1. 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 - aka matrix elements of the Hamiltonian - between nearest neighbors only. To describe the layered nature of the compounds we assume that the hopping integral $-t_1$ between nearest neighbors in x- or y-direction is different from the hopping integral $-t_2$ between nearest neighbors in z-direction 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 $E_{\mathbf{k}}$ where $\mathbf{k} = (k_x, k_y)$ is a two-dimensional wave vector. Show that for small $|\mathbf{k}| \ll \frac{\pi}{a}$ this can be approximated by

$$E_{\mathbf{k}} = E_0 + \frac{k^2}{2m^*} \tag{1}$$

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 $E_F = E_0 + \epsilon$ with $\epsilon \ll t_1$ so that (1) can be used for $\mathbf{k}$ on the Fermi surface. Find the Fermi momentum $k_{F,0}$.

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

$$E_{\mathbf{k}} = E_0 + \frac{k^2}{2m^*} - 2t_2\, cos(k_z\, a).$$

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

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

2. Calculation of the Thermal Conductivity using Boltzmann Equation

To estimate the thermal conductivity, we place ourselves in the case where only a thermal gradient is applied to the sample and no electrical or magnetic fields. We seek to calculate the resulting heat current defined as:

$$J_H = \int \frac{d\vec{k}}{4\pi^3}\left[E_n(\vec{k}) - \mu\right]\vec{v}_n(\vec{k}) f(\vec{r},\vec{k},t)$$

where E_n is the energy of band n that crosses the Fermi-level (we'll assume this is the only one), μ the chemical potential, $\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\nabla_k E_n$ the electron velocity in band n, and $f(\vec{k})$ the electron distribution function that we need to determine.
We first linearize the Boltzmann equation

$$\left.\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right|_{\text{Scattering}} = \frac{\partial f(\vec{r},\vec{k},t)}{\partial t} + \vec{v}_n(\vec{k})\cdot\frac{\partial f}{\partial \vec{r}} + \frac{\vec{F}}{\hbar}\cdot\frac{\partial f}{\partial \vec{k}}$$

and place ourselves in the relaxation time approximation, that is we assume that:
$f(\vec{r},\vec{k},t) = f_0(E_n) + g(\vec{r},\vec{k},t)$, with $f_0 \ll g$ (f_0 is the Fermi-Dirac distribution) and that

$$\left.\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right|_{\text{Scattering}} = -\frac{g(\vec{k})}{\tau(\vec{k})}$$

a) We search for stationary solutions. Rewrite the Boltzmann equation (remember, no external fields are applied).

b) To evaluate this, we'll assume that at each point $\vec{r}$ of the sample local thermal equilibrium is achieved so that we can write: $\frac{\partial f}{\partial \vec{r}} \sim \frac{\partial f_0}{\partial \vec{r}}$. Show that $\frac{\partial f_0}{\partial T} = -\frac{\partial f_0}{\partial E_n}\left(\frac{E_n(\vec{k})-\mu}{T}\right)$ and $\frac{\partial f_0}{\partial \mu} = -\frac{\partial f_0}{\partial E_n}$, and that one can then write

$$g(\vec{k}) = \tau(\vec{k})\vec{v}_n(\vec{k})\frac{\partial f_0}{\partial E_n}\left\{\frac{\partial \mu}{\partial T} + \frac{E_n(\vec{k})-\mu}{T}\right\}\nabla T$$

c) Using the Sommerfeld expansion, one can show that $\mu(T) = E_F\left(1 - \frac{\pi^2}{12}\left(\frac{T}{T_F}\right)^2\right)$. Why can then the term $\frac{\partial \mu}{\partial T}$ be neglected in the previous expression in normal conditions to measure the thermal conductivity of a metal? Show that this yields:

$$\kappa = \int \frac{d\vec{k}}{4\pi^3}\frac{[E_n(\vec{k})-\mu]^2}{T}\vec{v}_n^2(\vec{k})\tau(\vec{k})\frac{\partial f_0}{\partial E_n}$$

