

nonvanishing mean velocity

$$\vec{v}_n(\vec{h}) = \frac{1}{\hbar} \vec{\nabla}_{\vec{h}} \mathcal{E}_n(\vec{h})$$

(136)

$\Rightarrow$  electron "moves forever" without degradation of its mean velocity.

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### Fermi Surface

for free electrons: grand state

$$\text{all 1-electron levels } \mathcal{E}(\vec{h}) = \frac{\hbar^2 k^2}{2m} < \mathcal{E}_F$$

are occupied

$\mathcal{E}_F$  determined by requirement that total number of 1-electron levels  $\mathcal{E} < \mathcal{E}_F$  is equal to the number of electrons.

for Bloch electrons: grand state

$N$  Bloch electrons

we have 1-electron levels  $\mathcal{E}_n(\vec{h})$

$$\mathcal{E}_n(\vec{h}) \neq \frac{\hbar^2 k^2}{2m}$$

rather,  $\mathcal{E}_n(\vec{h})$  is determined by

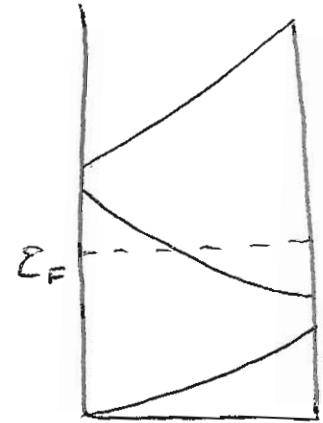
$$\left( \frac{\hbar^2}{2m} (\vec{h} - \vec{K})^2 - \mathcal{E}_n(\vec{h}) \right) c_{\vec{h}-\vec{K}} + \sum_{\vec{K}'} U_{\vec{K}'-\vec{K}} c_{\vec{h}-\vec{K}'} = 0$$



## 2) Partial filling

$E_F$  cuts through 1 or more bands

$\Rightarrow$  surface in  $\vec{k}$ -space separating occupied from unoccupied



set of all such surfaces called,  
the Fermi Surface

is a generalized Fermi sphere (for free electron case)

sometimes the Fermi surface is entirely within a single band

If it lies within 2 or more bands, this leads branches of the Fermi surface

The Fermi surface is such that

$$E_n(\vec{k}) = E_F = \text{constant energy}$$

all such  $\vec{k}$  points where this equation is true lie on the Fermi surface

Fermi surface is a constant energy surface.  
(or set of constant energy surfaces)

- repeated zone scheme
- reduced zone scheme

## Density of Levels

needed for the calculation of various weighted sums over electronic levels of one-electron properties

$$Q = 2 \sum_{n, \vec{h}} Q_n(\vec{h})$$

↑  
for  
spin

Same as for free-electron case, we can define

$$g = \lim_{V \rightarrow \infty} \frac{Q}{V} = 2 \sum_n \int_{\text{primitive cell}} \frac{d\vec{h}}{(2\pi)^3} Q_n(\vec{h})$$

if  $Q_n(\vec{h})$  depends on  $n$  and  $\vec{h}$  through the energy  $\epsilon_n(\vec{h})$ , then one can write

$$g = \int d\epsilon g(\epsilon) Q(\epsilon)$$

$$g(\epsilon) = \sum_n g_n(\epsilon)$$

$$g_n(\epsilon) = \int_{\text{primitive cell}} \frac{d\vec{h}}{4\pi^3} \delta(\epsilon - \epsilon_n(\vec{h})) = \text{density of levels in the } n^{\text{th}} \text{ band}$$

$$g = \int d\varepsilon g(\varepsilon) Q(\varepsilon) = 2 \sum_n \int \frac{d\vec{h}}{(2\pi)^3} Q_n(\vec{h}) \quad (140)$$

