PH 208 (Condensed Matter Physics)
Assignment 4

Name: Suman Kumar Pal

SR No.: 24974

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PH-208, Condensed Matter Physics- I

Instructor: Prof. Anindya Das

Assignment 4, Due: **31st March**,2025

Max. Marks: 35

Problem 1. Eigenstates of the Bloch Hamiltonian (7 points)

The eigenstate of Bloch Hamiltonian can be written as-

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{Nv}} \exp{(i\mathbf{k}\cdot\mathbf{r})} u_{n\mathbf{k}}(\mathbf{r})$$

where $\mathbf{K}$ is a wavevector in 1^{st}BZ, n is the band index, N is the number of sites in our box, and V is the volume of the unit cell. Is the following statement true? For a given band index n:

$$\int_v d^3\mathbf{r} u^*_{n\mathbf{k}'}(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) = \delta_{\mathbf{k},\mathbf{k}'}$$

Give reason(s) for your answer.

Problem 2. Nearly Free Elections in Dirac-Delta potentials (5 points)

Atoms are arranged in a one-dimensional chain with lattice spacing a. Each atom is represented by the potential $V(x) = aV_0\delta(x)$. Determine the energy gaps between the bands, assuming that the energy nearly free-electron approximation applies.

Problem 3. Empty Lattice Approximation (7 points)
Consider a BCC crystal lattice's free electron energy bands in the empty lattice approximation in the reduced zone scheme. Calculate and sketch roughly the energies of the first five bands in the [111] direction in $\mathbf{k}$-space.

Problem 4. Energy gap at the M point (6 points)

Consider electrons in a square lattice in two dimensions. The periodic the potential is given by

$$U(x, y) = 4U \cos\frac{2\pi x}{a} \cos\frac{2\pi y}{a}$$

with 'a' the lattice constant. Find approximately the energy gap at the corner point M with $k_M = \frac{\pi}{a}(\hat{x} + \hat{y})$ of the first Brillouin zone. It will suffice to solve a 2×2 determinantal equation.

Problem 5. Periodic Potential(10 points)

(i) Consider a two-dimensional lattice with a single-point basis with a valence of two. Treat the conduction electrons using the free electron model. Sketch roughly the Fermi surface for in the extended zone scheme and in the reduced zone scheme. [**5**]
(ii) Sketch the same for the case of electrons in a weak periodic potential- point out the main differences between the two situations.[**5**]

(1) Eigenstates of the Bloch Hamiltonian

$$\psi_{n\vec{k}}(\vec{r}) = \frac{1}{\sqrt{NV}} \exp(i\vec{k}.\vec{r})\, u_{n\vec{k}}(\vec{r})$$

$\vec{k}$ in 1st B.Z. : $-\frac{\pi}{a} \le |\vec{k}| \le \frac{\pi}{a}$

$$\psi^*_{nk}(r) = \frac{1}{\sqrt{NV}} e^{-i\vec{k}.\vec{r}}\, u^*_{nk}(r)$$

$$I = \int_V d^3r\, u^*_{nk'}(\vec{r})\, u_{nk}(\vec{r})$$

$$= \int_V d^3r\, (NV).\, e^{i\vec{k}'.\vec{r}} \psi^*_{n\vec{k}'}(\vec{r})\, e^{-i\vec{k}.r} \psi_{n\vec{k}}(\vec{r})$$

$$= NV \int_V d^3r\, e^{i(\vec{k}'-\vec{k}).\vec{r}}\, \psi^*_{nk'}(r)\, \psi_{nk}(r)$$

As we are inside 1st B.Z. $k'-k \neq G$ as G itself contains $\frac{2\pi}{a}$.

Probability density; $\rho_{nk}(r) = \psi^*_{nk}(r)\psi_{nk}(r)$

Now, over volume $e^{i(\vec{k}'-\vec{k}).r}$ takes values in all 4 quadrants of complex plane and we get the net result as "0".

So, only $\vec{k}' = \vec{k}$ gives non-zero result.

$$I = NV \int_V d^3r\, \delta_{k,k'}\, \psi^*_{nk'}(r)\, \psi_{nk}(r)$$

$$\Rightarrow I = NV\, \delta_{k,k'} \int_V d^3r\, \rho_{nk}(r) \; ; \; \rho_{nk}(r) = \psi^*_{nk}\psi_{nk}.$$

$\int_V d^3r\, \rho_{nk}(r)$ gives total probability of finding e^- inside unit cell of volume V and there are N sites inside cell.

