Universität Zürich[UZH]

Solid State Physics
Solution Sheet 12

FS17
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Discussion on 24th May

Due on 24th May

Exercise 1 *Tight binding model*

In the lecture, we derived the tight-binding expression for a two-dimensional square lattice:

$$\epsilon_k = -\epsilon_0 - 2t[\cos(k_x a) + \cos(k_y a)] \tag{1}$$

(a) Plot, using your favourite computer program, (1) the full three-dimensional band structure ϵ_k versus k_x and k_y as a surface-plot, (2) the band structure along the zone diagonal $k_x = k_y$, and (3) the Fermi surface ($\epsilon_k = \epsilon_\mathrm{F}$) for systems with $\mu = \epsilon_\mathrm{F}$ (metals), having the values $\epsilon_\mathrm{F} = -\epsilon_0$ and $\epsilon_\mathrm{F} = -\epsilon_0 \pm 2t$.

[Hint: Set $t = 1$ meaning that ϵ_k is plotted in units of t, set $\epsilon_0 = 0$, plot k_x, k_y in units of π/a]

Solution:

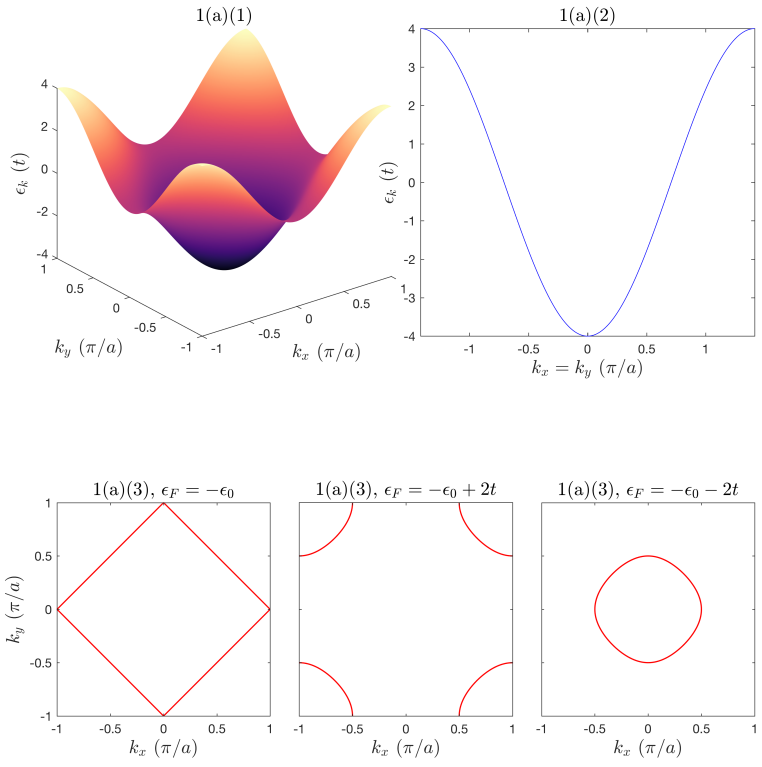

Figure 1: Solution 1(a)

(b) In the lecture, we developed the tight binding only to first order. Let's include second order terms. We define t' as the integral over next-nearest neighbours that are given by $\vec{\rho}_m = (\pm a, \pm a)$

and $(\pm a, \mp a)$. Show that the tight-binding dispersion becomes:

$$\epsilon_k = -\epsilon_0 - 2t[\cos(k_x a) + \cos(k_y a)] - 4t'[\cos(k_x a)\cos(k_y a)] \tag{2}$$

Solution:

$$\begin{aligned}\sum_m \exp(-i\vec{k}\vec{\rho}_m) &= e^{-i(k_x a + k_y a)} + e^{+i(k_x a + k_y a)} + e^{-i(k_x a - k_y a)} + e^{+i(k_x a - k_y a)} \\ &= 2[\cos(k_x a + k_y a) + \cos(k_x a - k_y a)] \\ &= 4\cos(k_x a)\cos(k_y a) \implies \text{eq. (2)}\end{aligned}$$

(c) Let's say that $\mu = -\epsilon_0 - 0.87t$. Compare the Fermi surfaces for $t' = 0$ and $t' = -0.2t$.

