

# Physics 141A Review

## Structure

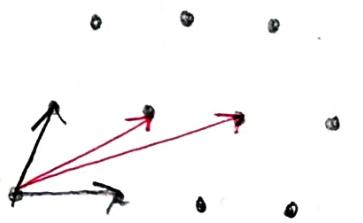
crystal: solid invariant under discrete translations

Braavis lattice: set of points in identical environment

$$\iff \text{set of points } \vec{R} = l\vec{a} + m\vec{b} + n\vec{c}$$

where  $\vec{a}, \vec{b}, \vec{c}$  are LI and  $l, m, n \in \mathbb{Z}$

\* primitive lattice vectors are not unique



unit cell: Region of space that, when translated by the lattice vectors, fills all space

Primitive unit cell: smallest possible unit cell (contains single lattice point)  
\* Primitive unit cells are not unique

Reciprocal lattice: Quantities associated with the lattice must also be periodic. E.g.  $\rho(z)$  for a 1D lattice,

$$\rho(z) = \sum_k \tilde{\rho}(k) e^{ikz} \quad \text{where } \rho(z) = \rho(z+a) \quad (\text{lattice const. } = a)$$

$$\Rightarrow \sum_k \tilde{\rho}(k) e^{ikz} = e^{ika} \sum_k \tilde{\rho}(k) e^{ikz}$$

$$\Rightarrow e^{ika} = 1$$

$$\Rightarrow k_n = \frac{2\pi n}{a}$$

Finding  $\tilde{p}_n = \tilde{p}(k_n) = \tilde{p}\left(\frac{2\pi n}{a}\right)$ :

$$\int_0^L dz p(z) e^{-ik_n z} = \int_0^L dz \left( \sum_n \tilde{p}_n e^{ik_n z} \right) e^{-ik_n z}$$

$$= \sum_n \tilde{p}_n \underbrace{\int_0^L dz e^{i(k_n - k_n)z}}_{L \delta_{nn}}$$

Thus,  $\tilde{p}_n = \frac{1}{L} \int_0^L dz p(z) e^{-ik_n z}$

Now for 3D:  $p(\vec{r}) = p(\vec{r} + \vec{R}_{\text{rec}})$

$$p(\vec{r}) = \sum_{\vec{G}} \tilde{p}_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$$

Periodicity

$$e^{i\vec{G} \cdot \vec{R}} = 1$$

where  $\vec{G}$  = reciprocal vector

$\vec{R}$  = real lattice vector

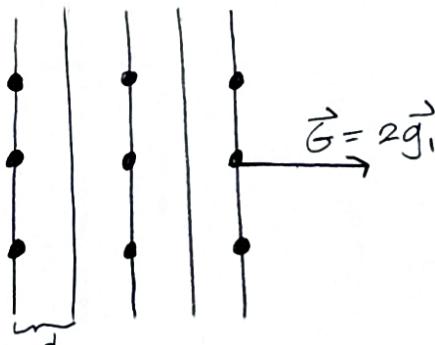
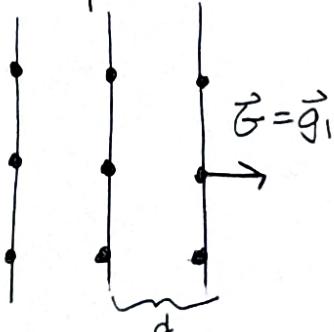
\*The set of allowed reciprocal lattices form a Bravais lattice where

$$\vec{G} = h\vec{g}_1 + j\vec{g}_2 + k\vec{g}_3$$

$$\vec{g}_1 = \frac{2\pi (\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} ; \vec{g}_2 = \frac{2\pi (\vec{a}_3 \times \vec{a}_1)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} ; \vec{g}_3 = \frac{2\pi (\vec{a}_1 \times \vec{a}_2)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

1st Brillouin zone: Wigner-Seitz unit cell of the reciprocal lattice

Family of lattice planes: For each reciprocal lattice vector,  $\vec{G}$ , we can imagine plotting the phase-fronts of the corresponding plane wave  $e^{i\vec{G} \cdot \vec{r}}$ . This set of phase-fronts will intersect all lattice points.



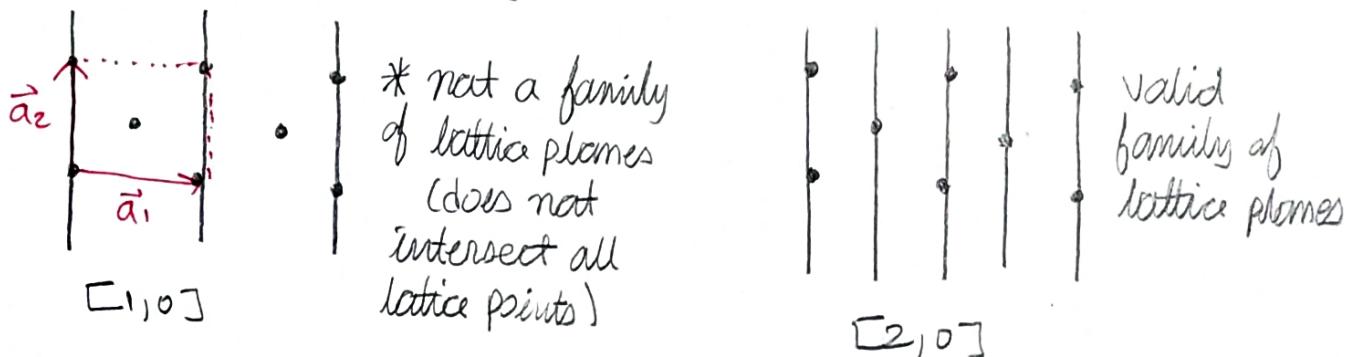
$$d = \frac{2\pi}{|\vec{G}|}$$

Miller Indices : For reciprocal lattice vector

$$\vec{G}_{hkl} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$$

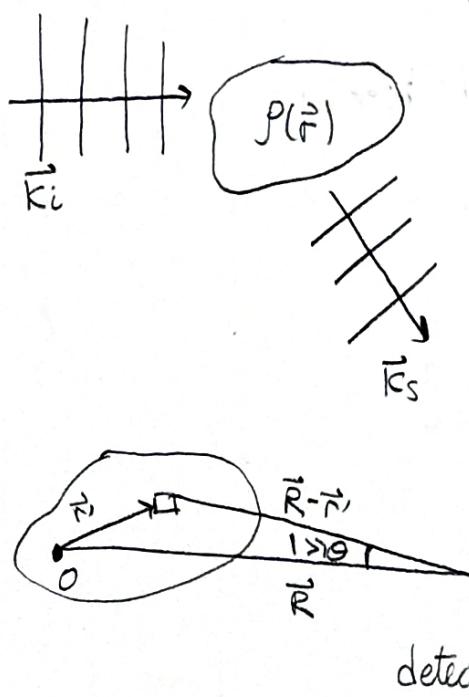
The corresponding family of lattice lines is described by the Miller indices  $[hkl]$

Conventional vs. primitive unit cell : Suppose we have body-centered crystal but we assume (incorrectly) that it has a conventional unit cell. Then, in scattering experiments where we probe the reciprocal lattice vectors, we will observe some Miller indices as "missing".



## Elastic Scattering

Suppose we scatter off an arbitrary charge density.