So, $\int_V d^3r\, \rho_{nk}(r) = \left(\frac{1}{N}\right) \cdot \left(\frac{1}{V}\right)$

probability of finding over N unit cells

Probability of finding in volume V inside a unit cell

Thus, $I = NV\, \delta_{k,k'} \frac{1}{N}\frac{1}{V}$

$$\Rightarrow \int_V d^3r\, u^*_{nk'}(r)\, u_{nk}(r) = \delta_{k,k'} \quad \text{(proved)}$$

The condition is proved for 1st B.Z.

For 1st B.Z only we need $\vec{k}' = \vec{k}$ condition for getting $e^{i(\vec{k}'-\vec{k}).\vec{r}} = 1$ inside integrand and from there we get $\delta_{k,k'}$ term.

But in higher B.Z., we can have $\vec{k}$ and $\vec{k}'$ s.t.

$|\vec{k}' - \vec{k}| \geq \frac{2\pi}{a}$. For $\vec{k}' - \vec{k} = \vec{G}$; where $\vec{G}$ represents reciprocal lattice vector and $\vec{G}.\vec{r} = 2\pi$ or some multiple of 2π.

Thus; $e^{i(\vec{k}'-\vec{k}).\vec{r}} = 1$ even if $\vec{k}' \neq \vec{k}$.

Thus for higher B.Z. we don't get $\delta_{k',k}$ term and condition given is not true.

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② Nearly Free Electrons in Dirac-Delta potentials

Total potential;
$$V(x) = \sum_{n=1}^{N} a V_0 \, \delta(x-na)$$

For periodic potential and nearly free e^- model;

E_k is almost even function of k; i.e. $E(k) = E(-k)$.

Also, condition for scattering is $k - k' = G$ or some multiple of G. For transition $-\frac{\pi}{a}$ to $\frac{\pi}{a}$ (1 Brillouin zone boundary to another boundary); E remains same. In this case we need to use degenerate perturbation theory.

$$H = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{H_0} + \underbrace{V(x)}_{H_1} \quad , \quad H_0 |\psi_k^{(0)}\rangle = H_0|k\rangle = E_k^{(0)}|k\rangle$$

(Box normalization is applied)

Consider k and $k' = -k$; $E_{k'}^{(0)} = E_k^{(0)}$. $E_k^{(0)} = \frac{\hbar^2 k^2}{2m}$.

$|\psi_k^{(0)}\rangle = \frac{e^{ikx}}{\sqrt{Na}} = |k\rangle$. ; $|k\rangle$ forms orthonormal basis.

Consider; $|\psi\rangle = \alpha|k\rangle + \beta|k'\rangle$. (a general state)

$H|\psi\rangle = E_k|\psi\rangle$.

$$H(\alpha|k\rangle + \beta|k'\rangle) = E_k(\alpha|k\rangle + \beta|k'\rangle)$$

Now; $\langle k|k'\rangle = 0$. Act $\langle k|$ in the above equation;

$$\alpha\langle k|H|k\rangle + \beta\langle k|H|k'\rangle = E_k\alpha$$

$$\Rightarrow \alpha\langle k|H_0|k\rangle + \alpha\langle k|V(x)|k\rangle + \beta\underbrace{\langle k|H_0|k'\rangle}_{\to 0} + \beta\langle k|V(x)|k'\rangle = E_k\alpha$$

$$\Rightarrow \alpha(E_k^{(0)} + V_0) + \beta\langle k|V(x)|k'\rangle = E_k\alpha$$

$$\Rightarrow \beta = \frac{\alpha(E_k - E_k^{(0)} - V_0)}{\langle k|V(x)|k'\rangle}$$

$$\langle k|V(x)|k\rangle = \int V(x)\,dx = \sum_n \int a V_0 \frac{\delta(x-na)}{Na}\,dx = \frac{V_0}{N}\sum_{n=1}^{N} 1 = V_0$$

$$\langle k|V(x)|k'\rangle = \sum_n \int a V_0 \, \delta(x-na) \frac{e^{i(k'-k)x}}{Na}\,dx$$
$$= \frac{V_0}{N}\sum_{n=1}^{N}\int e^{-iGx}\,\delta(x-na)\,dx$$
$$= \frac{V_0}{N}\sum_{n=1}^{N} e^{-iGna}$$

Now; G is multiple of $\frac{2\pi}{a}$.

So; $e^{-iGna} = 1$.

Thus: $\langle k | V(x) | k' \rangle = \frac{V_0}{N} \sum_{n=1}^{N} 1 = V_0$.