d) For the calculation of the electrical conductivity, we saw in class a useful way to perform such integral using constant energy surfaces. Use the same trick to show that κ can simply be rewritten as:

$$\kappa = \frac{1}{Te^2} \int dE_n \left(\frac{\partial f_0}{\partial E_n} \right) \sigma(E_n)[E_n - \mu]^2$$

e) Use the Sommerfeld expansion $\int dE \left(-\frac{\partial f_0}{\partial E}\right) G(E) \sim G(E_F) + \frac{\pi^2}{6}(k_B T)^2 \frac{\partial^2 G}{\partial E^2}\Big|_{E=E_F}$ to explicit κ and retrieve Wiedemann-Franz law. Estimate the Lorentz number.

f) Based on this, we can estimate the Seebeck S thermoelectric coefficient that quantifies the electrical current induced by a thermal gradient. It can be defined as follows: $\mathbf{J_q} = \sigma \mathbf{E} - S\sigma \nabla T$. Show that S can be written as

$$S = \frac{\pi^2 k_B^2 T}{3q} \frac{\partial \ln \sigma}{\partial E_n}\Big|_{E=E_F}.$$

g) It can be useful to introduce generalized transport coefficients that relates electrical and heat transport:

$$J_q = L_{11}\mathbf{E} + L_{12}\left(\frac{-\nabla T}{T}\right)$$

$$J_H = L_{21}\mathbf{E} + L_{22}\left(\frac{-\nabla T}{T}\right)$$

Express the L_{xx} coefficients as function of S,σ and T.

3. Hall-Effect

In order to find the Hall coefficient in the context of the Boltzmann equation, one may proceed in the following way:
Begin with the Boltzmann equation and reduce it first. Now guess a solution of the form $g = ak_x + bk_y$. Assume $\vec{B} = (0, 0, B)$ and $\vec{E} = (E_x, E_y, 0)$.

a) Determine a and b.

b) Compute currents along x and y and find the total conductivity tensor. Express the resistivity sensor in terms of the Hall coefficient R.

c) How does the result changes in the case of $\vec{E}$ assumed to be parallel to $\vec{B}$?

4. Tight-Binding Band

Consider a two-dimensional metal with a square lattice of lattice spacing a. The conduction band is described by the tight-binding approximation,

$$E = E_0 + E_1\,(2 - \cos k_x a - cos k_y a)$$

and the relaxation time τ is independent of the electron momentum or energy. The band is half-filled and the resulting Fermi line is shown in Figure 1.

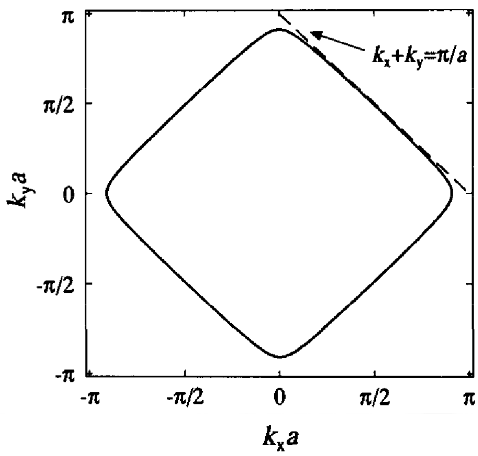

Figure 1: Fermi line for a two-dimensional tight-binding model with nearly half-filled band

a) Using the solution of the Boltzmann equation, calculate the conductivity tensor. (Hint: Use $\vec{v_n}(\vec{k}) = \frac{1}{\hbar}\frac{\partial E(\vec{k})}{\partial \vec{k}}$ an integral only depending in the velocity.)

b) Compare the result of a) to the conductivity from the Drude model. Use the same electron density and relaxation time. What is the relevant effective mass?