Band structure for electrons in weak periodic potential.

Use position / momentum states:

$$|\vec{k}\rangle \rightarrow \langle \vec{k}|\vec{k}'\rangle = \delta_{\vec{k},\vec{k}'} \qquad \vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$$

$$|\vec{r}\rangle \rightarrow \langle \vec{r}|\vec{r}'\rangle = \delta(\vec{r}-\vec{r}')$$

$$\langle \vec{r}|\vec{k}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} = \psi_{\vec{k}}(\vec{r})$$

$$|\vec{k}\rangle = \frac{1}{\sqrt{V}}\int d^3\vec{r}\, e^{i\vec{k}\cdot\vec{r}}\, |\vec{r}\rangle \quad ; \quad |\vec{r}\rangle = \frac{1}{\sqrt{V}}\sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}}\, |\vec{k}\rangle .$$

Hamiltonian:

- $$H = \sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m} |\vec{k}\rangle\langle\vec{k}| + \int d^3\vec{r}\; U(\vec{r})\, |\vec{r}\rangle\langle\vec{r}|$$

- $U(\vec{r}) = U(\vec{r}+\vec{R})$, Bravais lattice vectors $\vec{R}$.

Bloch's theorem

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \overbrace{\sum_{\vec{K}} C_{\vec{K}}\, e^{i\vec{K}\cdot\vec{r}}}^{u_{n\vec{k}}(\vec{r})} \quad ; \vec{k} \in \text{B.Z.}$$

$$\Rightarrow \quad |\psi_{n\vec{k}}\rangle = \sum_{\vec{K}} C_{\vec{K}} |\vec{k}+\vec{K}\rangle.$$

- For this to hold, potential should only mix $|\vec{k}\rangle$ with $|\vec{k}+\vec{K}\rangle$ if $\vec{K}$ is RLV....

Fourier transform potential term:

$$H = \sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m} |\vec{k}\rangle\langle\vec{k}| + \sum_{\vec{k},\vec{K}} \tilde{U}(\vec{K}) |\vec{k}+\vec{K}\rangle\langle\vec{k}|$$

- Sum on $\vec{K}$ is over RLV's only.
- $$\tilde{U}(\vec{k}) = \frac{1}{V}\int d^3\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\, U(\vec{r}) = \begin{cases} 0\ ; & \vec{k} \text{ not RLV} \\ \tilde{U}(\vec{K})\ ; & \vec{k} = \vec{K}, \text{ RLV} \end{cases}$$
- This factor of $\frac{1}{V}$ ensures $\tilde{U}(\vec{K}) \to$ constant in $V \to \infty$ limit.

d=1 example

$$U(r) = U_0\left(e^{iKr} + e^{-iKr}\right) = 2U_0 \cos(Kr)$$

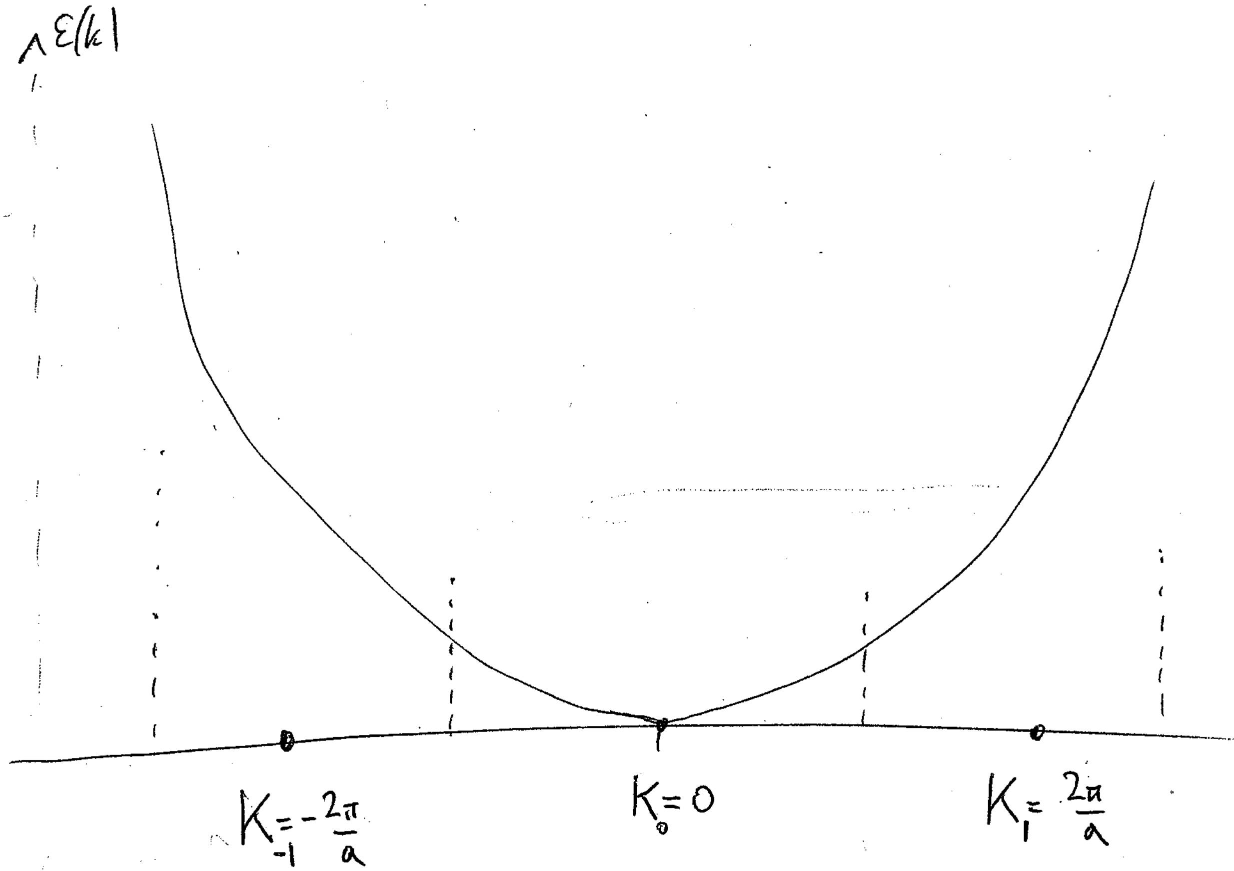
$$\tilde{U}(k) = \frac{U_0}{L}\int_0^L dr\, e^{-ikr}\left(e^{iKr} + e^{-iKr}\right) = U_0 \cdot \frac{\cancel{L}}{\cancel{L}}\left[\delta_{k,K} + \delta_{k,-K}\right]$$