So; $\alpha E_k^{(0)} + \alpha V_0 + \beta V_0 = \alpha E_k$

$\Rightarrow \alpha (E_k^{(0)} + V_0 - E_k) + \beta V_0 = 0$

We have; $(H_0 + v(x)) (\alpha |k\rangle + \beta |k'\rangle) = E_k (\alpha |k\rangle + \beta |k'\rangle)$

If we operate $\langle k' |$; we will get;

$\alpha \langle k' | V(x) | k \rangle + \beta (E_k^{(0)} + V_0) = \beta E_k$

$\Rightarrow \alpha V_0 + \beta (E_k^{(0)} + V_0 - E_k) = 0.$

Thus; $$\begin{pmatrix} \frac{\hbar^2 k^2}{2m} + V_0 - E_k & V_0 \\ V_0 & \frac{\hbar^2 k^2}{2m} + V_0 - E_k \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0.$$

For non trivial solution $\left(E_k^{(0)} = \frac{\hbar^2 k^2}{2m}\right)$.

$$\begin{vmatrix} \frac{\hbar^2 k^2}{2m} + V_0 - E_k & V_0 \\ V_0 & \frac{\hbar^2 k^2}{2m} + V_0 - E_k \end{vmatrix} = 0.$$

$\Rightarrow E_k = \frac{\hbar^2 k^2}{2m} + V_0 \pm \sqrt{(V_0)^2}$

$\Rightarrow E_+ = \frac{\hbar^2 k^2}{2m} + 2V_0$

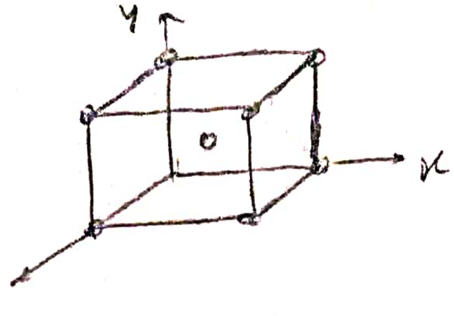
and $E_- = \frac{\hbar^2 k^2}{2m}$.

Energy gaps between bands $E_g = E_+ - E_-$

$\Rightarrow E_g = 2 V_0$ (Ans.)

③ Empty Lattice Approximation

BCC:



In empty lattice approximation,

$$E_{nk} = \frac{\hbar^2}{2m}(k+G_n)^2$$

Premitive lattice vectors: $\vec{a_1} = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z})$, $\vec{a_2} = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z})$

$\vec{a_3} = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})$

Reciprocal lattice vectors:

$$\vec{b_1} = \frac{a_2 \times a_3}{a_1.(a_2 \times a_3)} 2\pi = \frac{2\pi}{a}(\hat{y}+\hat{z})$$

$$\vec{b_2} = \frac{a_3 \times a_1}{a_1.(a_2 \times a_3)} 2\pi = \frac{2\pi}{a}(\hat{x}+\hat{z})$$

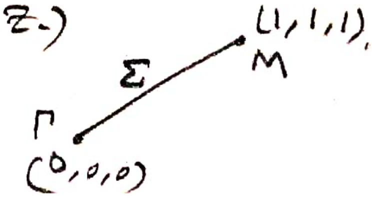
$$\vec{b_3} = \frac{a_1 \times a_2}{a_1.(a_2 \times a_3)} 2\pi = \frac{2\pi}{a}(\hat{x}+\hat{y})$$

$\vec{G_n} = n_1\vec{b_1} + n_2\vec{b_2} + n_3\vec{b_3}$ (translation vector in reciprocal space)

$$\Rightarrow \vec{G_n} = \frac{2\pi}{a}\left[(n_2+n_3)\hat{x} + (n_1+n_3)\hat{y} + (n_1+n_2)\hat{z}\right].$$

for [1 1 1] direction; $\vec{k} = \frac{\pi}{a}\xi(\hat{x}+\hat{y}+\hat{z})$ (in 1st B.Z.)

ξ varies from 0 to 1. Also; $|k| \in [0, \frac{\pi}{a}\sqrt{3}]$



$$E_{nk} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2\left[(\xi+2n_2+2n_3)\hat{x} + (\xi+2n_1+2n_3)\hat{y} + (\xi+2n_1+2n_2)\hat{z}\right]^2$$

(1) (n_1, n_2, n_3): $(0,0,0)$

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\xi^2(\hat{x}+\hat{y}+\hat{z})^2$$

$$\Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}3\xi^2$$

$\xi = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(0,3)$

(2) (n_1, n_2, n_3) : $(1,0,0)$ or $(0,1,0)$ or $(0,0,1)$.

