the crystal and the nature of the phonon modes. The intensity and width of the peaks will depend on factors like temperature and the interaction strength between the photons and the phonons.