Solution:

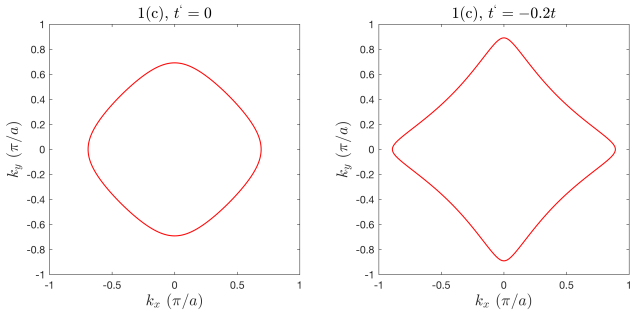

Figure 2: Solution 1(c)

(d) Figure 3 displays a Fermi surface of a two-dimensional electron gas (2DEG) produced by depositing potassium on an insulating substrate (Ca_2RuO_4). Extract the Fermi momentum k_F.

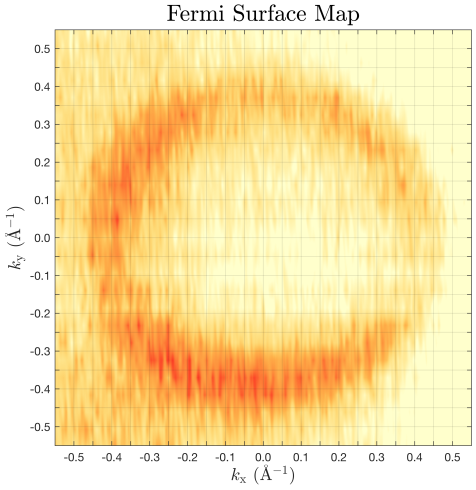

Figure 3: Fermi surface of a 2DEG on Ca_2RuO_4. Dark colours correspond to high intensities.

(e) Show that in two dimensions, the electron density is given by $n = k_F^2/(2\pi)$. Compare this with the results for three-dimensions.

Solution:
Analogous to three dimensional case, where the Fermi-circle has an area of $k_\mathrm{F}^2\pi$ and one allowed wavevector for the area element $(2\pi/L)^2$ in reciprocal space, the total number of orbitals are (incl. factor 2 for spin-degeneracy):

$$N = 2 \cdot \frac{k_\mathrm{F}^2 \pi}{(2\pi/L)^2} = \frac{k_\mathrm{F}^2 A}{2\pi} \tag{3}$$

and thus the electron density $n = N/A = k_\mathrm{F}^2/(2\pi)$

(f) The lattice constant is $a = 3.89\,\text{Å}$. What is the area of the Fermi surface? What is the Brillouin zone area and what is the ratio between the two? How does it relate to the electron density?

Solution:
The electron density is directly related through:

$$n = (2A_\mathrm{FS}/A_\mathrm{BZ})/a^2 \approx 0.03\,\text{Å}^{-2} \tag{4}$$

(g) Calculate the electronic density of state in two-dimensions. Show that it is independent of ϵ_k. Compare with the three-dimensional result.

Solution:
With the result from e) and $\epsilon_k = \frac{\hbar^2 k^2}{2m^*}$ the density of states is:

$$\mathcal{D}_{2D} = \frac{\mathrm{d}N}{\mathrm{d}\epsilon_k} = \frac{m^* A}{\pi\hbar^2}, \tag{5}$$

independent of ϵ_k, compared to $\mathcal{D}_{3D} \propto \epsilon_k^{1/2}$.