Quantum Theory of Condensed Matter

Prof. Milena Grifoni Room H33
Dr. Andrea Donarini Wednesdays at 13:15

Sheet 6

1. Fermi surface in 2D: square lattice

Consider a two-dimensional square crystal, with the ions at coordinates $\vec{R} = n\vec{a}_1 + m\vec{a}_2$, where $a = |\vec{a}_1| = |\vec{a}_2|$ is the lattice constant, and n and m are integers. The Hamiltonian for (non-interacting) valence electrons on this lattice, in the Wannier basis and in the limit of next nearest neighbours:

$$H = -t \sum_{\langle ij \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} - t' \sum_{[ij], \sigma} c^\dagger_{i\sigma} c_{j\sigma}$$

where $\langle ij \rangle$ indicates nearest neighbours, and $[ij]$ denotes next nearest neighbours.

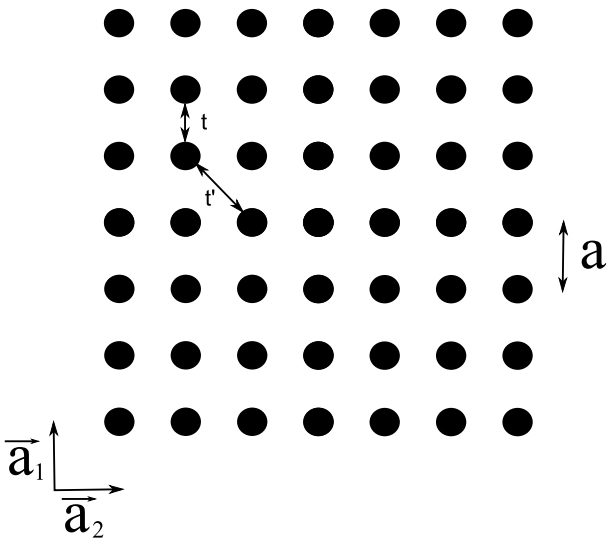

Fig.1

1. Which is the first Brillouin zone of the system? Calculate the band structure for the Hamiltonian. How many bands do you find?
2. Prove that in the case $t' = 0$ the Fermi energy is zero for a density of (valence) electrons corresponding to one electron per ion. Calculate analytically the form of the Fermi surface for this case.
3. Calculate the Fermi surface for very low electron density: namely for Fermi energies $\epsilon_F = -4(t + t') + \delta$ with $\delta/t \ll 1$.
4. Sketch the Fermi surface in the following 3 cases (you can use *e.g.* Maple)
   - $t' = 0$, $\epsilon_F = 0$, (just a check of the analytics!)
   - $t' = 0$, $\epsilon_F = -0.2t$
   - $t' = 0.1t$, $\epsilon_F = -0.2t$

2. Biatomic square lattice

Consider now the model described by the following Hamiltonian:

$$H = \sum_{i \in W,\sigma} \epsilon_W c^\dagger_{i\sigma} c_{i\sigma} + \sum_{i \in B,\sigma} \epsilon_B c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ij \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma}$$

where W and B represent respectively the "white" and "black" sublattices and the hopping part of the tight binding matrix concerns this time only nearest neighbours (as indicated in the Fig.2).

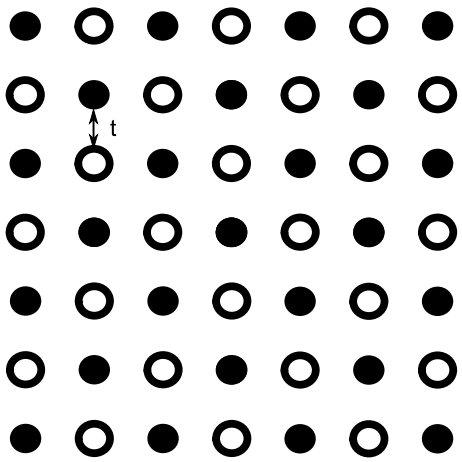

Fig.2

1. How many atoms are there in the unit cell? Draw the first Brillouin zone for the system.
2. Write the tight binding equations for this system and by solving them find the band structure. How many bands do you obtain?
3. Consider the system with the valence electron density corresponding to one electron per ion: is it a metal, a semiconductor or an insulator? Why?
4. In the case of identical atoms $\epsilon_W = \epsilon_B$ the model studied in this exercise reduces to the one of exercise 1 in the limit $t' = 0$. Prove that the band structures calculated in the two exercises coincide.

   Hint: Concentrate on how the different Brillouin zones map into each other.

Frohes Schaffen!