- We choose $\tilde{U}(\vec{K}=0) = 0$. (constant shift of potential.)

- Goal: Understand effect of $U(\vec{r})$ on the dispersion relation $\varepsilon(\vec{k})$. Do this in perturbation theory.

- First, understand band structure of free electrons $(U(\vec{r})=0)$

(d=1 for simplicity)

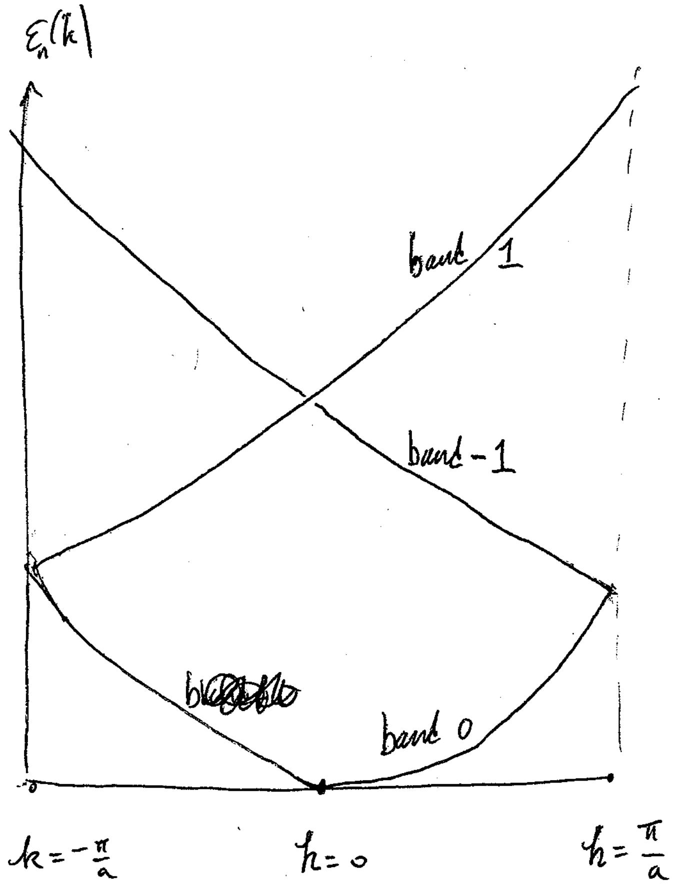


- Can always write wavevector as: $\vec{k} = \underbrace{\vec{k}}_{\text{lies in first Brillouin Zone}} + \underbrace{\vec{K}}_{\text{RLV}}$

- So $\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} e^{i\vec{K}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(\vec{r})$

$$u_{n\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{K}_n\cdot\vec{r}}$$

- Energy: $\mathcal{E}_n(\vec{k}) = \frac{\hbar^2}{2m}\left(\vec{k}+\vec{K}_n\right)^2$



- We plot energies versus crystal momentum $\vec{k}$ in first Brillouin zone.

- Now we want to understand how this picture gets corrected for weak potential $U(\vec{r})$.

- Two cases:

(1) Pick $\vec{k}$ so that $\varepsilon(\vec{k})$ is far from* $\varepsilon(\vec{k}+\vec{K})$ for all RLV's $\vec{K}$. (* means on the scale of $U(\vec{r})$)

Then it's simple exercise to show $\varepsilon(\vec{k}) \to \varepsilon(\vec{k}) + \mathcal{O}(U^2)$, only second-order shift.