Incident wave :  $A_i e^{i\vec{k}_i \cdot \vec{r}}$

Scattered wave :  $dA_s \propto A_i e^{i\vec{k}_i \cdot \vec{r}} (p(\vec{r}_i) dV)$

$$dA_s(\vec{r}_i, \vec{R}) \propto \left[ A_i e^{i\vec{k}_i \cdot \vec{r}} p(\vec{r}_i) dV \right] e^{\frac{i(\vec{k}_s - \vec{k}_i) \cdot (\vec{R} - \vec{r}_i)}{R}}$$

↑ element detector

$$\approx \frac{A_i}{R} e^{i\vec{k}_i \cdot \vec{r}} p(\vec{r}_i) dV e^{i\vec{k}_s \cdot (\vec{R} - \vec{r}_i)}$$

$$= \left[ \frac{A_i}{R} e^{i\vec{k}_s \cdot \vec{R}} \right] p(\vec{r}_i) dV e^{-i(\vec{R}_s - \vec{k}_i) \cdot \vec{r}}$$

Spherical sum  
(far-field approx)

$$\text{Thus, } A_s(\vec{R}) \propto \frac{4ie^{i\vec{E}_s \cdot \vec{R}}}{R} \int d\vec{r} \rho(\vec{r}) e^{-i(\vec{E}_s - \vec{E}_i) \cdot \vec{r}}$$

If we define the scattering vector,

$$\vec{K} = \vec{E}_s - \vec{E}_i$$

$$|A_s(\vec{R})|^2 \propto \int d\vec{r} \rho(\vec{r}) e^{i\vec{K} \cdot \vec{r}}$$

↑  
Scatter intensity

↑ spatial Fourier transform of  $\rho(\vec{r})$

Scattering for crystals: Now suppose  $\rho(\vec{r})$  is periodic

$$\rho(\vec{r}) = \sum_{\vec{G}} \tilde{\rho}_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$$

$$\text{Thus, } |A_s(\vec{R})|^2 \propto \int d\vec{r} \sum_{\vec{G}} \tilde{\rho}_{\vec{G}} e^{-i(\vec{R} - \vec{G}) \cdot \vec{r}} = \sum_{\vec{G}} \tilde{\rho}_{\vec{G}} \underbrace{\int d\vec{r} e^{-i(\vec{R} - \vec{G}) \cdot \vec{r}}}_{VS(\vec{R} - \vec{G}) \text{ for an infinite crystal}}$$

$$|A_s|^2 \propto \sum_{\vec{G}} \tilde{\rho}_{\vec{G}} \delta(\vec{R} - \vec{G})$$



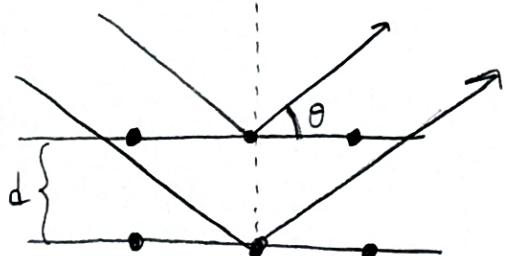
↑ = infinite crystal

↖ = finite crystal

Lau condition: For a crystal with reciprocal lattice vectors  $\vec{G}$ , the scattered waves must be of the form

$$\vec{E} = \vec{E}_s - \vec{E}_i = \vec{G} \quad \text{and} \quad |\vec{E}_i| = |\vec{E}_s|$$

Bragg Condition: Assume specular reflection off each family of lattice planes



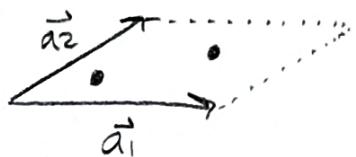
For constructive interference:

$$n\lambda = 2d \sin(\theta) \quad \text{for } n \in \mathbb{Z}$$

Structure Factor: For a crystal, each reciprocal lattice vector corresponds to a diffraction spot. We define the structure factor as,

$$S_G = \tilde{\rho}_G = \frac{1}{\sqrt{a_0^3}} \int_{a_0^3} d^3r \rho(\vec{r}) e^{iG \cdot \vec{r}}$$

Consider a unit cell,



We can write the charge density within the unit cell as  $\sum_{i=1}^N \rho_i (\vec{r} - \vec{r}_i)$

Thus,

$$\begin{aligned} \tilde{\rho}_G &= \frac{1}{V} \int d^3r \sum_{i=1}^N \rho_i (\vec{r} - \vec{r}_i) e^{iG \cdot \vec{r}} \\ &= \frac{1}{V} \sum_{i=1}^N \left( \int d^3r \rho_i (\vec{r} - \vec{r}_i) e^{iG \cdot \vec{r}} \right) \end{aligned}$$

let  $\vec{r}' = \vec{r} - \vec{r}_i$ , then,

$$\begin{aligned} \tilde{\rho}_G &= \frac{1}{V} \sum_{i=1}^N \int d^3r' \rho_i (\vec{r}') e^{iG \cdot (\vec{r}' + \vec{r}_i)} \\ &= \frac{1}{V} \sum_{i=1}^N \int d^3r' \rho_i (\vec{r}') e^{iG \cdot \vec{r}'} e^{iG \cdot \vec{r}_i} \\ &= \frac{1}{V} \sum_{i=1}^N e^{iG \cdot \vec{r}_i} \underbrace{\int d^3r' \rho_i (\vec{r}') e^{iG \cdot \vec{r}'}}_{f_i(G)} \end{aligned}$$

$f_i(G) \Rightarrow \text{form factor}$

Thus,

$$\tilde{\rho}_G = \sum_{i=1}^N f_i(G) e^{iG \cdot \vec{r}_i}$$

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## Heat capacity :

Heat capacity of a monoatomic ideal gas :  $3/2 k_B$  per atom

Heat capacity of a solid is :  $3k_B$  per atom for high temperature

Boltzmann model : Each atom in the solid is in a harmonic well  $\Rightarrow C = 3k_B$ ; but, this is wrong at low temperatures

$$E = \frac{p^2}{2m} + \frac{1}{2}kr^2$$

Classical partition function:  $Z \propto \underbrace{\int p^2 dr e^{-E(p,r)/k_B T}}_{\text{Integral over phase space}}$

$$U = -\frac{\partial \ln(Z)}{\partial \beta} \quad \text{where } \beta = \frac{1}{k_B T}$$

$$\text{Now, } Z \propto \int r^2 dr e^{-kr^2/2k_B T} \int p^2 dp e^{-p^2/2mk_B T}$$

Jacobian

$$\text{Let, } u = \frac{kr^2}{2k_B T}; v = \frac{p^2}{2mk_B T} \quad \text{some constant}$$

$$Z \propto \left(\frac{2k_B T}{K}\right)^{3/2} (2mk_B T)^{3/2} \int u^2 du e^{-u^2} \int v^2 dv e^{-v^2}$$

$$\propto \left(\frac{m}{K}\right)^{3/2} \left(\frac{1}{\beta}\right)^3$$

$$\text{Thus, } \ln(Z) = \text{const.} + 3\ln(1/\beta)$$

$$U = -\frac{\partial \ln(Z)}{\partial \beta} = 3/\beta = 3k_B T$$

$$C = \frac{\partial U}{\partial T} = 3k_B \iff \text{Dulong-Petit law}$$

Einstein calculation: Each atom is a quantum harmonic oscillator  
(allowed energies are quantized)

$$E_n = \hbar\omega(n+1/2)$$

$$Z_{10} = \sum_{n=1}^{\infty} e^{-\beta\hbar\omega(n+1/2)} = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}$$

$$U = -\frac{\partial \ln(Z)}{\partial \beta} = \hbar\omega(N_B(\beta\hbar\omega) + 1/2) \text{ where}$$

$$N_B(x) = \frac{1}{e^x - 1}$$

↑ Bose occupation

In the quantum regime:  $T \rightarrow 0, \beta \rightarrow \infty$

$$U \sim \hbar\omega e^{-\beta\hbar\omega} \implies c \sim e^{-\hbar\omega/kT}$$

Debye calculation: The model above predicts exponential behavior for low  $T$  when we actually measure  $c \propto T^3$

Debye calculation assumes periodic boundary conditions and the oscillation of the atoms given by sound modes.

$$U = 3 \sum_K \hbar\omega(K)(N_B(\beta\hbar\omega(K)) + 1/2)$$

↑ 1 mode / direction

$$= 3 \int_{all K} g(K) dK (N_B(\beta\hbar\omega(K)) + 1/2) \sim T^4$$

$$\text{density of states} = \left(\frac{L}{2\pi}\right)^3$$

$$\implies c \propto T^3 \quad (\text{but behavior for high-}T \text{ is wrong.})$$

Problem: not an infinite number of allowed  $K$ )

## Lattice Vibrations

### 1D monoatomic ring



- 1 atom/unit cell ( $N$  unit cells)
- Assume only longitudinal oscillations
- only nearest neighbor coupling

If  $u_n$  is the displacement of each atom, then,



$$\ddot{u}_{n+1} = \frac{k}{2} [u_{n+1} - u_n + (u_{n-1} - u_n)]$$

$$\ddot{u}_n = \frac{k}{2} [u_{n+1} + u_{n-1} - 2u_n]$$

Finding normal modes :  $u_n(t) = u_0 e^{-i\omega t}$

Plugging into eqn) applying boundary condition, we get

$$u_n^{(m)} = [u_0 e^{i(2\pi m/N)n}] e^{-i\omega_m t} = u_0 e^{i(k_m n - \omega_m t)} ; k_m = \left(\frac{2\pi}{Na}\right)m$$

