The Fermi surface

The ground state of N free electrons is constructed by occupying all one electron states with $\varepsilon(k) = \hbar^2 k^2/2m < \varepsilon_F$, where ε_F is determined by the density
Similarly for the Bloch electrons $\varepsilon_n(k) < \varepsilon_F$ and k should be confined to a single primitive cell of the recip. lattice
Two important cases:

(1) A certain # of bands is completely filled, all others remain empty. The difference in energy between the highest occupied level and the lowest unoccupied level is the band gap
When $\Delta_{gap} >> k_B T_{room}$ → insulators
$\Delta_{gap} \lesssim k_B T_{room}$ → semiconductors
The # of levels in each band = # of primitive cells in a crystal. Each level can accomodate 2 ($\uparrow\downarrow$) electrons ⇒ a configuration with a band gap can arise (though it need not) only if the # of electrons per primitive cell is even

(2) A number of bands may be partially filled. When this occurs, ε_F lies within the range of 1 or more bands. For each partially filled band there will be a surface in k-space separating the occupied from unoccupied levels. The set of all such surfaces → the Fermi surface. The parts of the FS arising from

individually partially filled bands are known as the branches of the FS.

Analytically the branch of the FS is determined by $E_n(\vec{k}) = E_F$ (*)

Since $E_n(k)$ is periodic in k, the solution of (*) is a k-surface with the periodicity of the recip. lattice. When the FS is represented by the full periodic structure → repeated zone scheme. If we use a single primitive cell → a reduced zone scheme.

Density of levels

One must often calculate weighted sums over the electronic levels

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

For each n the sum is over physically distinct levels $\Rightarrow$ $\Rightarrow$ all $\vec{k}$ are in one primitive cell of the rec. lat. In the limit of large volume of the crystal

$$\Delta k = \frac{(2\pi)^3}{V} \text{ is small, hence}$$

$$Q = 2 \sum_{n,k} Q_n(k) = 2 \left[\frac{(2\pi)^3}{V}\right]^{-1} \cdot \int_{\substack{\text{prim} \\ \text{cell}}} d^3k \; Q_n(k)$$

$$q = \frac{Q}{V} = \sum_n \int_{\substack{\text{prim} \\ \text{cell}}} \frac{d^3k}{(2\pi)^3} Q_n(k)$$

Often $Q_n(k)$ depends on n and $\vec{k}$ only through $\varepsilon_n(k)$, then

$$q = \int d\varepsilon \; g(\varepsilon) \, Q(\varepsilon) \quad \text{where}$$

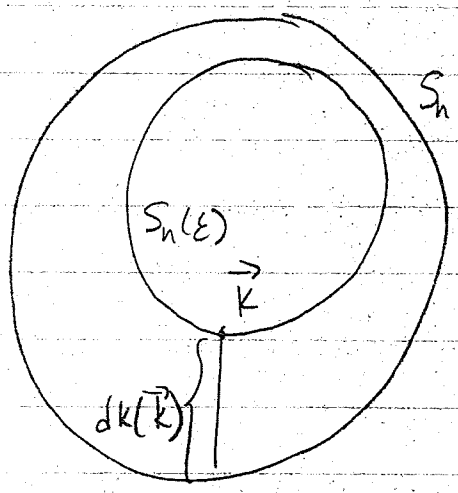
$$g(\varepsilon) = \sum_n g_n(\varepsilon)$$

$$g_n(\varepsilon) = 2 \int_{\text{prim cell}} \frac{d^3k}{(2\pi)^3} \, \delta(\varepsilon - \varepsilon_n(\vec{k}))$$

$$g_n(\varepsilon)\,d\varepsilon = \frac{2}{V} \times \left\{ \begin{array}{l} \text{the \# of allowed wavevectors} \\ \text{in the } n\text{-th band in the} \\ \text{energy range from } \varepsilon \text{ to } \varepsilon + d\varepsilon \end{array} \right.$$

$$\text{The \# of allowed } k = \frac{\text{Volume in } k \text{ space } \varepsilon < \varepsilon_n(k) < \varepsilon + d\varepsilon}{\Delta K}$$

$$g_n(\varepsilon)\,d\varepsilon = 2 \cdot \int \frac{d^3k}{(2\pi)^3} \times \left\{ \begin{array}{ll} 1, & \varepsilon \le \varepsilon_n(k) \le \varepsilon + d\varepsilon \\ 0, & \text{otherwise} \end{array} \right.$$



Let $S_n(\varepsilon)$ be the portion of the surface $\varepsilon_n(k) = \varepsilon$ lying within the primitive cell

δk – perpendicular distance

$$g_n(\varepsilon)\,d\varepsilon = \int_{S_n(\varepsilon)} \frac{dS}{4\pi^3} \cdot \delta k(\vec{k})$$

$$\varepsilon + d\varepsilon = \varepsilon + \left| \vec{\nabla}_k \varepsilon_n(k) \right| \delta k$$

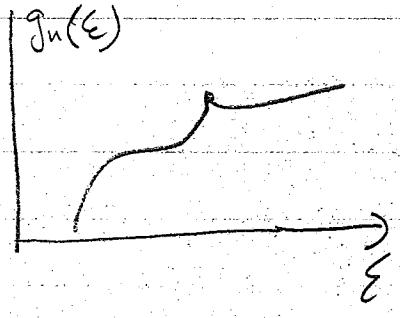
$$\delta k = \frac{d\varepsilon}{\left| \nabla \varepsilon_n(k) \right|}$$

$$g_n(\varepsilon) = \int_{S_n(\varepsilon)} \frac{dS}{4\pi^3} \frac{1}{\left| \vec{\nabla}_k \varepsilon_n(\vec{k}) \right|} \qquad (**)$$

From $\varepsilon_n(k)$ – periodic

Bounded above and below for $\forall n$

we must have values of k at which $|\nabla_k \varepsilon| = 0$ (e.g. $\vec{k}$ at maxima and minima). When $|\nabla \varepsilon| \neq 0$ the integrand in (**) diverges. In $d = 3$ such sing. are integrable with finite values of g_n. However $\frac{dg_n}{d\varepsilon}$ may diverge. In $d = 1$ even



$g_n(\varepsilon)$ will be infinite.

These are van Hove singularities.