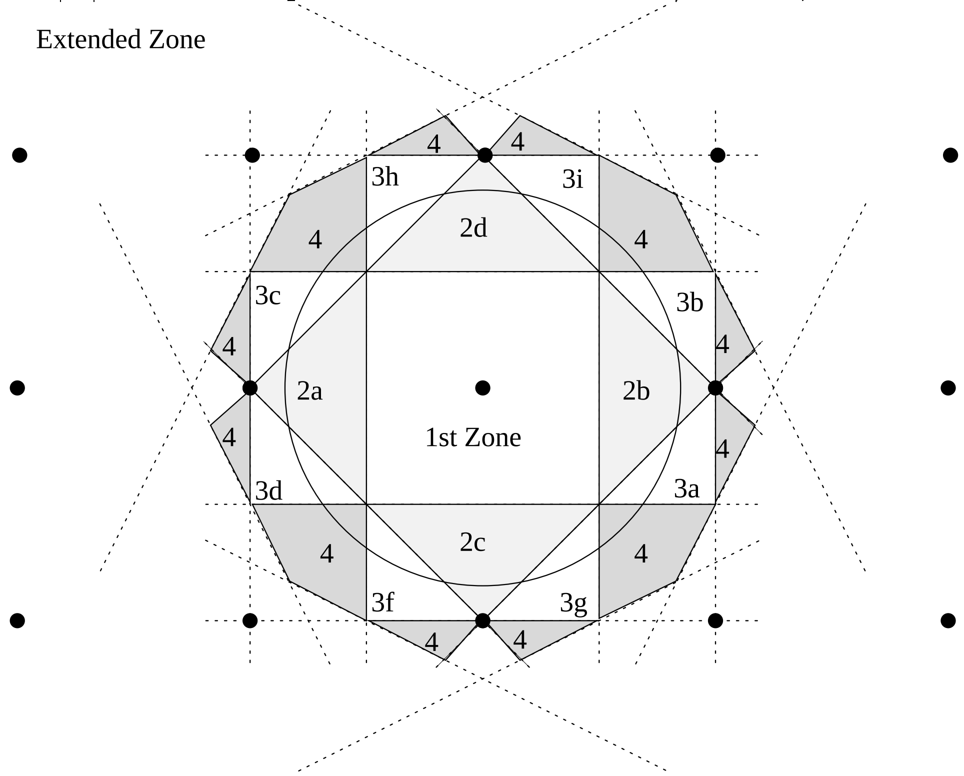
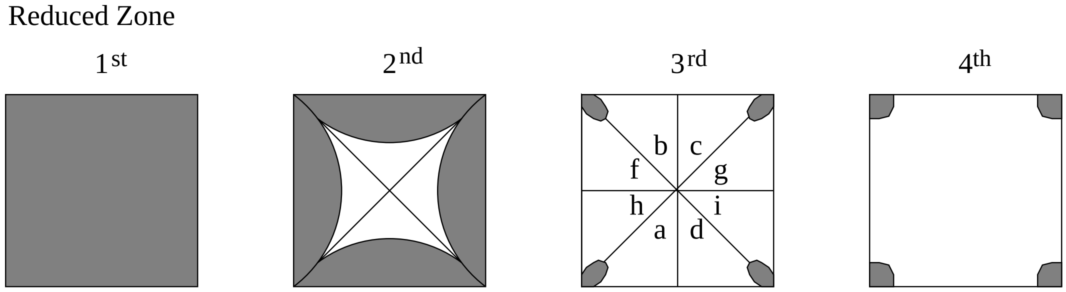
PHYS 551 Lecture #26

Title: The Fermi Surface

Since the "bulk" of electronic properties are determined by the location of the Fermi surface with respect to the band structure, it is extremely useful to examine the Fermi surface directly.

The zone boundries occur at all places where $\vec{k}\cdot\vec{G}/2 = |\frac{\vec{G}}{2}|^2$ or $2\vec{k}\cdot\vec{G} = G^2$ or $2\vec{k}\cdot\vec{G} - |\vec{G}|^2 = 0$. For a square lattice with 4 electrons/unit cell, the following occurs:





If there are 4 e^-'s/primitive lattice then

$$\pi k_F^2 = 2 \text{ Area } 1^{st} \text{ B.Z.} \quad = \quad 2\left(\frac{2\pi}{L}\right)^2 \quad \text{Let } |\vec{G}_{10}| = \frac{2\pi}{L}$$
$$\pi k_F^2 \quad = \quad G^2$$

$$k_F = \sqrt{\frac{2}{\pi}}G = .80|\vec{G}|$$

Now what happens if the electron is "nearly" free?

(1) Small energy gap form at all zone boundaries.