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[\xi_1 \hat{x} + (\xi_1+2)\hat{y} + (\xi_1+2)\hat{z}\right]^2$$

$$= \frac{\hbar^2\pi^2}{2ma^2}\left[\xi_1^2 + 2(\xi_1+2)^2\right]. \quad \Big| \xi_1 = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(8, 19)$$

(3) (n_1, n_2, n_3) : $(\bar{1},0,0)$ or $(0,\bar{1},0)$ or $(0,0,\bar{1})$

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[\xi_1^2 + (\xi_1-2)^2 + (\xi_1-2)^2\right]$$

$$= \frac{\hbar^2\pi^2}{2ma^2}\left[\xi_1^2 + 2(\xi_1-2)^2\right] \quad \Big| \xi_1 = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(8,3).$$

(4) (n_1, n_2, n_3) : $(1,1,0)$, $(1,0,1)$, $(0,1,1)$.

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[(\xi_1+2)^2 + (\xi_1+2)^2 + (\xi_1+4)^2\right].$$

$$= \frac{\hbar^2\pi^2}{2ma^2}\left[2(\xi_1+2)^2 + (\xi_1+4)^2\right]. \quad \Big| \xi_1 = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(24, 43)$$

(5) (n_1, n_2, n_3) : $(1,\bar{1},0)$, $(1,0,\bar{1})$, ... (6 possibilities).

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[(\xi_1-2)^2 + (\xi_1+2)^2 + \xi_1^2\right]$$

$$= \frac{\hbar^2\pi^2}{2ma^2}(3\xi_1^2 + 8). \quad \Big| \xi_1 = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(8, 11).$$

(6) (n_1, n_2, n_3) : $(\bar{1},\bar{1},0)$, ... (3 possibilities)

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[(\xi_1-2)^2 + (\xi_1-2)^2 + (\xi_1-4)^2\right]$$

$$= \frac{\hbar^2\pi^2}{2ma^2}\left[2(\xi_1-2)^2 + (\xi_1-4)^2\right]. \quad \Big| \xi_1 = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(24, 11)$$

(7) (n_1, n_2, n_3) : $(\bar{1},\bar{1},1)$, ... (3 possibilites).

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[2\xi_1^2 + (\xi_1-4)^2\right]. \quad \Big| \xi_1 = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(16, 11)$$

(8) (n_1, n_2, n_3) : $(2,0,0)$, ... (3 possibilities)

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[\xi_1^2 + 2(\xi_1+4)^2\right] \quad \Big| \xi_1 = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(32, 51)$$

(9) (n_1, n_2, n_3): $(\bar{2}, 0, 0), \ldots$ (3 possibilities)

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[\xi^2 + 2(\xi-4)^2\right] \quad \Big| \quad \xi = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(32, 19)$$

(10) (n_1, n_2, n_3): $(1,1,1)$

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\, 3(\xi+4)^2 \quad \Big| \quad \xi = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(48, 75)$$