We now plug this into eqn to find  $\omega_m$

$$-m\omega_m^2 u_0 = k u_0 (e^{ik_m a} + e^{-ik_m a} - 2)$$

$$m\omega_m^2 = 4k \sin^2(k_m a)$$

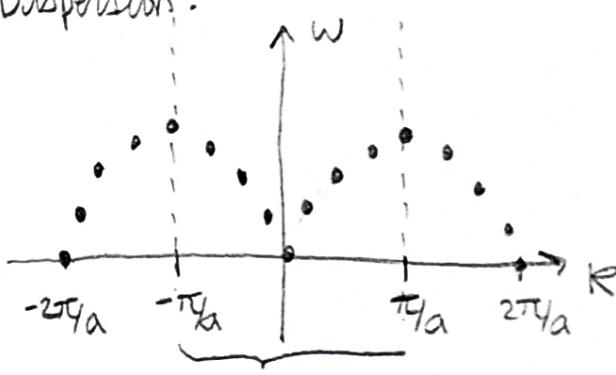
Thus,

$$u_n^{(m)}(t) = u_0 e^{i(k_m n - \omega_m t)}$$

$$k_m = \left(\frac{2\pi}{Na}\right)m$$

$$\omega_m = 2\sqrt{\frac{k}{m}} \left| \sin\left(\frac{k_m a}{2}\right) \right|$$

Dispersion:



Mode counting :  $e^{i(\frac{2\pi m}{N})} = e^{i(\frac{2\pi(m+N)}{N})}$

Thus  $k_m$  is indistinguishable from  $k_{m+N}$

⇒ there are  $N$ -distinguishable modes all between  $[-\pi/a, \pi/a]$  (1st BZ) separated by  $2\pi/Na$

Density of states : The density of states as a function of  $k$ ,

$$\# \text{ modes} = g(k) dk$$

For 1D ring:  $g(k) = N a / 2\pi = \text{length} / 2\pi$

Generalizing) 2D:  $g(k) = \frac{\text{Area}}{(2\pi)^2}$

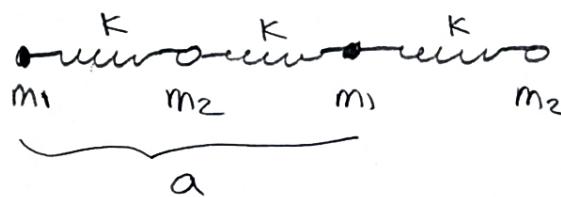
3D:  $g(k) = \frac{\text{Volume}}{(2\pi)^3}$

Density of states as a function of  $\omega$

$$g(k) dk = g(\omega) d\omega$$

$$g(\omega) = \frac{g(k)}{d\omega/dk}$$

1D tray model with basis : 2 atom basis



Made counting:

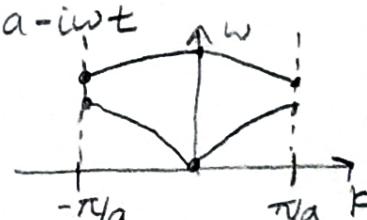
- We expect (# dimensions) (# atoms/cell) (# cell) = (1)(2)(N) =  $2N$  total modes
- expect  $N$  distinguishable  $k$
- Thus, we expect (# dim) (# atoms/cell) branches
- We expect 1 acoustical mode per dimension with the remaining being optical modes

Normal modes : by translational symmetry, we expect the phase between unit cells to be the same, thus,

$$u_{1n}(t) = u_1 e^{i k n a - i \omega t}$$

$$u_{2n}(t) = u_2 e^{i k n a - i \omega t}$$

we can find the com and find the dispersion



## Electronic Properties

Successive models of electronic properties

① classical picture (Drude model)

good: Drude conductivity  $\sigma(\omega)$

bad: specific heat of electrons

② Quantum picture of free electrons (Fermi gas)

good: specific heat, Pauli magnetic susceptibility

bad: crystal insulators, sign of Hall effect

③ Electrons in periodic potential (tight-binding and nearly free e-model)

good: Existence of insulators, Hall effect

bad: magnetism and superconductivity

④ Electrons in periodic potential interacting with other electrons  
and with lattice vibrations

good: magnetism and superconductivity

bad: topological states of matter

## Drude model

Applying the kinetic theory of gases to the understanding of e<sup>-</sup> motion within metals.

Assumptions:

- e<sup>-</sup> has scattering time  $\tau$ ; the probability of scattering in time  $dt$  is  $dt/\tau$
- After a scattering event, the e<sup>-</sup> moment becomes  $\vec{p} = 0$
- Between scattering events, the e<sup>-</sup>s respond to external  $\vec{E}$  and  $\vec{B}$  fields

## Electron in Fields

Suppose an  $e^-$  has momentum  $\vec{p}(t)$  and experiences force  $\vec{F} = d\vec{p}/dt$ . Then,

$$\begin{aligned}\langle \vec{p}(t+\Delta t) \rangle &= \left(1 - \frac{\Delta t}{\tau}\right) (\vec{p}(t) + \vec{F} \Delta t) + O(\Delta t^2) \\ &= \vec{p}(t) + \vec{F} \Delta t - \frac{\vec{p}(t)}{\tau} \Delta t - \cancel{\vec{F} \frac{\Delta t}{\tau^2}}\end{aligned}$$

$$\frac{\langle \vec{p}(t+\Delta t) \rangle - \vec{p}(t)}{\Delta t} = \vec{F} - \frac{\vec{p}(t)}{\tau}$$

$$\boxed{\frac{d\vec{p}}{dt} = \vec{F} - \frac{\vec{p}}{\tau}}$$

Electron in  $\vec{E}$ :  $\frac{d\vec{p}}{dt} = -e\vec{E} - \frac{\vec{p}}{\tau}$

In steady state,  $d\vec{p}/dt = 0$ , thus,

$$\vec{p} = -e\tau\vec{E}$$

$$m\vec{v} = -e\tau\vec{E}$$

$$\vec{j} = -en\vec{v} = \frac{e^2 n \tau}{m} \vec{E}$$

$$\Rightarrow \boxed{\vec{j} = \sigma \vec{E}; \sigma = \frac{e^2 \tau n}{m}}$$

↑ conductivity

## Electron in $\vec{E}$ and $\vec{B}$

$$\frac{d\vec{p}}{dt} = -e(\vec{E} + \vec{v} \times \vec{B}) - \frac{\vec{p}}{\tau}$$

In steady state,  $d\vec{p}/dt = 0$ , and with  $\vec{p} = m\vec{v}$ ,  $\vec{j} = -en\vec{v}$

$$0 = -e\vec{E} + \frac{\vec{j} \times \vec{B}}{n} + \frac{m}{ne\tau} \vec{j}$$

$$\vec{E} = \left( \frac{1}{ne} \vec{j} \times \vec{B} + \frac{m}{ne^2 \tau} \vec{j} \right)$$

$$\boxed{\vec{E} = L\vec{j}; \rho_{xx} = \rho_{yy} = \rho_{zz} = \frac{m}{ne^2 \tau}; \rho_{xy} = -\rho_{yx} = \frac{B}{ne}}$$

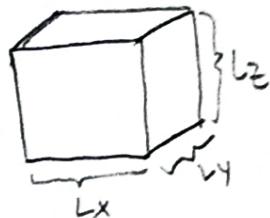
↑ resistivity tensor

↑ Hall resistivity

Hall coefficient:  $R_H = \frac{\rho_{yx}}{IB} = -\frac{1}{ne}$  (Drude model)