$$g(\varepsilon) = \sum_n g_n(\varepsilon)$$

$$= 2 \sum_n \int \frac{d\vec{h}}{(2\pi)^3} Q_n(\vec{h})$$

$$g = \sum_n \int \frac{d\vec{h}}{4\pi^3} Q_n(\vec{h})$$

$$= \int d\varepsilon \left[ \sum_n \int \frac{d\vec{h}}{4\pi^3} Q(\varepsilon) \right] \delta(\varepsilon - \varepsilon_n(\vec{h}))$$

$$= \int d\varepsilon \left[ \sum_n \int \frac{d\vec{h}}{4\pi^3} \delta(\varepsilon - \varepsilon_n(\vec{h})) \right] Q(\varepsilon)$$

$$= \int d\varepsilon g(\varepsilon) Q(\varepsilon)$$

$$\text{with } g(\varepsilon) = \sum_n \int \frac{d\vec{h}}{4\pi^3} \delta(\varepsilon - \varepsilon_n(\vec{h}))$$

$$= \sum_n g_n(\varepsilon)$$

$$\text{with } g_n(\varepsilon) = \int \frac{d\vec{h}}{4\pi^3} \delta(\varepsilon - \varepsilon_n(\vec{h}))$$

prim  
cell

either sum over all of  $\vec{h}$ -space, or else sum over all  $n$  and over all  $\vec{h}$  within a single primitive cell of  $\vec{h}$ -space

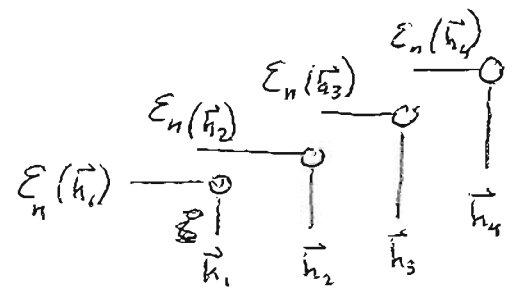
$$\sum_{\text{all } \vec{h}} \rightarrow \sum_{n, \vec{h} \text{ inside 1 prim cell}}$$

$$g_n(\epsilon) = \int \frac{d\vec{h}}{4\pi^3} \delta(\epsilon - \epsilon_n(\vec{h}))$$

$$g_n(\epsilon)d\epsilon = \left[ \frac{2}{V} \sum_{\text{prim cell}} \delta(\epsilon - \epsilon_n(\vec{h})) \right] d\epsilon$$

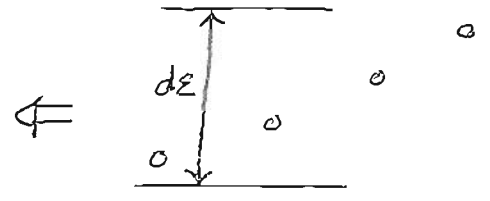
$$g_n(\epsilon)d\epsilon = \frac{2}{V} \left[ \sum_{\text{prim cell}} \delta(\epsilon - \epsilon_n(\vec{h})) \right] (d\epsilon)$$

$g_n(\epsilon)d\epsilon = \frac{2}{V} \times$  number of allowed wave vectors on the  $n^{\text{th}}$  band in the energy range  $\epsilon \rightarrow \epsilon + d\epsilon$



$$= \frac{2}{V} \times \left[ \frac{\text{\vec{h}-space volume with } \epsilon \leq \epsilon_n(\vec{h}) \leq \epsilon + d\epsilon}{\text{volume for 1 wave-vector}} \right]$$