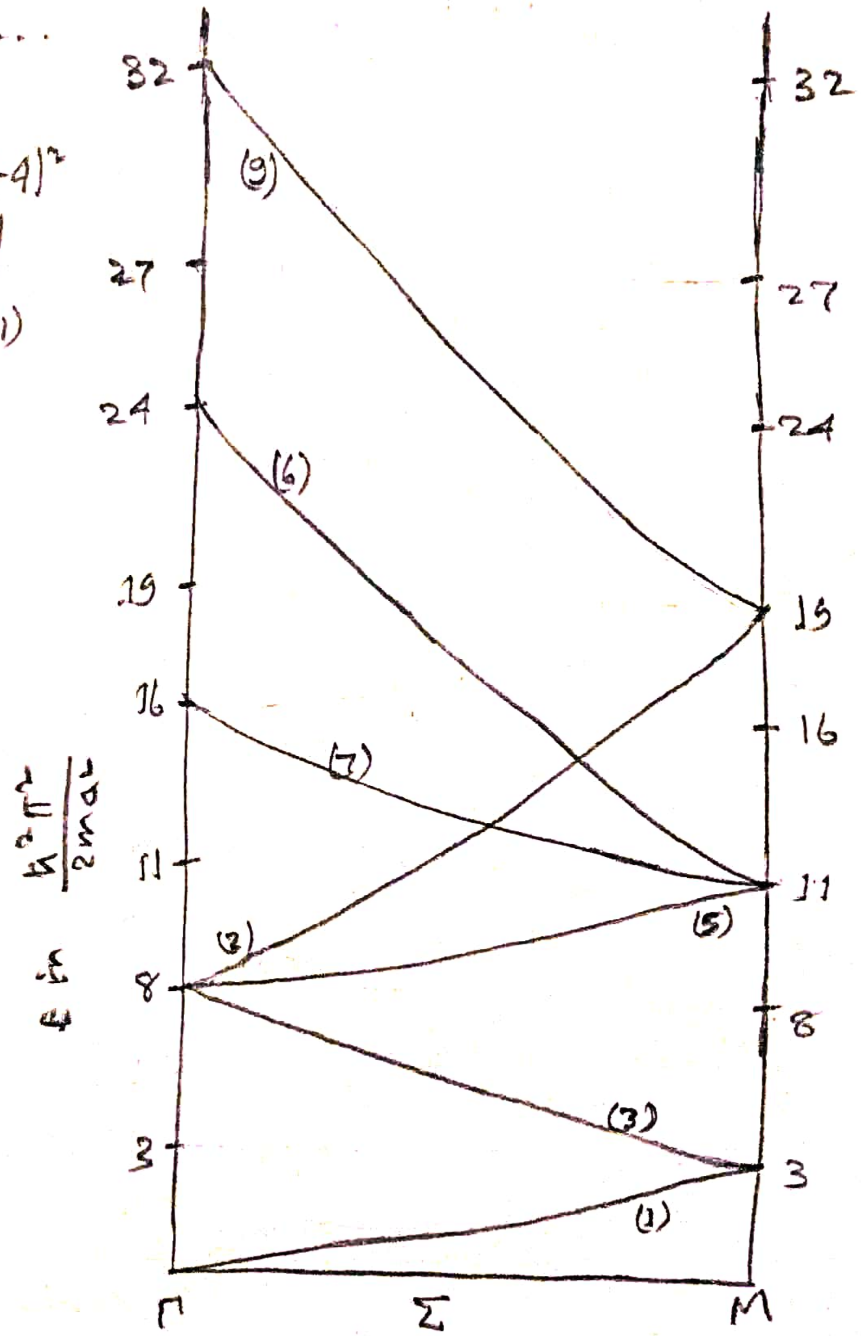
(11) (n_1, n_2, n_3): $(1, \bar{1}, 1), \ldots$ (3 possibilities)

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[2\xi^2 + (\xi+4)^2\right] \quad \Big| \quad \xi = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(32, 27)$$

(12) (n_1, n_2, n_3): $(\bar{2}, 1, 0), \ldots$
(6 possibilities)

$$E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}\left[(\xi-2)^2 + (\xi-4)^2 + (\xi-2)^2\right]$$

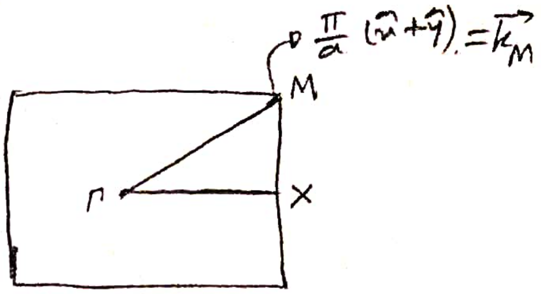
$$\xi = (0,1) \Rightarrow E_{nk} = \frac{\hbar^2\pi^2}{2ma^2}(24, 11)$$



④ Energy gap at the M point

$U(x,y) = 4U \cos\frac{2\pi x}{a} \cos\frac{2\pi y}{a}$

The Hamiltonian of the system is;



$H = H_0 + U(x,y)$

$H_0 = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$

(free particle Hamiltonian)

for $H_0|k\rangle = E_k^{(0)}|k\rangle$; $E_k^{(0)} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2)$

$|k\rangle = \frac{1}{\sqrt{Na}}\frac{1}{\sqrt{Na}} e^{ik_x x} e^{ik_y y} = \frac{1}{Na} e^{i\vec{k}\cdot\vec{r}}$

(Box normalization is applied)

Consider; $H|\psi\rangle = E_k|\psi\rangle$.

We can take; $\vec{k}_M' = \frac{\pi}{a}(-\hat{x}, -\hat{y})$. Then $\vec{k}_M - \vec{k}_M' = \frac{2\pi}{a}(\hat{x}+\hat{y})$
$= 2\vec{k}_M$

$\vec{k}_M - \vec{k}_M'$ represents a translation vector $\vec{G} = \frac{2\pi}{a}(\hat{x}+\hat{y})$ in reciprocal space. Thus $\vec{k}_M$ to $\vec{k}_M'$ scattering is possible.

Now; for H_0; $E_{\vec{k}_M}^{(0)} = E_{\vec{k}_M'}^{(0)} = \frac{\hbar^2 k_M^2}{2m}$

Thus, here we have degeneracy and we have to use degenerate perturbation theory.