## Fermi Gas

In our model: an e<sup>-</sup> is confined in a box with no other potential and periodic boundary conditions



$$H = \frac{p^2}{2m}; \hat{H}\psi = E\psi$$

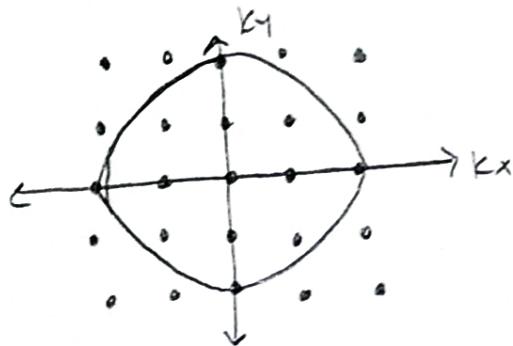


quantized bc of boundary conditions

$$\text{Eigenstates: } e^{i\vec{k} \cdot \vec{r}}; E = 2\pi \left( \frac{n_x}{L_x} \hat{x} + \frac{n_y}{L_y} \hat{y} + \frac{n_z}{L_z} \hat{z} \right)$$

$$\text{Eigenenergies: } E(\vec{k}) = \frac{\pi^2 k^2}{2m}$$

$$\text{Density of states: } g(E) = \frac{2}{\Delta k_x \Delta k_y \Delta k_z} = \frac{2L_x L_y L_z}{(2\pi)^3} = \frac{2 \cdot \text{Volume}}{(2\pi)^3}$$



\* ground state fills out radially because  $E \propto k^2$  and pauli exclusion principle

Fermi wavevector: occupied states lie in a sphere in k-space with radius  $k_F$  (Fermi wavevector)

Number of states for  $k_F$ :

$$N = \left(\frac{4}{3}\pi k_F^3\right) g(k) = \left(\frac{4}{3}\pi k_F^3\right) \left(\frac{V}{4\pi^3}\right)$$

$$N = \frac{\sqrt{V} k_F^3}{3\pi^2}$$

Fermi surface: At  $T=0$ , the Fermi surface is the location in k-space where there is a discontinuity in the e<sup>-</sup> occupation number

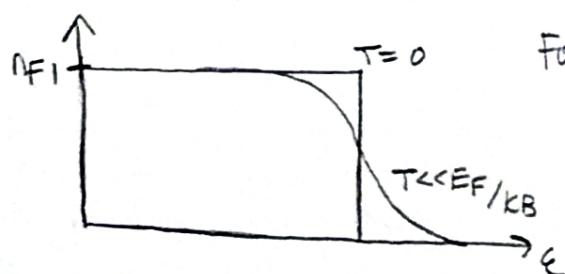
$$\boxed{\text{Fermi Energy: } E_F = \frac{\pi^2 k_F^2}{2m}}$$

Fermi occupation Factor: The probability of an eigenstate with energy E being occupied is

$$\boxed{N_F = \frac{1}{e^{\beta(E-\mu)} + 1}}$$

Recall  $\beta = 1/k_B T$

$\mu$  = chemical potential



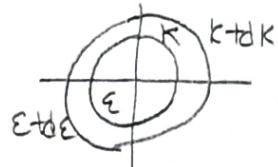
For  $k_B T \ll E_F / k_B$ ,  $\mu \approx E_F$

Electron Heat capacity:  $U(T) = \sum_k n_F(E) E(E)$

In the continuum approximation (many  $N$ ),

$$U(T) = \int (d^3k g(k)) f(\vec{E}) E(\vec{E})$$

$$= \int dE g(E) f(E) E$$



Density of states in energy:  $g(E) dE = g(k) (4\pi k^2 dk)$

$$= g(k) [4\pi k^2 \left(\frac{dk}{dE}\right) dE]$$

$$= \left[\frac{2V}{(2\pi)^3}\right] (4\pi k^2) \left(\frac{m}{\hbar^2 c}\right) dE$$

$$= \frac{V m k}{\pi^2 \hbar^2} dE = \frac{(2m)^{3/2}}{2\pi^2 \hbar^3} \sqrt{E} dE$$

[skipping steps] In the Sommerfeld expansion for  $T \ll E_F/k_B$ , we get

$$C = \frac{\pi^2}{3} g(E_F) k_B^2 T$$

### Electron in periodic potential

Bloch's Theorem Solutions to SE in periodic potential

$$\hat{H}\psi = E\psi$$

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \text{ where } V(\vec{r}) = V(\vec{r} + \vec{R}_{\text{lattice}})$$

let's define the translation operator  $\hat{T}(\vec{a})$  such that  $\hat{T}(\vec{a}) \hat{V}(\vec{r}) = \hat{V}(\vec{r} + \vec{a})$

$$[\hat{T}(\vec{a}), \hat{V}(\vec{r})] = [\hat{T}(\vec{a}), d/dx] = 0 \implies \hat{T}(\vec{a}) \text{ commutes with } \hat{H}$$

$\implies \hat{T}(\vec{a}) \text{ shares same eigenvectors as } \hat{H}$

Find the eigenvalues of  $\hat{T}(\vec{a})$ :

$$\hat{T}(\vec{a}) \psi(\vec{r}) = f(\vec{a}) \psi(\vec{r})$$

We know  $\hat{T}(\vec{a})^n = \hat{T}(n\vec{a})$ , thus,

$$f^n(\vec{a}) = f(n\vec{a})$$

$$\implies f(\vec{a}) = e^{i\vec{k} \cdot \vec{a}} \text{ for some } \vec{k} \text{ (discrete bc of periodic boundary conditions)}$$

Thus,  $\hat{T}(\vec{a})\psi(\vec{r}) = f(\vec{a})\psi(\vec{r})$

$$\psi_{\vec{k}}(\vec{r} + \vec{a}) = e^{i\vec{k} \cdot \vec{a}} \psi_{\vec{k}}(\vec{r}) \quad \text{where } \psi_{\vec{k}}(\vec{r}) \text{ is an energy eigenstate}$$

Observe :

- ① Eigenstates of  $\hat{A}$  (and  $\hat{T}(\vec{a})$ ) can be indexed by the wavevector  $\vec{k}$
- ②  $\psi(\vec{r} + \vec{a}) \neq \psi(\vec{r})$  unless  $k=0$ ; the wave function is not periodic  
However shifting by  $\vec{a}$  (lattice vector) only adds a phase,

$$|\psi(\vec{r} + \vec{a})|^2 = |\psi(\vec{r})|^2$$

- ③ Bloch's theorem can alternatively be expressed as

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{R} \cdot \vec{r}} u_{\vec{k}}(\vec{r})$$

where  $u_{\vec{k}}(\vec{r})$  is an eigenstate for some  $k$  and  $u_{\vec{k}}(\vec{r})$  is periodic in the unit cell

\* Note: we can write  $u_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} u_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$

2 Toy models for solving the SE :

- ① Tight-binding: assume effect of neighbor atoms are weak (act as a weak perturbation). Useful in insulating/semiconductor states. Bloch states: linear combination of atomic orbitals.
- ② Nearly free electrons: assume the atomic periodic potential is a weak perturbation (possible bc screening of coulomb force in metals). Bloch states: linear combination of plane waves.

## Perturbation Theory

Suppose we understand  $\hat{H}_0 |\psi_n\rangle = E_n |\psi_n\rangle$

and we want to understand  $\hat{H} = \hat{H}_0 + \lambda \hat{V}$  for  $\lambda \ll 1$

### Time-independent non-degenerate:

$$E_n' = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + O(\lambda^3)$$

$$= E_n^{(0)} + \lambda \langle \psi_n^{(0)} | \hat{V} | \psi_n^{(0)} \rangle + \lambda^2 \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | \hat{V} | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}} + O(\lambda^3)$$

$$|\psi_n'\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | \hat{V} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} |\psi_m^{(0)}\rangle + O(\lambda^2)$$

### Time-independent degenerate

Suppose  $E_1 = E_2 = \epsilon$

$$\hat{H}_0 = \begin{pmatrix} 0 & & & \\ & \ddots & & \\ & \vdots & \ddots & \\ & \vdots & \vdots & 3\epsilon \end{pmatrix} \text{ and } \hat{V} = \begin{pmatrix} \vdots & \ddots & & \\ \vdots & \boxed{\vdots} & \vdots & \\ \vdots & \vdots & \ddots & \\ \vdots & & & \vdots \end{pmatrix}, \tilde{v} = \begin{pmatrix} \vdots & \vdots \end{pmatrix}$$

$$\det(\tilde{v} - \mu \hat{1}) = 0 \implies v_1, \vec{v}_1 = \begin{pmatrix} A \\ B \end{pmatrix} \implies \psi_I = A\psi_1 + B\psi_2$$

