5. Repetition

- What is wrong with the Drude Model?
- What is typically E_F? What temperature does that relate to? How fast are electrons at the Fermi energy?
- What is the meaning of the real and imaginary part of the electrical conductivity as a function of frequency?
- What relationship can you find between the electrical and thermal conductivity of a metal?
- State Bloch's theorem in your own words.

6. Fermi surface of Iron-pnictide superconductors

Iron-pnictide superconductors such as KFe_2As_2 are layered half-metals with weakly overlapping valence and conduction bands, and this results in a special kind of Fermi surface. As a simplest model we consider a 3-dimensional simple cubic lattice with lattice constant a and hopping integrals (=matrix elements of the Hamiltonian) between nearest neighbors only. To describe the layered nature of the compounds we assume that the hopping integral between nearest neighbors in x- or y-direction $(-t_1)$ is different from the hopping integral between nearest neighbors in z-direction $(-t_2)$ and $t_1 \gg t_2$ whereby $t_1, t_2 > 0$.

a) Consider a single $(x-y)$ plane (i.e. $t_2 = 0$) and find the dispersion relation $E(\boldsymbol{k})$ where $\mathbf{k} = (k_x, k_y)$ is a two-dimensional wave vector. Show that for small $|k| \ll \frac{\pi}{a}$ this can be approximated by $E(\boldsymbol{k}) \sim E_0 + \frac{k^2}{2m^*}$ (1)
and express the effective mass m^* and the shift E_0 in terms of t_1 and a.

b) Assume that the band is almost empty i.e. the Fermi energy is $E_F \sim E_0 + \varepsilon$ with $\varepsilon \ll t_1$ so that equation (1) above can be used for $\mathbf{k}$ on the Fermi surface. Find the Fermi momentum k_F.

c) Consider now the case $t_2 \neq 0$. Show that for a 3D momenta $\boldsymbol{k} = (k_x, k_y, k_z)$with $k_x^2 + k_y^2 \ll \frac{\pi}{a}, \forall k_z$, the dispersion relation can be written as

$$E(\boldsymbol{k}) \sim E_0 + \frac{k^2}{2m^*} - 2t_2 cos(k_z a)$$

Then discuss the shape of the Fermi surface for the case $E_F \sim E_0 + \varepsilon$ with $t_2 \ll \varepsilon \ll t_1$ (Hint: let $\boldsymbol{k}_F = (k_{F,x}, k_{F,y}, k_{F,z})$ be a wave vector on the Fermi surface and find the relationship between $k_{F\parallel} = \left({k_{F,x}}^2 + {k_{F,y}}^2\right)^{1/2}$ and $k_{F,z}$). Sketch the resulting Fermi surface.

d) What changes if the band is almost full rather than almost empty?

7. Charge Screening and Thomas Fermi Approximation

a) Use the set of equations we established in the lecture in order to derive the general expression for the dielectric function

$$\epsilon(\boldsymbol{q}) = 1 - \frac{1}{\epsilon_0 q^2}\chi(\boldsymbol{q}) = 1 - \frac{1}{\epsilon_0 q^2}\frac{\rho^{ind}(\boldsymbol{q})}{\phi^{tot}(\boldsymbol{q})}$$

b) What are the assumptions made for the Thomas Fermi approximation?

c) Using these assumptions, one can write $\rho^{ind}(r) = -e\{n_0(\boldsymbol{r}) - n_0\}$, where n_0 is the homogeneous charge carrier concentration of the unperturbed system. Moreover, $n_0(\boldsymbol{r}) = n_0(\mu + e\phi^{tot}\{\boldsymbol{r}\})$, leading to

$$\rho^{ind}(r) = -e\{n_0(\mu + e\phi^{tot}\{\boldsymbol{r}\}) - n_0(\mu)\}$$

Show that

$\epsilon(\boldsymbol{q}) = 1 + \frac{k_s^2}{q^2}$ with $k_s = \sqrt{\frac{e^2}{\varepsilon_0}\frac{D(E_F)}{V}}$

What happens for $q \to 0$?

[Hints: you can assume $e\phi^{tot} \ll \mu$ and use $\frac{D(E_F)}{V} = (\partial n_0 / \partial \mu)_{\mu = E_F}$]

d) How large is the screening length $\lambda = 1/k_s$ roughly for copper? How much for silicon? Compare them to the interatomic spacing.