



Discussion on 24<sup>th</sup> May

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### Exercise 1 *Tight binding model*

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

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

(a) Plot, using your favourite computer program, (1) the full three-dimensional band structure  $\epsilon_k$  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 ( $\epsilon_k = \epsilon_F$ ) for systems with  $\mu = \epsilon_F$  (metals), having the values  $\epsilon_F = -\epsilon_0$  and  $\epsilon_F = -\epsilon_0 \pm 2t$ .

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

(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:

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

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

(d) Figure 1 displays a Fermi surface of a two-dimensional electron gas (2DEG) produced by depositing potassium on an insulating substrate ( $\text{Ca}_2\text{RuO}_4$ ). Extract the Fermi momentum  $k_F$ .

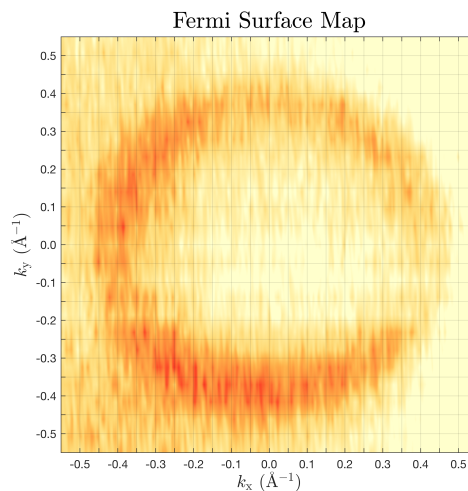


Figure 1: Fermi surface of a 2DEG on  $\text{Ca}_2\text{RuO}_4$ . Dark colours correspond to high intensities.

(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.

(f) The lattice constant is  $a = 3.89 \text{ \AA}$ . 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?

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