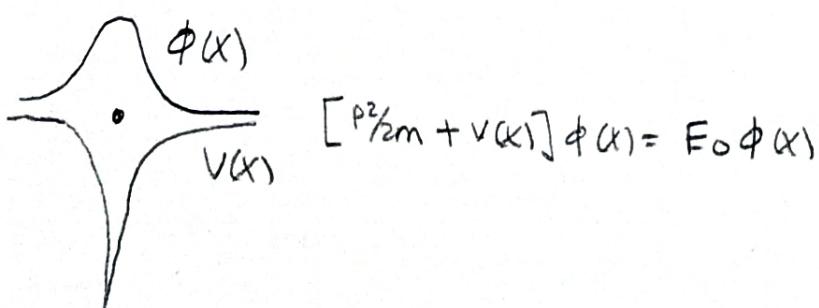
$$v_2, \vec{v}_2 = \begin{pmatrix} C \\ D \end{pmatrix} \implies \psi_{II} = C\psi_1 + D\psi_2$$

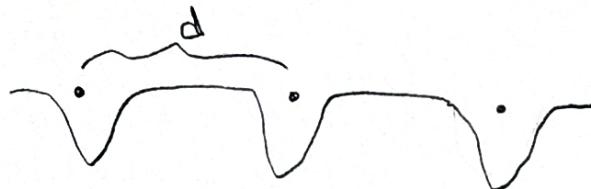
$$E_I = \epsilon + \lambda + \sum_{m \neq I, II} \frac{|\langle \psi_m^{(0)} | \hat{V} | \psi_I \rangle|^2}{\epsilon - E_m^{(0)}} + O(\lambda^3)$$

$$E_{II} = \epsilon + \lambda + \sum_{m \neq I, II} \frac{|\langle \psi_m^{(0)} | \hat{V} | \psi_{II} \rangle|^2}{\epsilon - E_m^{(0)}} + O(\lambda^3)$$

### Tight-Binding model in 1D

Suppose we have a 1D chain of atoms with separation  $a$ , potential  $V(x)$  and a single orbital  $\phi(x)$  where  $\phi(x)$  is the solution to the SE for a single atom.





- If  $d \gg 1$ , we expect the eigenstate to have energy  $E_0$  and the entire system to be degenerate

- We assume the perturbed eigenstate is a linear combo of each orbital  $\phi(x-na)$
- Furthermore, the eigenstate must satisfy Bloch's theorem. Thus, we assume the ansatz,

$$\Psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} \phi(x-na)$$

↑                              ↓  
 Normalization      atomic orbital

where  $k = \left(\frac{2\pi}{na}\right)m$  for  $m \in \mathbb{Z}$   
 ↑  
 BC Periodic boundary condition  $\Rightarrow$  only  $N$ -distinguishable  $k$ -states

Solve for eigenenergies :  $\hat{H} = \frac{\hat{p}^2}{2m} + \sum_n \hat{V}(x-na)$

$$\begin{aligned} E(k) &= \langle \Psi_k(x) | \hat{H} | \Psi_k(x) \rangle \\ &= \frac{1}{N} \sum_{n,n'} e^{iK(n-n')} \underbrace{\langle \phi(x-n'a) | \hat{H} | \phi(x-na) \rangle}_{H_{nn'}} \end{aligned}$$

lets find  $H_{nn'}$  :  $\hat{H} |\phi(x-na)\rangle = \left[ \frac{\hat{p}^2}{2m} + \hat{V}(x-na) + \sum_{m \neq n} \hat{V}(x-na) \right] |\phi(x-na)\rangle$

$$= \left( E_0 + \sum_{m \neq n} \hat{V}(x-na) \right) |\phi(x-na)\rangle$$

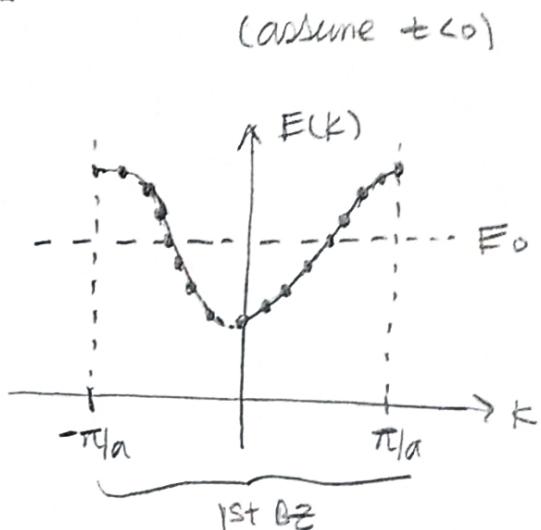
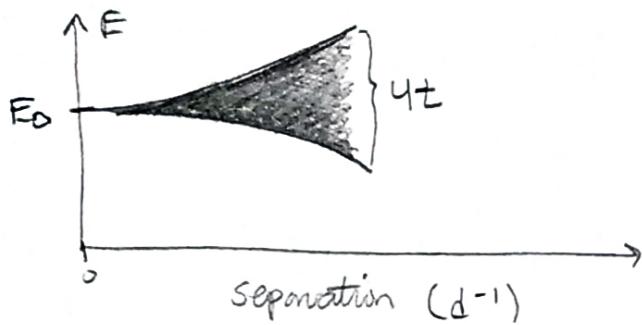
$$H_{nn'} = \langle \phi(x-n'a) | \hat{H} | \phi(x-na) \rangle$$

$$H_{nn'} = E_0 \underbrace{\langle \phi(x-n'a) | \phi(x-na) \rangle}_{\text{assume } 0} + \sum_{m \neq n} \underbrace{\langle \phi(x-n'a) | \hat{V}(x-na) | \phi(x-na) \rangle}_{\text{assume } t \text{ for } n' = n \pm 1}$$

$$H_{nn'} = E_0 \delta_{n,n'} + t \delta_{n,n \pm 1}$$

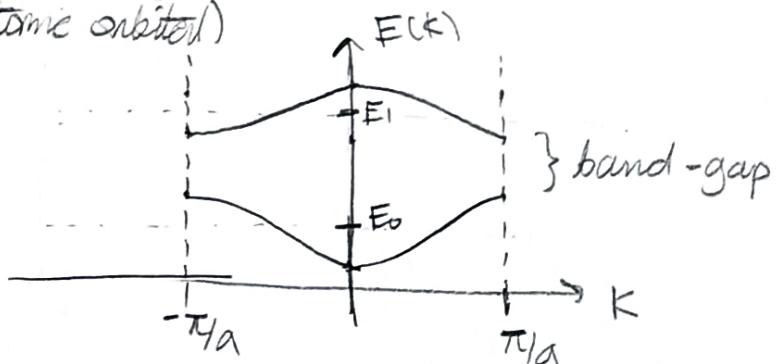
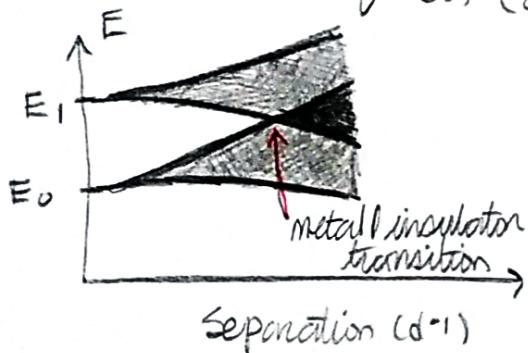
$$\text{Finally, } E(k) = \frac{1}{N} \sum_{n,n'} e^{ik(n-n')} H_{nn'} \\ = \frac{1}{N} \sum_n [E_0 + t(e^{ika} + e^{-ika})]$$

$$E(k) = E_0 + 2t \cos(ka)$$



Multiple bands: we can perform the same process to higher energy eigenstates of V(x) (other atomic orbitals)

$\Rightarrow N$  k-states  
 $\Rightarrow 2N$  total states



Band filling: In 1D, a filled band carries no current because the system can not respond to an external field (no additional states to move to).