(2) Since $|\vec{v}| \perp$ Zone Boundary $\rightarrow 0$, or $\hat{n} = \vec{G}/|\vec{G}|$ and $\vec{v} = \frac{1}{\hbar}\nabla_k E$

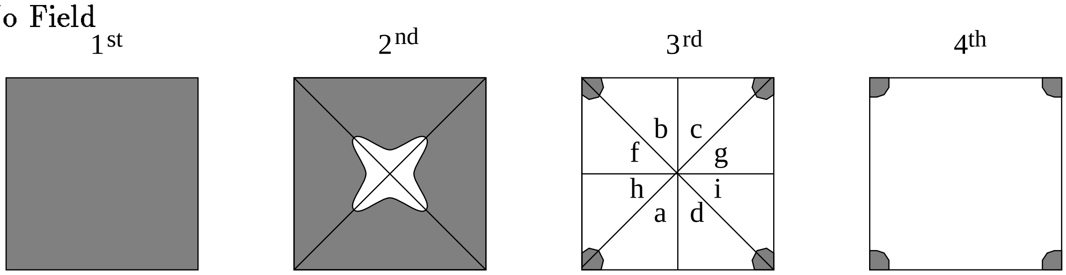
$$\text{so } \vec{v}\cdot\hat{n} = \tfrac{1}{\hbar}\nabla_k E(k)\cdot\vec{G}/|\vec{G}| = 0$$

$$\tfrac{1}{\hbar}\nabla_k E(k)\cdot\vec{G} = 0$$

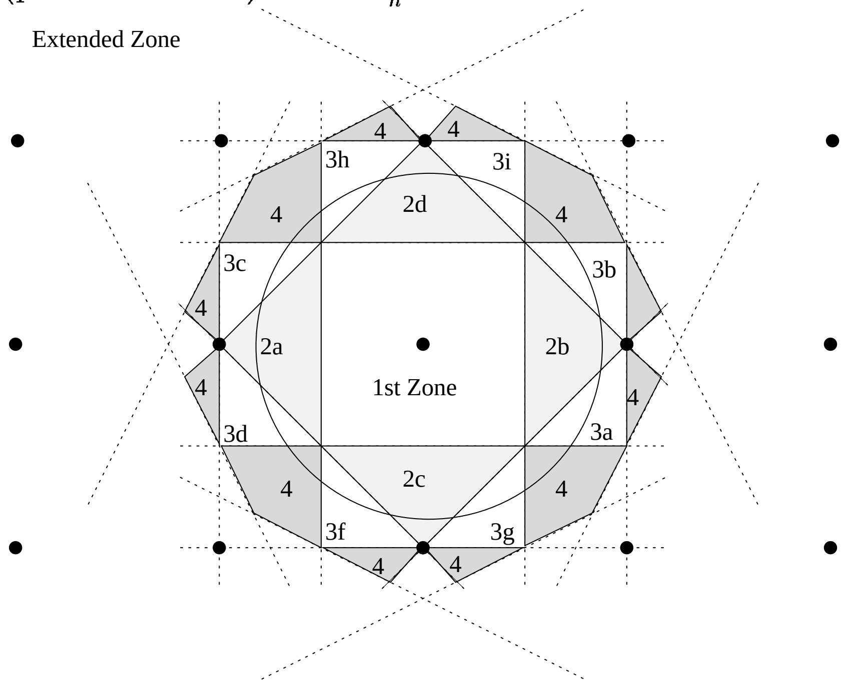
Since $\nabla_k E\cdot\vec{G} = 0, \nabla_k E(k) \perp \vec{G}$ or the energy contours are parallel to $\vec{G}$.

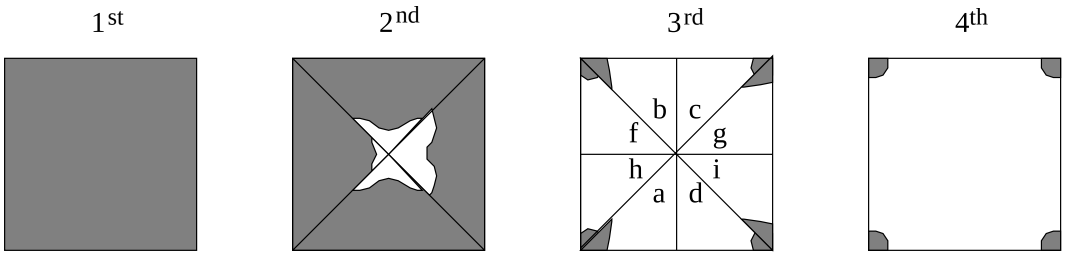
(3) The total volume within the Fermi surface is fixed.

No Field

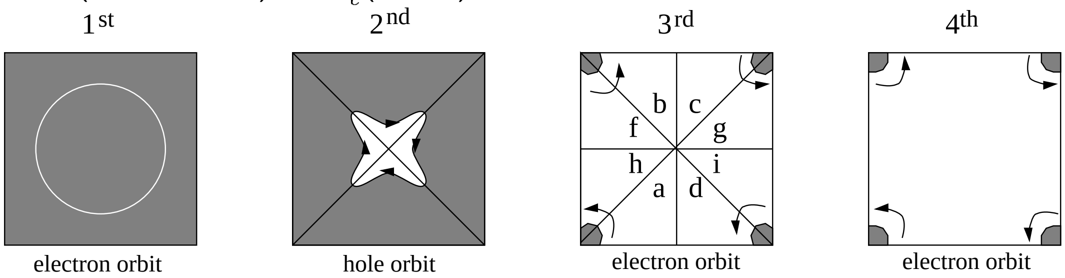


E-field (points to the left) $\Delta k = -\frac{e\vec{E}}{\hbar}\tau$





B-field (out of paper) $\vec{F} = \frac{q}{c}(\vec{v} \times \vec{B})$



So, once again, what parameters are important for conduction? (In a metal)