In this case,  $\Delta n = 4$

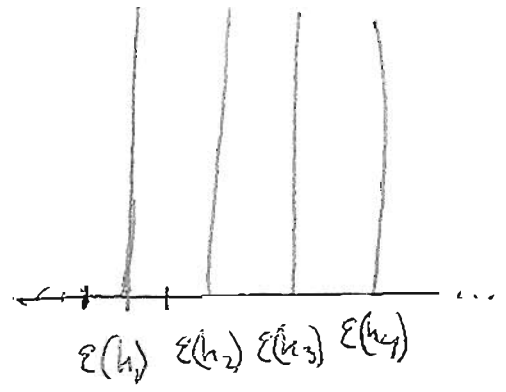


$$= \frac{2}{V} \left[ \frac{\int d\vec{h} (\epsilon \leq \epsilon_n(\vec{h}) \leq \epsilon + d\epsilon)}{\frac{(2\pi)^3}{V}} \right]$$

$$\Delta n = \int \delta(\epsilon - \epsilon_n(\vec{h})) d\epsilon$$

$$= \int \frac{d\vec{h}}{4\pi^3} \text{ if } \epsilon \leq \epsilon_n(\vec{h}) \leq \epsilon + d\epsilon$$

$$= 0 \text{ if } \epsilon_n(\vec{h}) \text{ not within } \epsilon \rightarrow \epsilon + d\epsilon$$



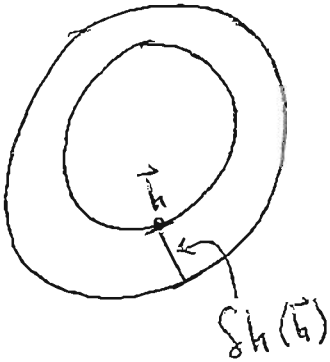
Express  $g_n(\epsilon)$  as a surface integral

(142)

$$g_n(\epsilon) d\epsilon = \int_{\text{prim cell}} \frac{d\vec{h}}{4\pi^3}$$

but  $d\vec{h} = dS \delta h(\vec{h})$

$$\Rightarrow \int_{\text{prim cell}} \frac{dS \delta h(\vec{h})}{4\pi^3}$$



but

$$d\epsilon = \left[ \vec{\nabla}_{\vec{h}} \epsilon_n(\vec{h}) \right] \delta h(\vec{h})$$

$$\Rightarrow \delta h(\vec{h}) = \frac{d\epsilon}{\left| \vec{\nabla}_{\vec{h}} \epsilon_n(\vec{h}) \right|}$$

$$\Rightarrow g_n(\epsilon) d\epsilon = \int_{\text{prim cell}} \frac{dS d\epsilon}{4\pi^3 \left| \vec{\nabla}_{\vec{h}} \epsilon_n(\vec{h}) \right|}$$

$$\Rightarrow g_n(\epsilon) = \int_{\text{prim cell}, S_n(\epsilon)} \frac{dS}{4\pi^3} \frac{1}{\left| \vec{\nabla}_{\vec{h}} \epsilon_n(\vec{h}) \right|}$$

Explicit Relation between Density of Levels  $[g_n(\epsilon)]$  and Band Structure  $[\epsilon_n(\vec{h})]$

$$g_n(\varepsilon) = \int_{S_n(\varepsilon)} \frac{dS}{4\pi^3} \frac{1}{|\vec{\nabla}_k \varepsilon_n(\vec{k})|} \quad \text{Density of Levels}$$

within prim cell

The integral is over the constant energy surface  $S_n(\varepsilon)$  within a single primitive cell

IF  $\vec{\nabla}_k \varepsilon_n(\vec{k}) = 0$  anywhere on that constant energy surface, then there will be a singularity in  $\frac{1}{|\vec{\nabla}_k \varepsilon_n(\vec{k})|}$

$\Rightarrow$  van Hove singularities

In 3-D, they are integrable

$\Rightarrow g_n(\varepsilon)$  is finite at

In real solid, there will be such singularities because

$\vec{\nabla}_k \varepsilon_n(\vec{k})$  will be  $= 0$  at certain points within each unit cell (i.e. at <sup>local</sup> max and min of  $\varepsilon_n(\vec{k})$ )

due to 1) boundedness, and 2) periodicity of each  $\varepsilon_n(\vec{k})$