(2) Degenerate case. $\vec{k}$ is such that $\varepsilon(\vec{k}) = \varepsilon(\vec{k}+\vec{K})$.
(For simplicity, we assume happens for only one RLV $\vec{K}$, but can have more than double degeneracy.)

- Write $\varepsilon_0 = \varepsilon(\vec{k}) = \varepsilon(\vec{k}+\vec{K})$ $\quad |1\rangle = |\vec{k}\rangle \quad |2\rangle = |\vec{k}+\vec{K}\rangle$

Degenerate perturbation theory: $\quad \langle k|q+\vec{k}\rangle\langle q|k+\vec{K}\rangle$

$$H_{eff} = \begin{pmatrix} \langle 1|H'|1\rangle & \langle 1|H'|2\rangle \\ \langle 2|H'|1\rangle & \langle 2|H'|2\rangle \end{pmatrix} = \begin{pmatrix} 0 & \tilde{U}^*(\vec{K}) \\ \tilde{U}(\vec{K}) & 0 \end{pmatrix}$$

$\Rightarrow$ energies are: $\boxed{\varepsilon = \varepsilon_0 \pm \sqrt{|\tilde{U}(\vec{K})|^2}}$ $\rightarrow$ splitting linear in $U(\vec{r})$

Note, case (2) also applies when

$$\varepsilon(\vec{k}) \approx \varepsilon(\vec{k}+\vec{K}) \approx \varepsilon_0$$

and $\varepsilon_0 - \varepsilon(\vec{k}) \sim \varepsilon_0 - \varepsilon(\vec{k}+\vec{K}) \sim U$.

Then: $$H_{eff} = \begin{pmatrix} \varepsilon(\vec{k})-\varepsilon_0 & \tilde{U}^*(\vec{K}) \\ \tilde{U}(\vec{K}) & \varepsilon(\vec{k}+\vec{K})-\varepsilon_0 \end{pmatrix}$$

- This is important, since it occurs for $\vec{k}$ near degeneracy points.

In general, $$\varepsilon_{\pm} = \left(\frac{\varepsilon(\vec{k})+\varepsilon(\vec{k}+\vec{K})}{2}\right) \pm \sqrt{\left(\frac{\varepsilon(\vec{k})-\varepsilon(\vec{k}+\vec{K})}{2}\right)^2+|U|^2}$$

Summary I

A

- $$H = \sum_{k} \overset{\varepsilon(\vec{k})}{\cancel{\frac{\hbar^2 k^2}{2m}}} |\vec{k}\rangle\langle\vec{k}| + \sum_{\vec{k},\vec{K}} \tilde{V}(\vec{K}) |\vec{k}+\vec{K}\rangle\langle\vec{k}|$$

$$\varepsilon(\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m}$$

- Label states by $\vec{k} \in$ B.Z. ~~, $\vec{k} = \vec{k} + \vec{K}$~~

  & discrete index n

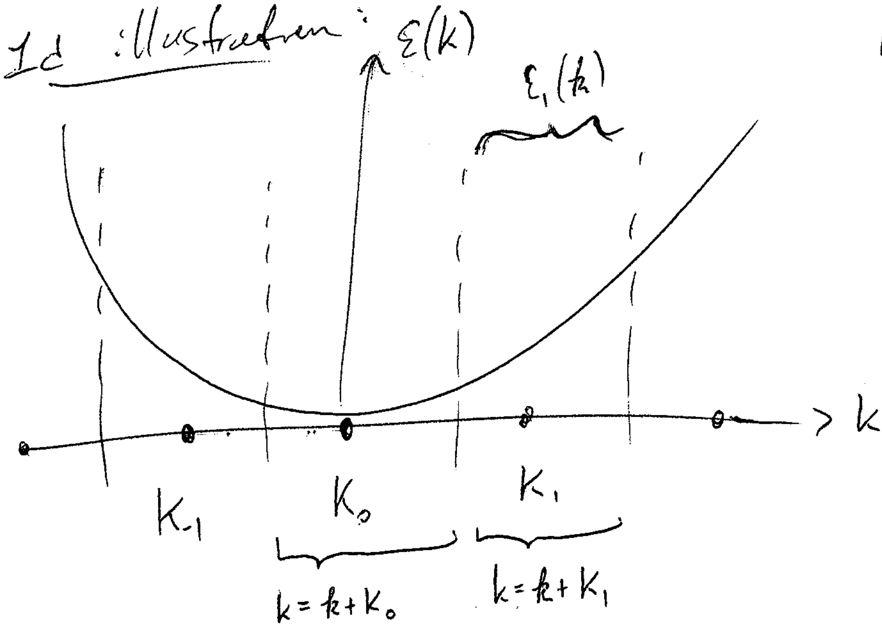
  n labels RLV's.