$$\vec{j} = -ne\vec{v} = -e \; v_{fermi_{\vec{E}_x}} \; \# \text{ unbalanced electrons/volume}$$

$$\begin{aligned} \text{If one-dimensional} \quad \Delta\vec{k} &= \frac{-e\vec{E}}{\hbar}\tau \\ \# \text{ unbalanced} &= \Delta\vec{k}\,\frac{dN}{dk} \end{aligned}$$

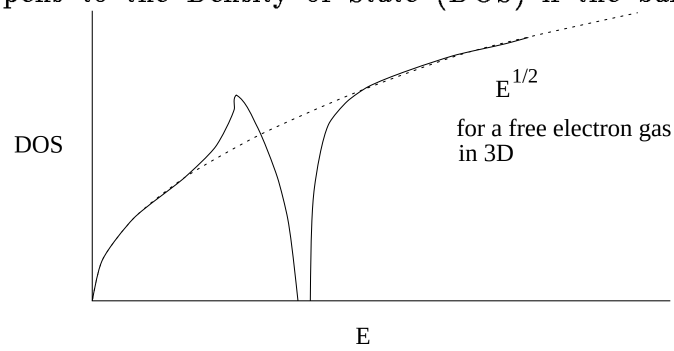
$$\begin{aligned} \text{so} \quad \vec{j} &\sim -e \; v_{Fermi}\frac{-e\;\vec{E}}{\hbar}\tau\frac{dN}{dk} \\ &\sim -e^2\tau\vec{E}\; v_{Fermi}\;\frac{dN}{dk} \qquad \frac{dN}{dk} = \frac{dN}{d\epsilon}\frac{d\epsilon}{dk} = \mathcal{D}(\epsilon_F)\hbar v_F \end{aligned}$$

thus

$$\vec{j} \sim e^2 v_F^2 \mathcal{D}(\epsilon_F)\tau\vec{E}$$

Hence the major parameters as $\underline{\mathcal{D}(\epsilon_F)}$, $\underline{v_F}$ and $\underline{\tau_{Fermi}}$.

What happens to the Density of State (DOS) if the band gaps are modest.



Clearly there is a cusp in $D(\varepsilon)$ as k approaches the zone boundary and $E(k)$ becomes flat. Then the DOS decreases to zero. Finally, it increases again and approaches the $\sqrt{\epsilon}$ behavior

Now that we have "beaten to death" the various subleties of the Free Electron Gas model, it is perhaps useful to get another perspective.

LCAO or Tight Binding:

Tight Binding (or linear conbinations of atomic orbitals) is perhaps the simplest method for describing energy bands. For a single atom, the electron "orbitals" form a set of discrete energy levels. Hence a periodic lattice might be expected to be best described by a superposition of these atomic states.

One atom: eigenfunction $\phi_A(\vec{r})$ and eigenvalue E_A.

Lattice: eigenfunction $\Gamma \sum_R \phi_A(\vec{r}-R)$ and eigenvalues E_A's.

Both satisfy the Schrödinger equation $-\frac{\hbar^2}{2m}\nabla^2\phi_A + U_A\phi_A = E_A\phi_A$.

However in a periodic crystal, the electron wavefunction must satisfy the Bloch condition

$$\psi(\vec{k},\vec{r}+\vec{R}') = e^{i\vec{k}\cdot\vec{R}'}\psi(\vec{k},\vec{r})$$

Hence for a lattice with one atom and one electron per unit cell,

$$\psi(\vec{k},\vec{r}) = \Gamma \sum_R e^{i\vec{k}\cdot\vec{R}}\phi_A(\vec{r}-\vec{R})$$

thus the degeneracy is broken.

What are the TRANSLATIONAL PROPERTIES?

$$\psi(\vec{k},\vec{r}+\vec{R}') = \Gamma \sum_R e^{i\vec{k}\cdot\vec{R}}\phi_A(\vec{r}-\vec{R}+\vec{R}')$$

but $-\vec{R}+\vec{R}'$ is another lattice vector, let $\vec{R}'' = \vec{R}-\vec{R}'$

$$\begin{aligned}
\psi(\vec{k},\vec{r}+\vec{R}') &= \Gamma \sum e^{i\vec{k}\cdot(\vec{R}'+\vec{R}'')}\phi(\vec{r}-\vec{R}'') \\
&= e^{i\vec{k}\cdot\vec{R}'}\Gamma \sum e^{i\vec{k}\cdot\vec{R}''}\phi(\vec{r}-\vec{R}'') \\
\psi(\vec{k},\vec{r}+\vec{R}') &= e^{i\vec{k}\cdot\vec{R}'}\psi(k,r)
\end{aligned}$$

and thus the Bloch condition is satisfied.