Take, $|\psi\rangle = \alpha|k_M\rangle + \beta|k_M'\rangle$

$H|\psi\rangle = E_k|\psi\rangle$; $H_0|k_M\rangle = E_k^{(0)}|k_M\rangle$, $H_0|k_M'\rangle = E_k^{(0)}|k_M'\rangle$

$H = H_0 + U(x,y)$

also; $\langle k_M|k_M'\rangle = 0$, $\langle k_M|k_M\rangle = 1$

so; $\alpha E_k^{(0)}|k_M\rangle + \alpha U|k_M\rangle + \beta E_k^{(0)}|k_M'\rangle + \beta U|k_M'\rangle$

$= \alpha E_k|k_M\rangle + \beta E_k|k_M'\rangle$

Operating by $\langle k_M|$;

$\alpha E_k^{(0)} + \alpha\langle k_M|U_{(x,y)}|k_M\rangle + \beta\langle k_M|U_{(x,y)}|k_M'\rangle = \alpha E_k$

$$\langle k_M | U(x,y) | k_M \rangle = \frac{4U}{(Na)^2} \int_0^{Na}\int_0^{Na} \cos\frac{2\pi x}{a} \cos\frac{2\pi y}{a}\, dx\,dy$$

$$= \frac{4U}{(Na)^2}\left(\frac{a}{2\pi}\right)^2 \sin\frac{2\pi x}{a}\Big|_0^{Na} \sin\frac{2\pi y}{a}\Big|_0^{Na}$$

$$= 0$$

Similarly, $\langle k_{M'} | U(x,y) | k_{M'} \rangle = 0$.

$$\langle k_M | U(x,y) | k_{M'} \rangle = \frac{4U}{(Na)^2} \int_0^{Na}\int_0^{Na} \cos\frac{2\pi x}{a} \cos\frac{2\pi y}{a}\, e^{i(\vec{k}_{M'}-\vec{k}_M)\cdot\vec{r}}$$

$$= \frac{4U}{(Na)^2} \int_0^{Na} e^{-\frac{2\pi i}{a}x} \cos\frac{2\pi x}{a}\, dx \int_0^{Na} e^{-\frac{2\pi i}{a}y} \cos\frac{2\pi x}{a}\, dx \quad \Bigg| \; (\vec{k}_{M'}-\vec{k}_M)\cdot\vec{r} = -\frac{2\pi}{a}(x+y)$$

$$= \frac{4U}{(Na)^2}\left(\frac{a}{2\pi}\right)^2 \left(\int_0^{2\pi N} e^{-i\eta} \cos\eta\, d\eta\right)^2; \quad \eta \equiv \frac{2\pi x}{a},\ d\eta = \frac{2\pi}{a}dx$$

$$= \frac{4U}{(2\pi N)^2}\left[\frac{1}{2}\int_0^{2\pi N} (1+\cos 2\eta)\, d\eta + \frac{i}{2}\int_0^{2\pi N} \sin 2\eta\, d\eta\right]^2$$

$$= \frac{U}{(2\pi N)^2}\left[2\pi N + \underbrace{\frac{1}{2}\sin 2\eta\Big|_0^{2\pi N}}_{0} + \underbrace{i\,\frac{1}{2}\cos 2\eta\Big|_{2\pi N}^{0}}_{0}\right]^2$$

$$= \frac{U}{(2\pi N)^2}(2\pi N)^2 = U$$

$$\Rightarrow \langle k_M | U(x,y) | k_{M'} \rangle = \langle k_{M'} | U(x,y) | k_M \rangle = U$$

Also, $E_k^{(0)} = \dfrac{\hbar^2 k_{M}^2}{2m} = \dfrac{\hbar^2}{2m}\cdot\dfrac{\pi^2}{a^2}(1+1) = \dfrac{\hbar^2\pi^2}{ma^2}$

Thus; $\alpha\cdot\dfrac{\hbar^2\pi^2}{ma^2} + \alpha\cdot 0 + \beta\cdot U = \alpha E_k$.

Similarly, operating by $\langle k_{M'}|$;

$$\alpha\langle k_{M'} | U(x,y) | k_M \rangle + \beta E_k^{(0)} + \beta\langle k_{M'} | U(x,y) | k_{M'} \rangle = \beta E_k$$

$$\rightarrow \alpha\cdot U + \beta\frac{\hbar^2\pi^2}{ma^2} = \beta E_k.$$

Thus:
$$\begin{pmatrix} \frac{\hbar^2\pi^2}{ma^2} & U \\ U & \frac{\hbar^2\pi^2}{ma^2} \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = E_k\begin{pmatrix}\alpha \\ \beta\end{pmatrix}$$