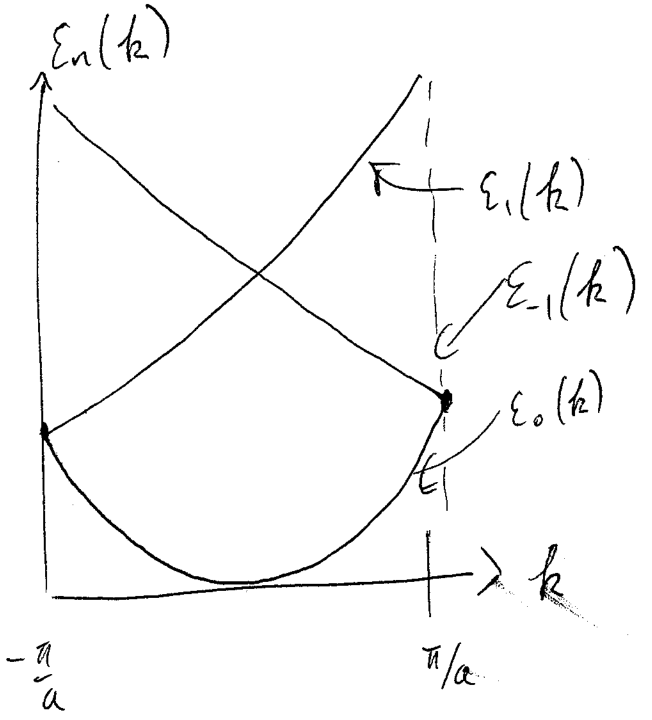
$$|\vec{k}\rangle = |\vec{k} + \vec{K}_n\rangle \longrightarrow |\vec{k}, n\rangle \text{ "Bloch state"}$$

$$\varepsilon_n(\vec{k}) = \varepsilon(\vec{k} + \vec{K}_n)$$

1d illustration:

$$K_n = \frac{2\pi n}{a}$$





Summary 2

(B)

~~What~~ Size at deg. @ edge?

P.T. in $V(\vec{r})$:

- Most important cases are degenerate points:

$$\varepsilon(\vec{k}) \approx \varepsilon(\vec{k}+\vec{K}) \quad (\text{can be more than } 2)$$

$$\varepsilon(\vec{k}_0) = \varepsilon(\vec{k}_0+\vec{K}) \equiv \varepsilon_0$$

$$|1\rangle = |\vec{k}\rangle \qquad |2\rangle = |\vec{k}+\vec{K}\rangle$$

$$(H_{eff})_{\alpha\beta} = \langle\alpha|H|\beta\rangle = \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & \varepsilon_0 \end{pmatrix} + \begin{pmatrix} \varepsilon_0 - \varepsilon(\vec{k}) & \tilde{V}^*(\vec{K}) \\ \tilde{V}(\vec{K}) & \varepsilon_0 - \varepsilon(\vec{k}+\vec{K}) \end{pmatrix}$$

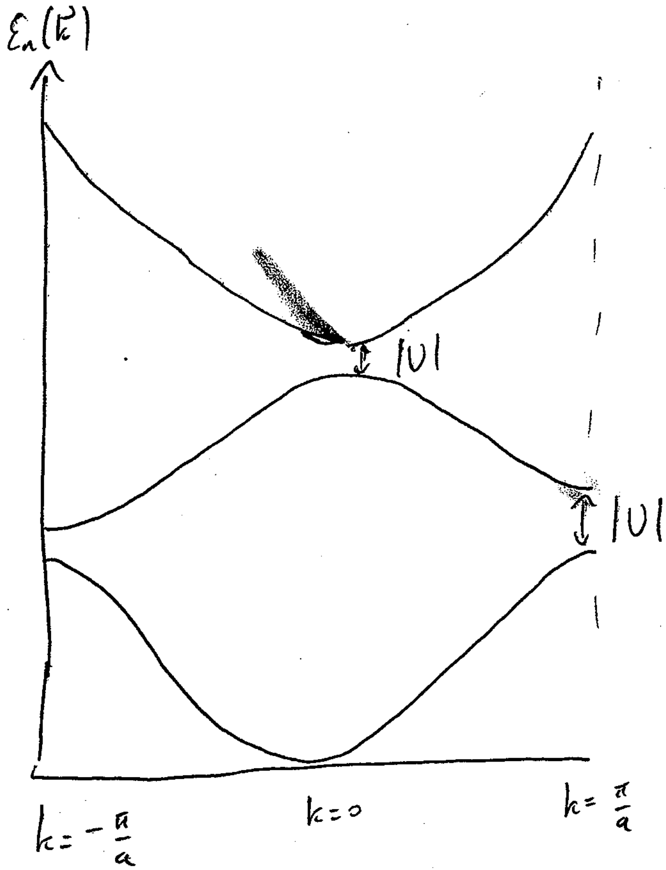
Summary 3

C

Energy: $\mathcal{E}_{\pm}(\vec{k}) = \left(\frac{\mathcal{E}(k) + \mathcal{E}(k+K)}{2}\right) \pm \sqrt{\left(\frac{\mathcal{E}(\vec{k}) - \mathcal{E}(\vec{k}+\vec{K})}{2}\right)^2 + |\tilde{V}(\vec{K})|^2}$