Effective mass: expanding the dispersion relation for small  $k$ ,

$$E(k) \approx \text{const.} + \frac{1}{2} m^* k^2$$

$$\text{For a free electron, } E(k) = \frac{\hbar^2 k^2}{2m}$$

Thus, we define the effective mass  $m^*$ ,

$$\frac{\hbar^2 k^2}{2m^*} = \frac{1}{2} m^* k^2$$

$$m^* = \frac{\hbar^2}{2t a^2}$$

## Nearly free electron model

Note: this derivation does not explicitly mention perturbation theory, but we would get the same result]

The nearly free e- model the periodic potential as a small perturbation of the free electron wave function. Recall from Bloch's theorem that  $\psi(\vec{r})$  in a periodic potential must be of the form

$$\begin{aligned}\psi_K(\vec{r}) &= e^{i\vec{k} \cdot \vec{r}} u_K(\vec{r}) \text{ where } u_K(\vec{r}) = u_K(\vec{r} + \vec{R}_{\text{latt}}) \\ &= e^{i\vec{k} \cdot \vec{r}} \left[ \sum_G \tilde{u}_{K,G} e^{-iG \cdot \vec{r}} \right] \xrightarrow{\text{Fourier series}} \text{lattice vector} \\ &= \sum_G \tilde{u}_{K,G} e^{i(\vec{k} - \vec{G}) \cdot \vec{r}}\end{aligned}$$

Now, let's calculate  $\tilde{u}_{K,G}$

$$\begin{aligned}\tilde{u}_{K,G} &= \int_{\text{cell}} d^3r u_K(\vec{r}) e^{iG \cdot \vec{r}} = \int_{\text{cell}} d^3r \underbrace{[\psi_K(\vec{r}) e^{-i\vec{k} \cdot \vec{r}}]}_{\text{Bloch thm.}} e^{iG \cdot \vec{r}} \\ &= \boxed{\int_{\text{cell}} d^3r \psi_K(\vec{r}) e^{-i(\vec{k} - \vec{G}) \cdot \vec{r}}} = \tilde{u}(\vec{k} - \vec{G})\end{aligned}$$

$$\text{Thus, } \psi_K(\vec{r}) = \sum_G \tilde{u}_{K,G} e^{i(\vec{k} - \vec{G}) \cdot \vec{r}}$$

$$\boxed{\psi_K(\vec{r}) = \sum_G \tilde{u}(\vec{k} - \vec{G}) e^{i(\vec{k} - \vec{G}) \cdot \vec{r}}}$$

\* Note: normalization factor has been dropped

where  $K = \left(\frac{2\pi}{N_a}\right)m$  for  $m \in \mathbb{Z}$   
and in the 1st BZ

$$\text{Now, the SE : } \hat{H} \psi_K(\vec{r}) = E(\vec{k}) \psi_K(\vec{r})$$

$$\text{where } \hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{r}) = \frac{\hat{p}^2}{2m} + \underbrace{\sum_G \tilde{V}_G e^{-iG \cdot \vec{r}}}_{\text{periodic potential}} \quad \text{Fourier coefficient of } V(\vec{r})$$

$$\text{kinetic term : } \frac{\hat{p}^2}{2m} \left[ \sum_G \tilde{u}(\vec{k} - \vec{G}) e^{i(\vec{k} - \vec{G}) \cdot \vec{r}} \right] = \sum_G \frac{\hbar^2 |\vec{k} - \vec{G}|^2}{2m} \tilde{u}(\vec{k} - \vec{G}) e^{i(\vec{k} - \vec{G}) \cdot \vec{r}}$$

Potential term:  $V(\vec{r}) \Psi_{\vec{k}}(\vec{r}) = \left[ \sum_{G_1} \tilde{V}_{G_1} e^{i(G_1 \cdot \vec{r})} \right] \left[ \sum_{G_1} \tilde{U}(E - G_1) e^{i(E - G_1) \cdot \vec{r}} \right]$

$$V(\vec{r}) \Psi_{\vec{k}}(\vec{r}) = \sum_{G_1 \in G} e^{i(E - \vec{k} - \vec{G}_1) \cdot \vec{r}} \tilde{U}(\vec{k} - \vec{G}_1) \tilde{V}_{G_1}$$

For,  $\vec{G}^{\parallel} = \vec{G} + \vec{G}'$

$$\begin{aligned} V(\vec{r}) \Psi_{\vec{k}}(\vec{r}) &= \sum_{(G, G')} e^{i(E - G^{\parallel}) \cdot \vec{r}} \tilde{U}(\vec{k} - \vec{G}^{\parallel} + \vec{G}') \tilde{V}_{G'} \\ &= \sum_{G^{\parallel}} \left[ e^{-i(E - G^{\parallel}) \cdot \vec{r}} \sum_{G'} \tilde{U}(E + \vec{G}' - \vec{G}^{\parallel}) \tilde{V}_{G'} \right] \\ &= \sum_{G^{\parallel}} \left[ e^{-i(E - \vec{G}') \cdot \vec{r}} \sum_{G'} \tilde{U}(E + \vec{G}' - \vec{G}) \tilde{V}_{G'} \right] \end{aligned}$$

Finally, the SE becomes:

$$\sum_{G^{\parallel}} \left[ e^{i(E - \vec{G}') \cdot \vec{r}} \left\{ \left[ \frac{\hbar^2 |\vec{k} - \vec{G}|^2}{2m} - E(\vec{k}) \right] \tilde{U}(\vec{k} - \vec{G}') + \sum_{G_1} \tilde{V}_{G_1} \tilde{U}(\vec{k} + \vec{G}' - \vec{G}) \right\} \right] = 0$$

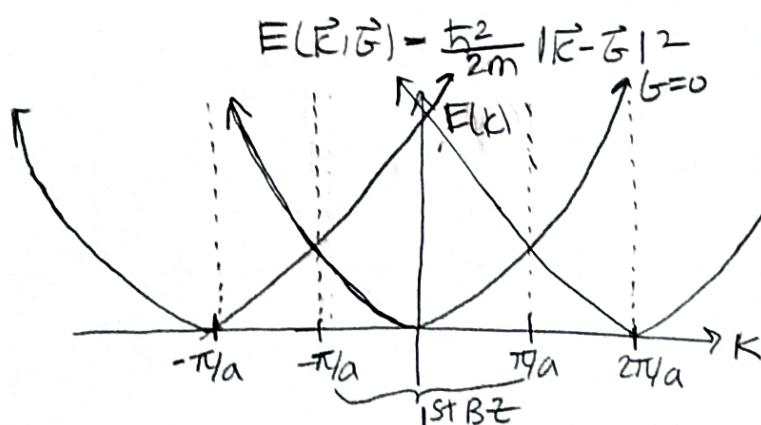
For some  $E$ , and each value of  $\vec{G}$ , each term must be zero for the expression to hold

$$\left[ \frac{\hbar^2 |\vec{k} - \vec{G}|^2}{2m} - E(\vec{k}) \right] \tilde{U}(\vec{k} - \vec{G}') + \sum_{G_1} \tilde{V}_{G_1} \tilde{U}(\vec{k} + \vec{G}' - \vec{G}) = 0$$

for some  $\vec{k}$  and each  $\vec{G}$

Free electron:  $V(\vec{r}) = 0 \implies \tilde{V}_G = 0 \forall G$ . Thus, eq ① becomes

$$\left[ \frac{\hbar^2 |\vec{k} - \vec{G}|^2}{2m} - E(\vec{k}) \right] \tilde{U}(\vec{k} - \vec{G}') = 0$$



$G = 2\pi/a$  while  $V(\vec{r}) = 0$ , we treat the system as periodic with  $N$  unit cells and  $k$  values can be mapped to the 1st BZ

Cos Potential : Notice that eq ① is a coupled set of equations in  $\tilde{v}$  where the number of equations is equal to the number of Fourier coefficients of  $V(\vec{r})$

$$\begin{aligned} \text{Suppose } V(x) = -V_0 \cos\left(\frac{2\pi x}{a}\right) &= -\frac{V_0}{2} (e^{i2\pi x/a} + e^{-i2\pi x/a}) \\ &= -\frac{V_0}{2} (e^{i6\pi x} + e^{-i6\pi x}) \end{aligned}$$

We can find  $E(\vec{r})$  using eq ① but let's use Perturbation theory instead.  
For a free electron,  $|K\rangle = e^{i\vec{K} \cdot \vec{r}} (\sqrt{\nu})$

$$\hat{H}_0 |K\rangle = \epsilon_0(\vec{K}) |K\rangle = \frac{\hbar^2 K^2}{2m} |K\rangle$$

Now, for  $H = H_0 + \tilde{V}(\vec{r})$ , First note :

$$\langle \vec{K}' | \tilde{V} | \vec{E} \rangle = \frac{1}{V} \int d\vec{r} e^{i(\vec{K}' - \vec{E}') \cdot \vec{r}}$$

$$\boxed{\langle \vec{K}' | \tilde{V} | \vec{E} \rangle = \tilde{V}_{\vec{E} - \vec{E}'}}$$

↑ Fourier coefficient of  $V(\vec{r})$

1st order perturbation :  $E(\vec{E}) = \epsilon_0(\vec{E}) + \langle \vec{K}' | \tilde{V} | \vec{E} \rangle = \epsilon_0(\vec{E}) + \tilde{V}_0$

This is a global shift for all eigenstates, so why we can ignore this term.