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$$\Rightarrow \begin{pmatrix} \frac{\hbar^2\pi^2}{ma^2} - E_k & U \\ U & \frac{\hbar^2\pi^2}{ma^2} - E_k \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

For nontrivial solution; $\left(\frac{\hbar^2\pi^2}{ma^2} - E_k\right)^2 - U^2 = 0.$

$$\Rightarrow E_k = \frac{\hbar^2\pi^2}{ma^2} \pm U$$

Thus; energy of 2 new nondegenerate states will be; $E_+ = \frac{\hbar^2\pi^2}{ma^2} + U$ and $E_- = \frac{\hbar^2\pi^2}{ma^2} - U.$

Energy gap; $E_g = E_+ - E_-$

$$\Rightarrow E_g = 2U. \quad \text{(Ans.)}$$

⑤ Periodic Potential (2D)

5.(i) Consider N sites and lattice parameter "a", valence = 2.
If k_F radius of Fermi surface (circle in 2D);
total number of e^- = $2N = 2 \cdot \frac{\pi k_F^2}{(2\pi/L)^2}$

spin degeneracy

Distance between consecutive k points = $\frac{2\pi}{L}$; consider the space to be L×L.
$L^2 = Na^2$.

So, $k_F^2 = \frac{N}{\pi} \frac{4\pi^2}{L^2}$

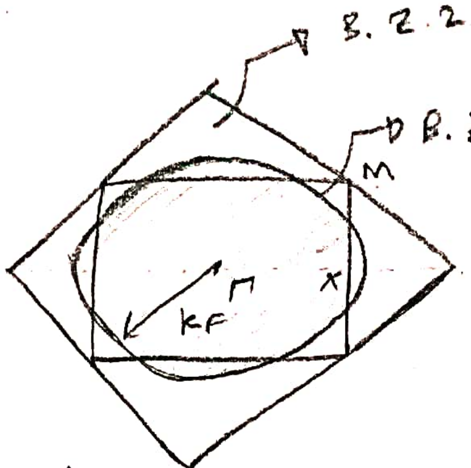
$\Rightarrow k_F = \frac{2\pi}{a}\sqrt{\frac{1}{\pi}}$

$k_F = \frac{\pi}{a}\sqrt{\frac{4}{\pi}}$

$2 > \frac{4}{\pi} > 1 \Rightarrow \frac{2\pi}{a} > k_F > \frac{\pi}{a}$.

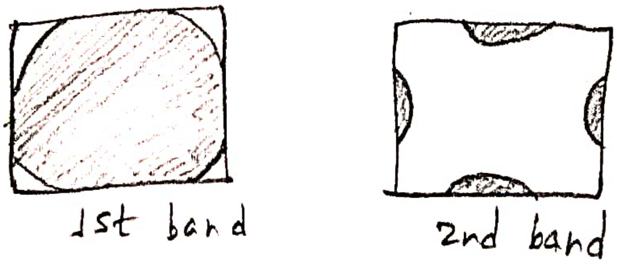
$\frac{4}{\pi} < \sqrt{2} \Rightarrow k_F < \sqrt{2}\,\frac{\pi}{a}$

Thus; the Fermi surface is contained only in 1st and 2nd Brillouin zones.



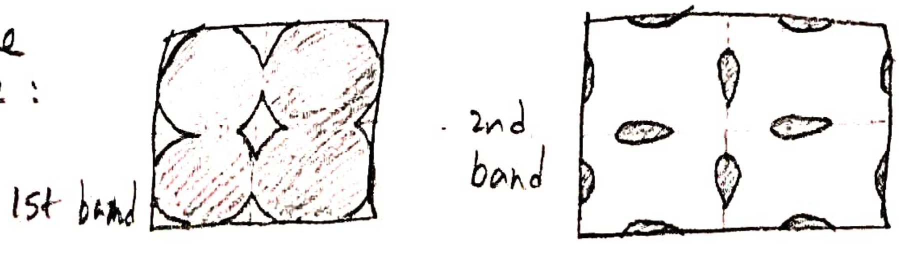
(Extended zone scheme)

For reduced zone scheme; we need to shift the domains outside B.Z.1 by $\frac{2\pi}{a}$ to bring those in range $-\frac{\pi}{a} < k < \frac{\pi}{a}$ range.