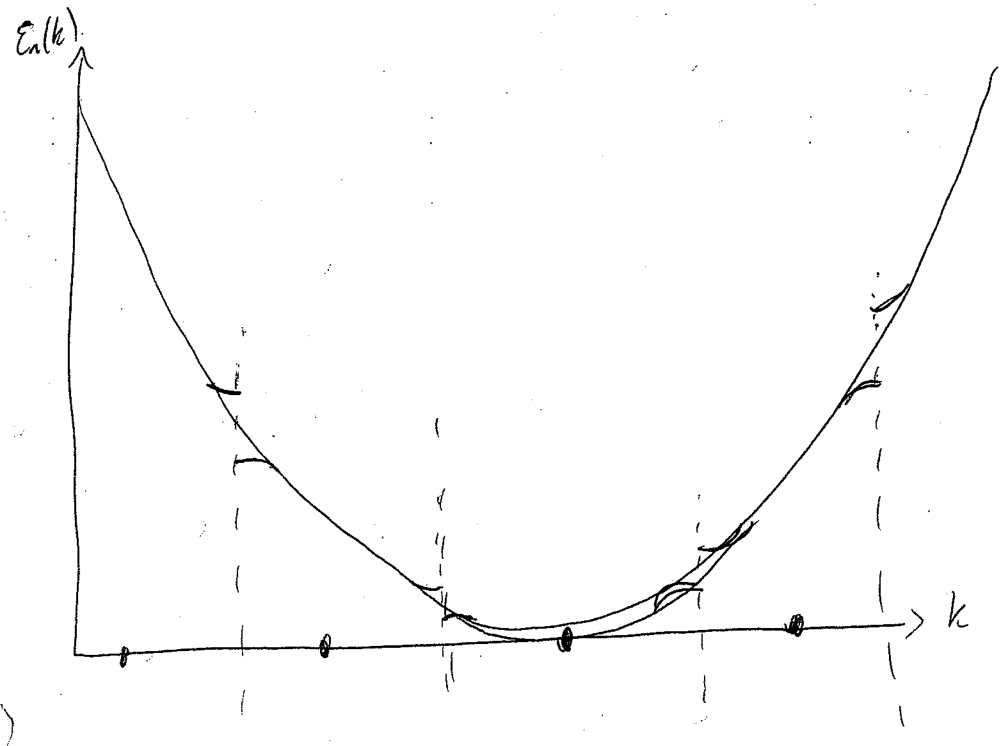
For $\vec{k} = \vec{k}_0$, $\quad \mathcal{E}_{\pm}(\vec{k}_0) = \mathcal{E}_0 \pm |\tilde{V}(\vec{K})|$

- In 1d case:

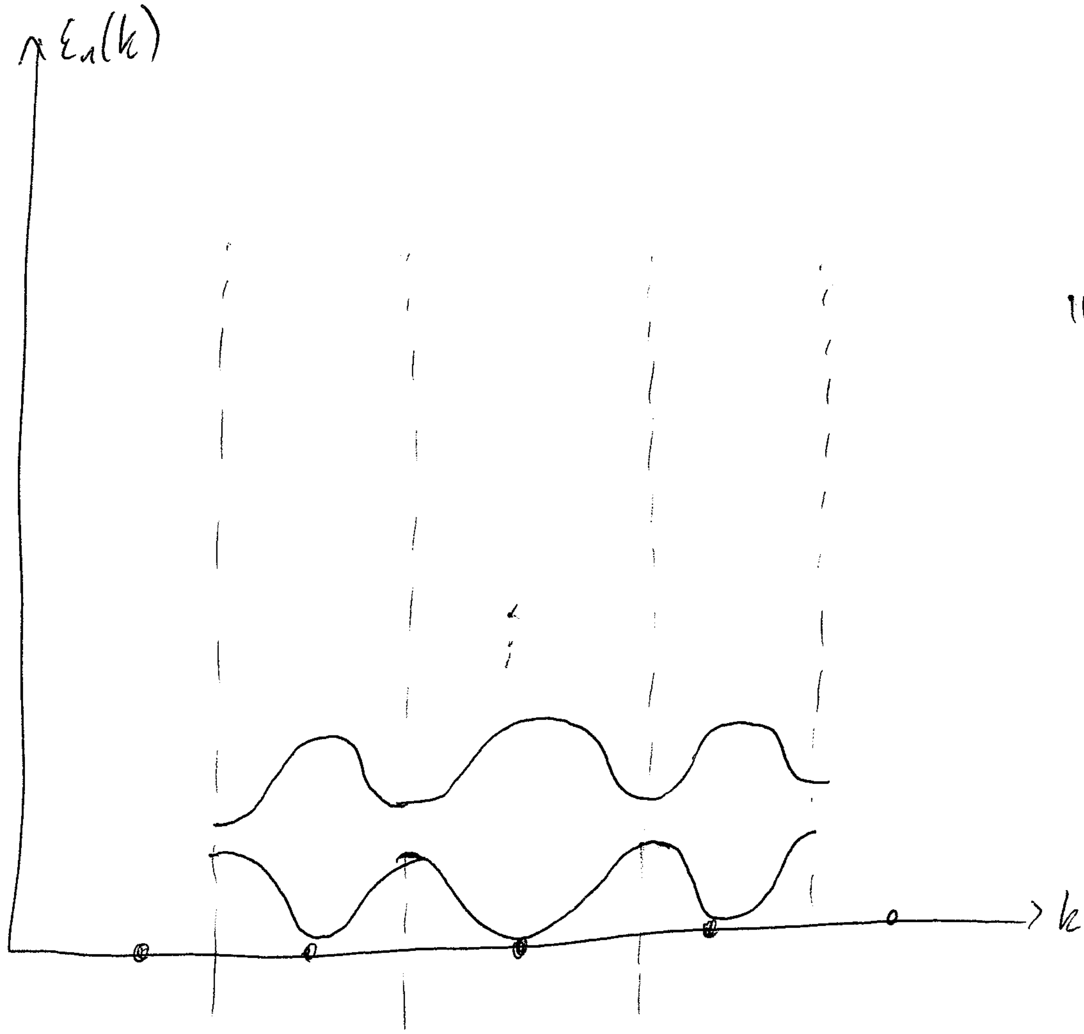


"Reduced zone scheme" ~~⇔~~

→ Only plot within Brillouin zone.



"Extended Zone scheme"



"Repeated zone scheme"

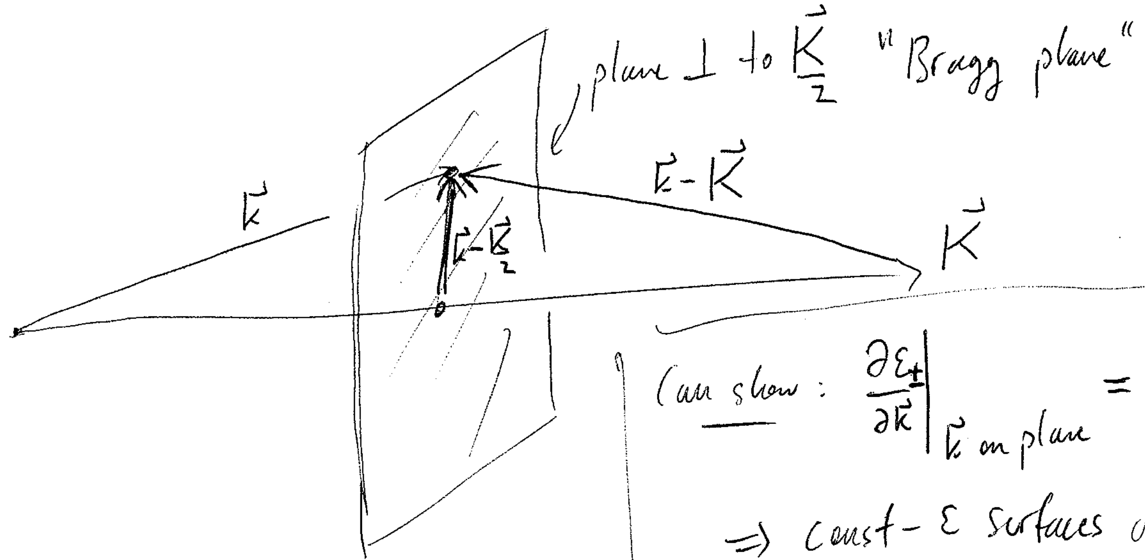
• Reduced zone scheme is most fundamental, ~~which~~ Others only <u>literally</u> make sense for weak $U(\vec{r})$, where every band can be identified as "coming from" some free electron band.

However, other pictures also useful sometimes.

Higher dimensions.

degeneracy

- $\varepsilon(\vec{k}) = \varepsilon(\vec{k}-\vec{K})$ when $|\vec{k}| = |\vec{k}-\vec{K}|$

