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Fachbereich Physik

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Einführung in die Theoretische Festkörperphysik

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Exercise 9

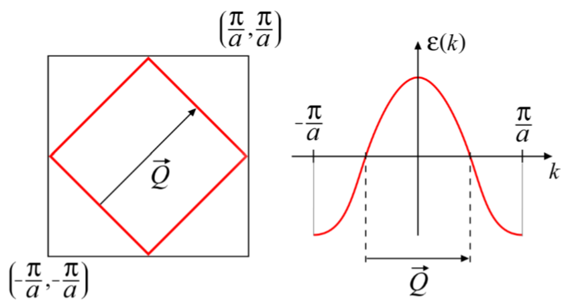
(Due date: 13.01.2020)

Problem 1 (**Fermi Surface Nesting**) (5 points)

Fermi surface nesting describes the situation in which a part of the Fermi surface can be translated in k-space to another part of the Fermi surface by a single vector $\vec{Q}$,

$$\varepsilon_F(\vec{k}) = \varepsilon_F(\vec{k}+\vec{Q}). \tag{1}$$

This can lead to instability of the system to magnetic order; e.g. the nesting vector $\vec{Q} = (\pi/a, \pi/a)$ favors in two dimensions an antiferromagnetic order of the magnetic moments (Néel state).



The tight-binding cubic lattice models with nearest-neighbor hopping matrix elements t

$$\varepsilon(\vec{k}) = \varepsilon_0 + 2t\sum_{i=1}^{d}\cos(k_i a)$$

have nested Fermi surfaces in any dimension d (see the figure for 1D and 2D examples) when the band is half filled. The Fermi surface nesting is generally not preserved when the electron hopping between the second-nearest neighbors t' is added. In the special case of the 1D model, the Fermi surface would remain nested until the hopping amplitude reaches some critical value $(t'/t)^{(c)}$. Above this critical value it is, in one dimension, not possible to find a single vector which transforms the Fermi surface to itself.

(a) Write down the tight-binding dispersion relation for a 1D model with both the nearest-neighbor and the second nearest-neighbor hopping matrix elements.

(b) Determine the critical value $(t'/t)^{(c)}$ for half-filling.
(*Hint:* First, plot the dispersion relation for different relations of the hopping parameters. Second, think about the position of the Fermi energy in each case with the help of the equation for the number of electrons per band $N_e = \frac{1}{N}\sum_{\sigma\vec{k}}\Theta(E_F - \varepsilon(\vec{k}))$.

Problem 2 (**Sommerfeld Expansion**) (5 points)

The density of states of free electrons in two dimensions is a constant:

$$\rho(E) = \frac{V}{N}\frac{m}{\pi\hbar^2} \tag{2}$$

a) Show that in 2-d all temperature-dependent terms in the Sommerfeld expansion for the particle number (respectively density) vanish. Deduce that $\mu = E_F$ at any temperature.

b) We want to find the relation between chemical potential and Fermi energy using a different approach. Calculate the electron number from the density of states without the Sommerfeld expansion and show that:

$$\mu + k_B T \ln(1 + e^{-\mu/k_B T}) = E_F \tag{3}$$

What does that mean for the Sommerfeld expansion in two dimensions? *Hint:* The following integral could be useful:

$$\int \mathrm{d}x \frac{1}{\mathrm{e}^x + 1} = x = \ln(\mathrm{e}^x + 1) \tag{4}$$

Problem 3 (**Effective Mass**) (5 points)

Consider a band with two-dimensional tight-binding dispersion,

$$E(\mathbf{k}) = E_0 - 2t_1 \cos(k_x a) - 2t_1 \cos(k_y a) \tag{5}$$

Calculate the effective mass of the electrons for the cases:

a) The band is nearly empty.

b) The band is nearly full.

Interpret your results.

Frohe Festtage und einen guten Rutsch ins neue Jahr!