2nd order perturbation :  $E(\vec{E}) = \epsilon_0(\vec{E}) + \tilde{V}_0 + \sum_{\vec{K}' \neq \vec{E}} \frac{|\langle \vec{K}' | \tilde{V} | \vec{E} \rangle|^2}{\epsilon_0(\vec{E}') - \epsilon_0(\vec{K}')} \quad ^0$

In 1D, degeneracy occurs when  $K' = -k = \frac{n\pi}{a}$  for  $n \in \mathbb{Z}$

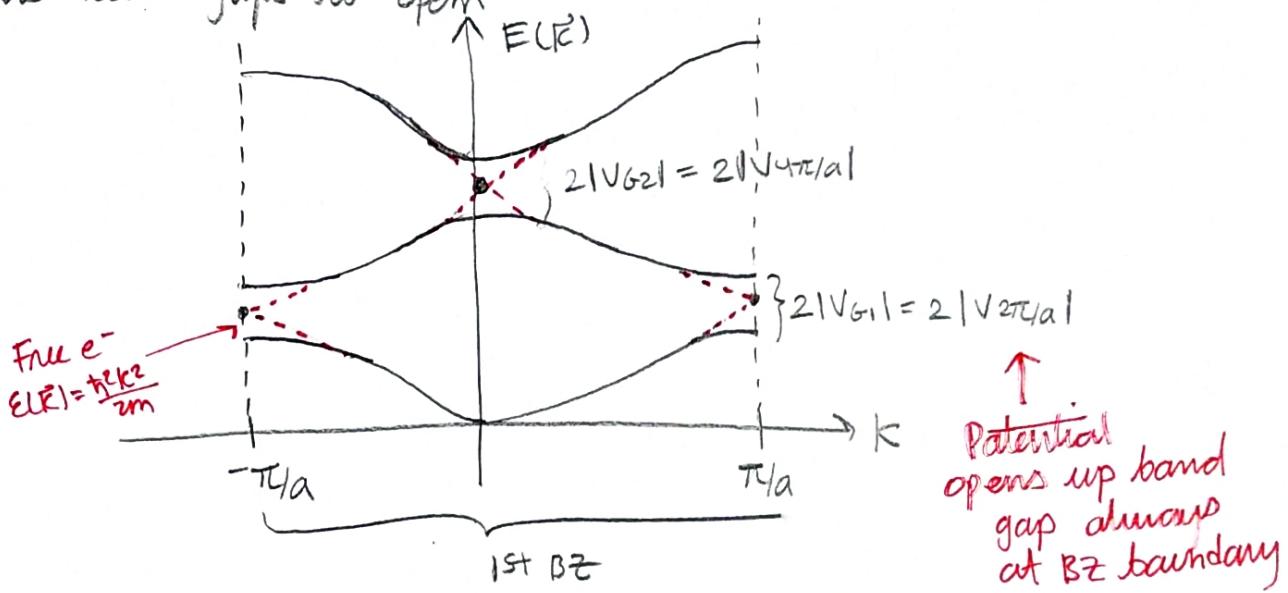
If  $|K\rangle$  and  $|E'\rangle = |K + G\rangle$  are degenerate, degenerate perturbation theory,  
 $|4\rangle = \alpha |K\rangle + \beta |E'\rangle$

$$\begin{pmatrix} \langle \vec{K}' | \tilde{V} | \vec{E}' \rangle & \langle \vec{K}' | \tilde{V} | \vec{K}' \rangle \\ \langle \vec{K}' | \tilde{V} | \vec{K}' \rangle & \langle \vec{K}' | \tilde{V} | \vec{E}' \rangle \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \implies \boxed{E_{\pm} = \epsilon_0(\vec{E}') \pm |\tilde{V}_G|}$$

$$\begin{pmatrix} \epsilon_0(\vec{E}') & V-G = \tilde{V}_G \\ \tilde{V}_G & \epsilon_0(\vec{E}+G) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

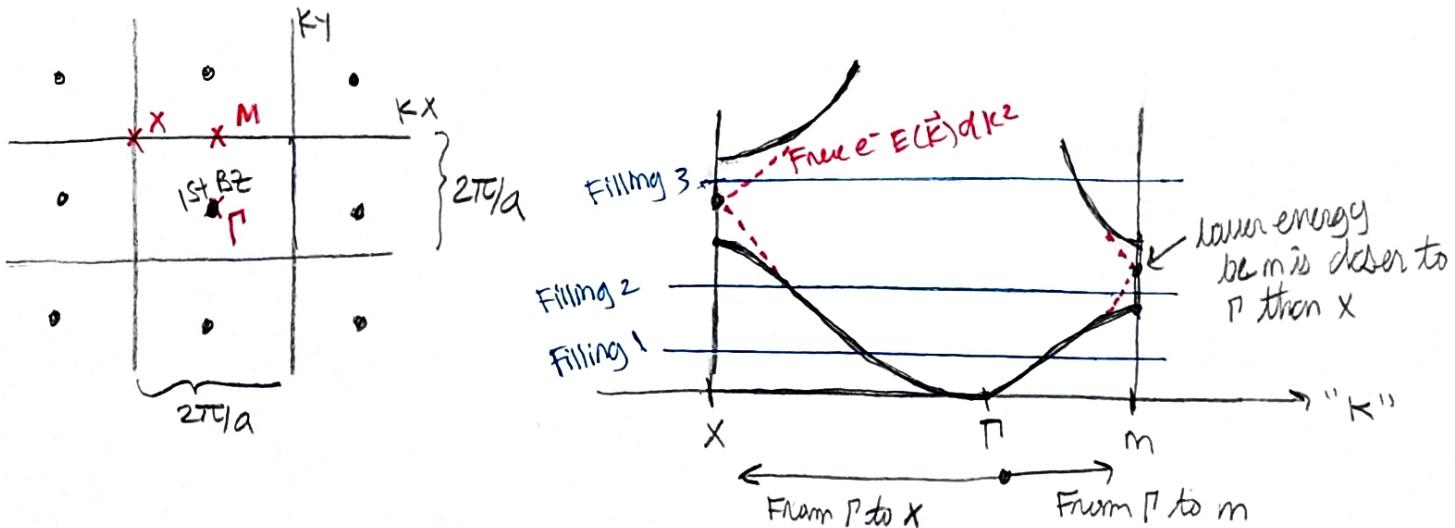
Notice that the degeneracy always occurs at the BZ boundary.

A potential with non-zero Fourier coefficients lifts the degeneracy and causes band gaps to open.

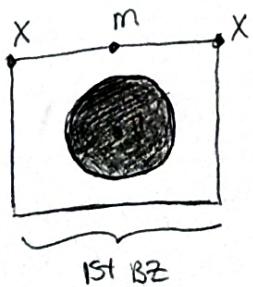


Fermi Surfaces: Recall the Fermi surface separates the filled and unfilled states at  $T=0$ .