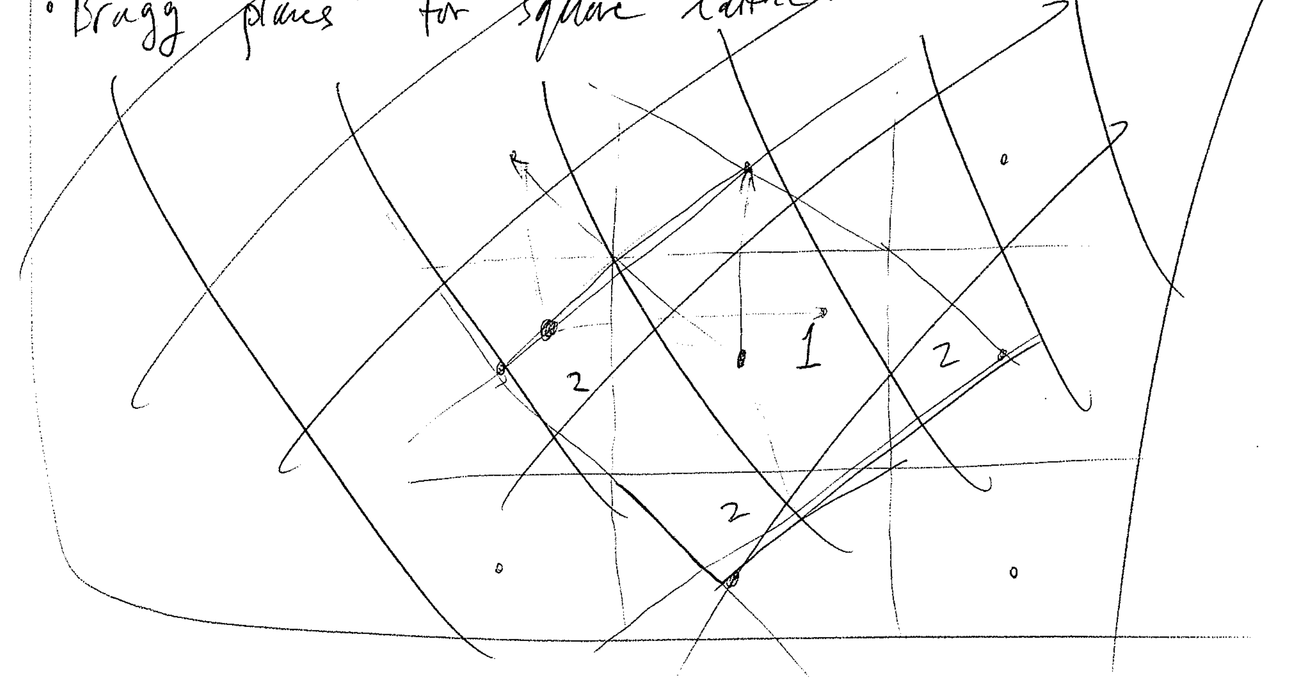


Can show: $\left.\frac{\partial \varepsilon_\pm}{\partial \vec{k}}\right|_{\vec{k}\text{ on plane}} = \frac{\hbar^2}{m}\left(\vec{k}-\frac{1}{2}\vec{K}\right)$

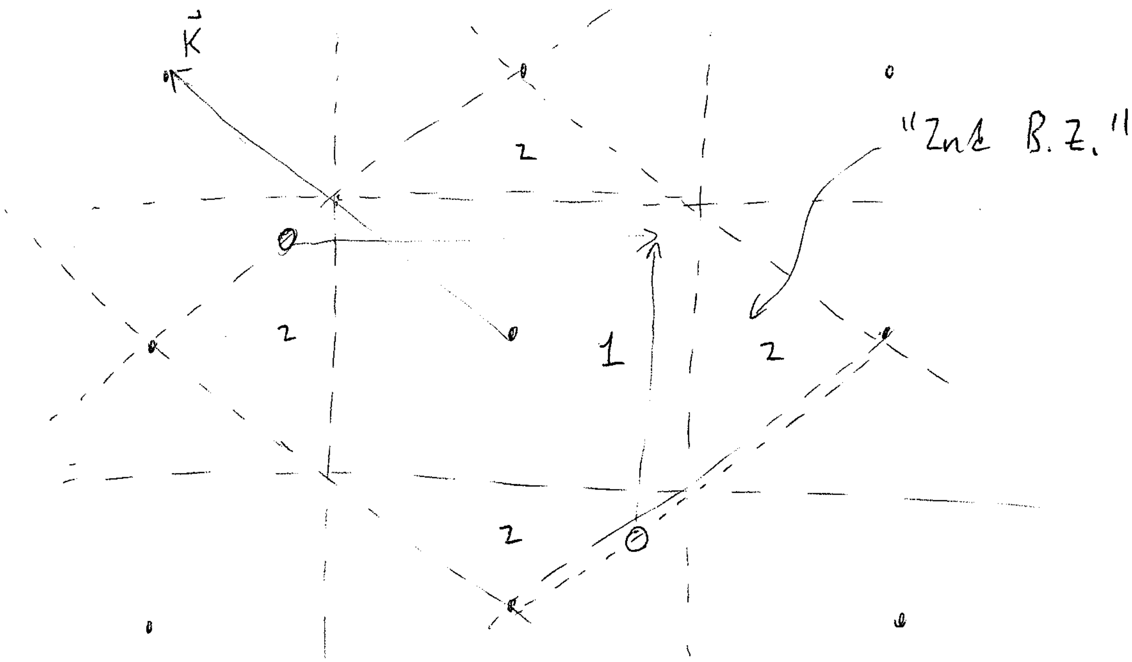
$\Rightarrow$ const-ε surfaces are ⊥ to plane.

- Have degeneracy whenever $\vec{k}$ lies on Bragg plane (if lies on more than one Bragg plane, $\Rightarrow$ multiple degeneracy).