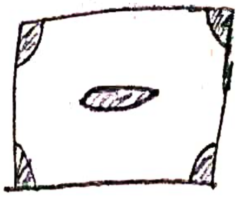


(Reduced zone scheme)

Repeated zone scheme:

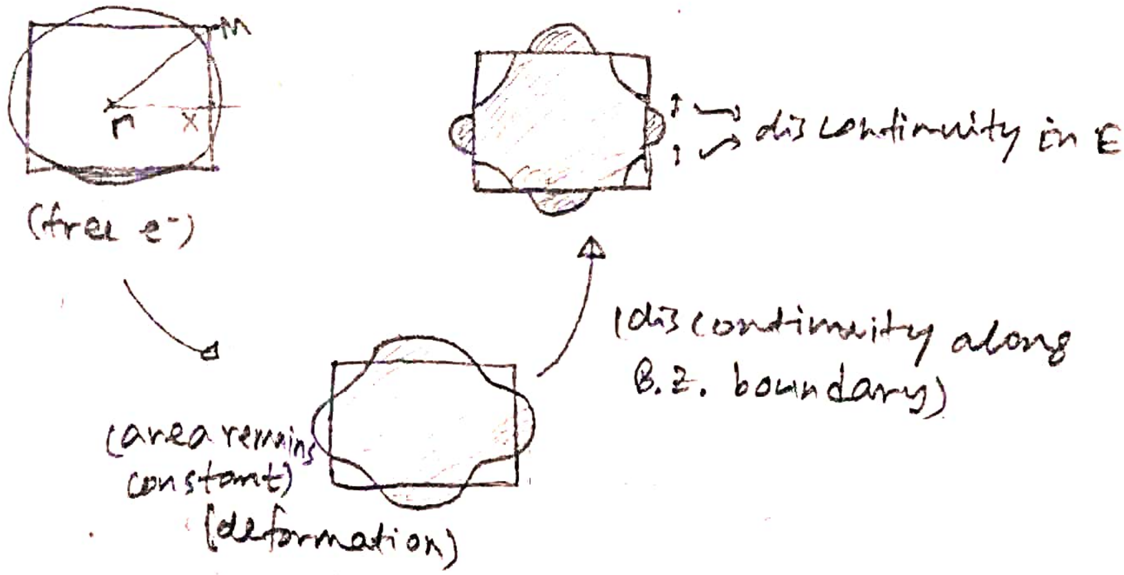


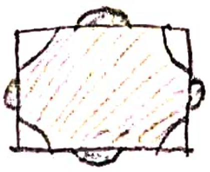
reduced zone:

1st band  2nd band 

5.(ii) For e^- in periodic potential; we will have discontinuity in E around boundary of Brillouin zones.

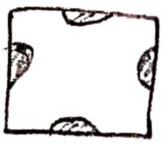
The diagrams for this case will be;





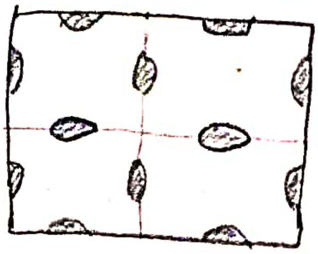
(extended zone)

1st band

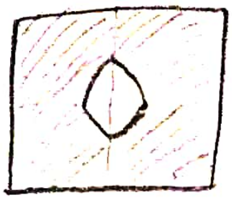
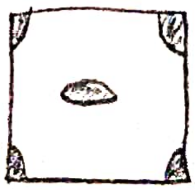


2nd band

(reduced zone)

1st band  2nd band 

(Repeated zone)

1st band  2nd band 

(Reduced zone)

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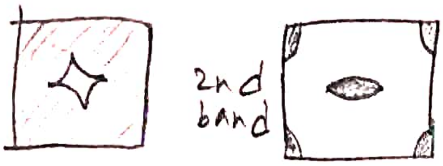
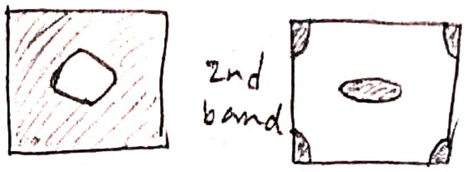
Main differences between 2 situations:

Free e^- model	Weak periodic potential
(i) Energy around Brillouin zone is continuous here	(i) Energy around Brillouin zone is discontinuous here.
(ii) Fermi surface is not perpendicular along B.Z. boundary.	(ii) Fermi surface is perpendicular along boundary of Brillouin zone.
(iii) 1st band  2nd band (Reduced zone)	(iii) 1st band  2nd band (Reduced zone)

Because of the deformation of Fermi surface around Fermi surface, around boundary the surface becomes perpendicular. This makes the slope of 2 Fermi surfaces in 2 consecutive bands having same slope. In reduced zone we see sharp corners in free e^- model at at that points the slope is not defined. But for reduced zone of weak periodic potential, the slope of Fermi surface is defined at every point and we have a totally smooth surface.

(iv) consider directions:

Along $X \Delta M$. (g).