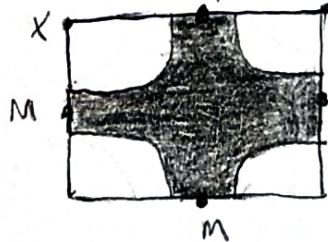
Consider a 2D square lattice in reciprocal space (also square)



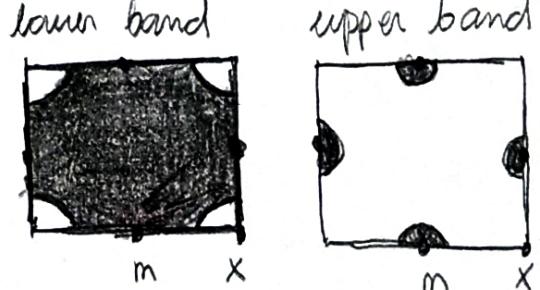
Filling 1



Filling 2



Filling 3



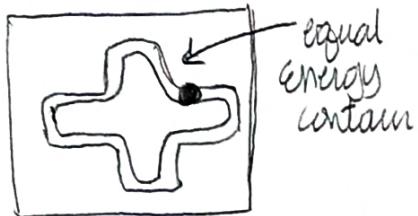
\* Circle becomes distorted as potential increases

# Semiclassical Dynamics

## Assumptions:

- ① electrons treated by  $\alpha m$ , but  $\vec{E}$  and  $\vec{B}$  treated as classical fields
- ② assume  $\hbar \omega < E_{\text{gap}} \Rightarrow$  trapped in a single band
- ③ assume fields are uniform (on the length scale of lattice constant).

wavepacket: a small region in reciprocal space



The wavepacket moves with group velocity,

$$\vec{v}_g(\vec{E}) = \frac{1}{\hbar} \nabla_{\vec{k}} \epsilon(\vec{E})$$

Force on wavepacket (with wavevector  $\vec{k}'$ )

Suppose we have a constant force  $\vec{F}$

$$\delta \epsilon(\vec{k}') = \vec{F} \cdot \delta \vec{t} = \vec{F} \cdot \vec{v}_g(\vec{E}) \delta t = \frac{\vec{E}}{\hbar} \cdot \nabla_{\vec{k}} \epsilon(\vec{E}) \delta t$$

$$\text{we also know, } \delta \epsilon(\vec{k}') = \nabla_{\vec{k}} \epsilon(\vec{E}) \cdot d\vec{E}$$

Thus,

$$\vec{F} = \frac{\hbar}{t} \frac{d\vec{E}}{dt}$$

For the crystal momentum  $\hbar \vec{k}$ , the force is equal to the time rate of change of  $\hbar \vec{k}$

## Tight-binding Band

$$\text{Recall } \epsilon(\vec{k}) = -2t \cos(ka)$$

- Under constant force,  $\vec{k}$  will increase linearly with time and eventually loop back to its starting value.  $\Rightarrow k(t) = \frac{F}{\hbar} t$

$$- v_g(k) = \frac{1}{\hbar} \frac{dk}{dt} = \frac{-2ta}{\hbar} \sin(ka)$$

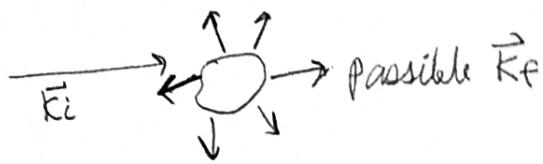
$$\text{Thus, } v_g(t) = v_g\left(\frac{Ft}{\hbar}\right) = -\frac{2ta}{\hbar} \sin\left(\frac{Fa}{\hbar}t\right)$$

$\Rightarrow$  group velocity oscillates in time

$\Rightarrow$  do not observe in lab because impurity will scatter the  $\vec{k}$  state of electrons

## Scattering

wavevector of  $e^-$  will be randomized upon encountering impurity, or phonons, etc.



Suppose we have an ensemble of  $N$  electrons with scattering time  $\tau_n$

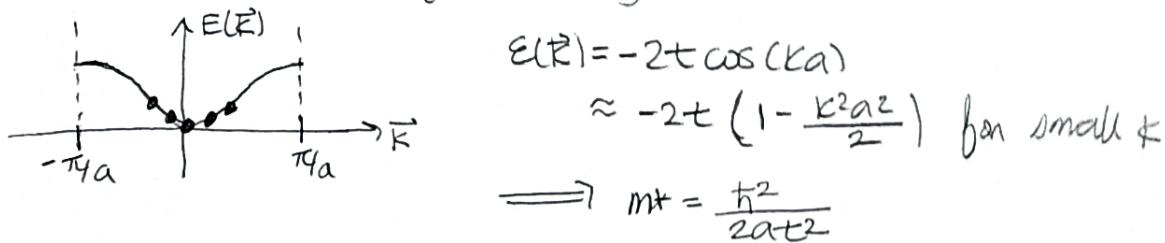
$$\langle \vec{K}(t) \rangle = \frac{1}{N} \sum_n \vec{K}_n(t) = \frac{1}{N} \sum_n \underbrace{[\vec{K}_n(t-\tau_n) + \vec{F}/\hbar \tau_n]}_{\text{assume collision in before present}}$$

Now,  $\sum_n \vec{K}_n(t-\tau_n)$  is the average of scattered  $K_s$  (random)  $\Rightarrow 0$ . Thus,

$$\langle \vec{K}(t) \rangle = \frac{\vec{F}}{\hbar} t \quad \leftarrow K \text{ becomes steady-state}$$

average scattering time

Current in sponse (tight-binding) band



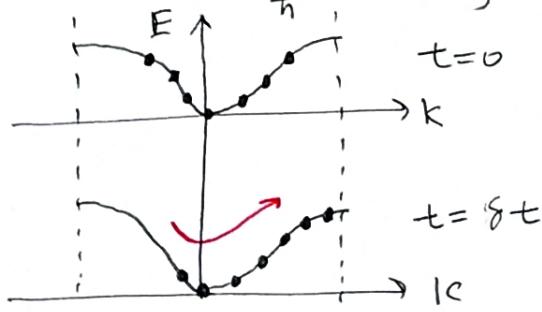
For 1D, the current becomes,

$$I = \lambda \langle v \rangle = (-ne) \left( \frac{\hbar}{m*} \langle K \rangle \right) = \left( \frac{-ne\hbar}{m*} \right) \left( -eE \frac{\pi}{\hbar} \right)$$

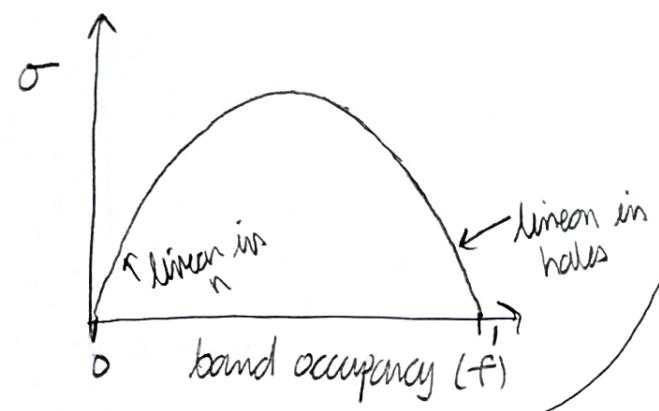
$$\overbrace{\frac{1}{I} = \frac{ne^2 \tau}{m*} \vec{E}}^{\sigma \text{ (Drude formula)}} \quad (\text{generalized to 3D for } n = N/V)$$

## Current with long band occupancy

- We found previously that an electric field moves all states by an amount  $\frac{eE\tau}{\hbar}$  linearly as a function of time.

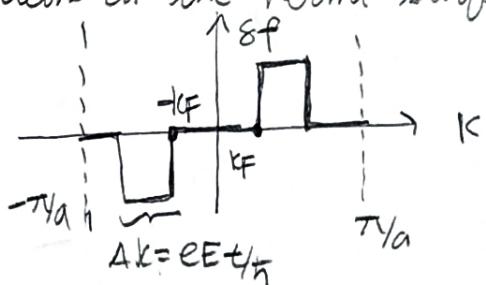


If a band is completely filled:  
shifting the bands does not change  
the overall state of the system.  
Thus, filled bands carry no current  
because  $\langle v \rangle \propto \langle k \rangle = 0$  for a filled band



$$I = \sigma \langle v \rangle \quad \text{change in occupancy from ground state } (\langle v \rangle = 0) \\ I = \sum_k \delta f(k) (-e) v_g(k) \quad \text{due to } \vec{E}$$

Recall the picture above, the shift in occupancy only occurs at the Fermi surface



In the limit,  $\Delta k \ll 1/a$   
 hopping integral (not time)

$$I = \underbrace{\left[ \frac{2e^2 \tau t a}{\pi \hbar^2} \sin(k_F a) \right]}_{\sigma} E$$

Simplifying, we get,

$$\sigma = \frac{e^2}{\pi \hbar} v_g(k_F) \tau = \frac{e^2}{\pi \hbar} l_F \quad \begin{matrix} \text{mean free path} \\ \uparrow \text{Fermi velocity} \end{matrix}$$

\* Conductivity depends on the properties of  $e^-$  at Fermi surface

\* In 2D/3D, the Fermi surface is more complex  $\Rightarrow \sigma \propto \langle l_F \rangle$