- Bragg "planes" for square lattice:

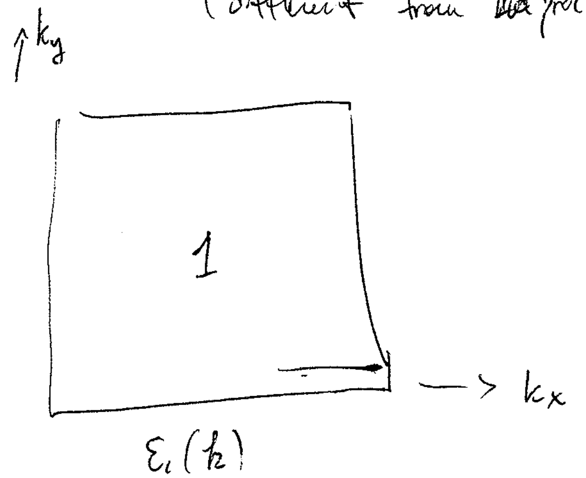


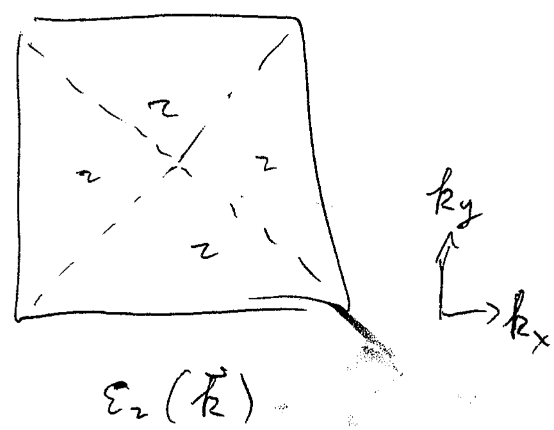
- Bragg "planes" for square lattice



O's have same $\vec{k}$ inside 1st B.Z.

- Can define $\varepsilon_n(\vec{k})$ as band obtained from nth B.Z.
  (different from ~~the~~ procedure we used in d=1 example)



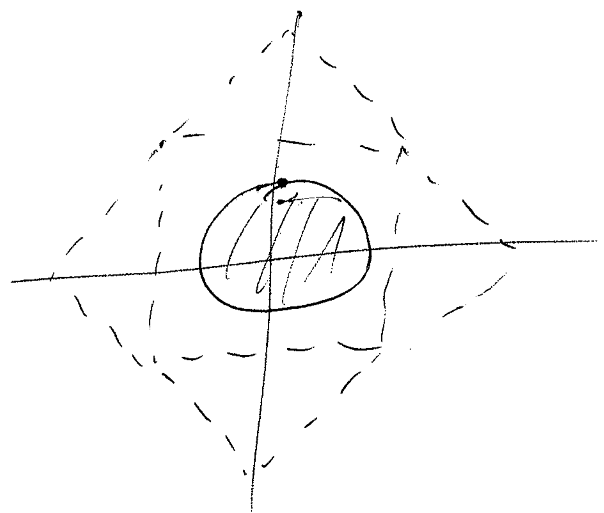


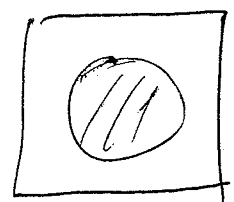
etc.

What does Fermi surface look like?

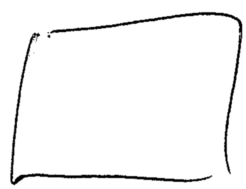
- Many pieces: nth piece given by $\varepsilon_n(\vec{k}) = \varepsilon_F$

Square lattice example:

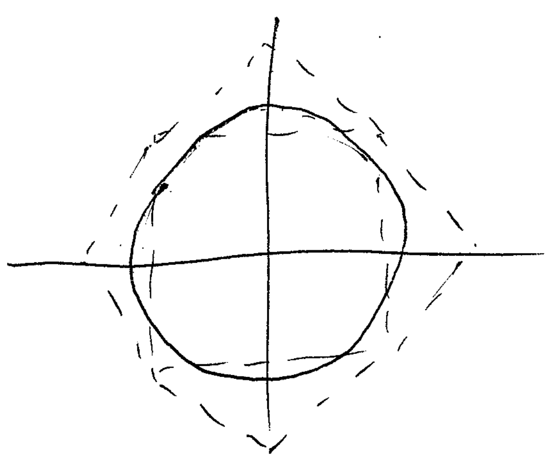


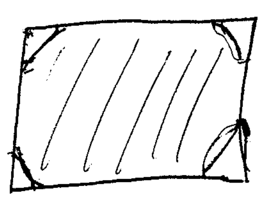


1st band

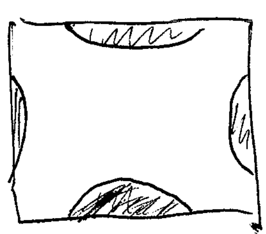


no F.S. in 2nd band





1st band



2nd band