Quantum theory of condensed matter I

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Thu 10:00 - 12:00 H33
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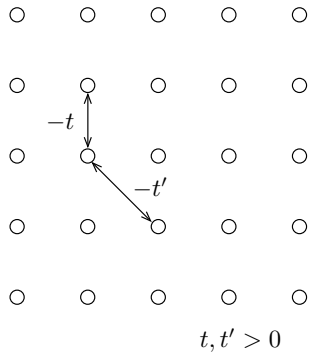
Sheet 3

1. Band structure and Fermi surface of a 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.



1. What is the Brillouin zone of the system? **(1 Point)**

Let us assume one atomic orbital ν per atom. The tight-binding Hamiltonian in the $|\nu\vec{R}\rangle$ basis can be written as

$$\hat{h} = \epsilon_\nu \sum_{\vec{R}} |\nu\vec{R}\rangle\langle\nu\vec{R}| - t \sum_{\substack{\vec{R}\vec{R}' \\ \text{nearest} \\ \text{neighbours}}} |\nu\vec{R}\rangle\langle\nu\vec{R}'| - t' \sum_{\substack{\vec{R}\vec{R}' \\ \text{next nearest} \\ \text{neighbours}}} |\nu\vec{R}\rangle\,\langle\nu\vec{R}'|,$$

or, in other words, $\gamma(\vec{a}_i) = -t$ and $\gamma(\pm(\vec{a}_1 \pm \vec{a}_2)) = -t'$.

2. Calculate the band structure for this Hamiltonian, assuming $t' = 0$ (use the LCAO secular approximation). How many bands do you find? **(2 Points)**
3. Assume $t' \neq 0$. How is the band structure modified with respect to the case from 1.2 ? **(1 Point)**

At zero temperature, electrons fill all available states below certain energy called Fermi energy E_F. The Fermi energy is thus determined by the band structure and by the density of electrons. The collection of all k such that $\epsilon(k) = E_F$ is called the Fermi surface. Naturally, the Fermi surface has $d-1$ dimensions in a d-dimensional crystal.

4. Prove that in the case of $t' = 0$ the Fermi energy is zero for a density of (valence) electrons corresponding to one electron per atom. Calculate analytically the form of the Fermi surface for this case. Take into account that the atomic levels (and thus also the Bloch states) are doubly spin-degenerate. **(2 Points)**

5. Calculate the Fermi surface for very low electron density: namely for Fermi energies $\epsilon_F = -4(t + t') + \delta$, with $\delta \ll t$. **(2 Points)**

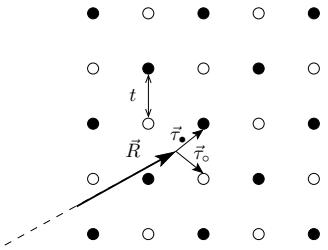
6. Sketch the Fermi surface in the following 3 cases (you can use e.g. Maple, Mathematica, Matlab...)

   - $t' = 0$, $\epsilon_F = 0$ (just a check of the analytics!)
   - $t' = 0$, $\epsilon_F = -0.2t$
   - $t' = 0.1t$, $\epsilon_F = -0.2t$

   (2 Points)

2. Diatomic square lattice (Oral)

Consider now a crystal shown below, with two atoms in a unit cell ($\bullet$ and $\circ$), and one orbital ν per atom.



1. Draw the first Brillouin zone for the system.

2. Write down the tight-binding Hamiltonian in the LCAO basis $\{|\nu_{\bullet/\circ}\vec{R}\rangle\}$, where $\varphi_{\nu(\bullet/\circ)}(\vec{r} - \vec{R} - \vec{\tau}_{\bullet/\circ}) := \langle\vec{r}|\nu_{\bullet/\circ}\vec{R}\rangle$, assuming that only overlap integrals between nearest neighbours are not zero. Calculate the band structure for this Hamiltonian (use the LCAO secular approximation).
   How many bands do you find?

3. Consider the system with the valence electron density corresponding to one electron per ion: is it a metal, a semiconductor, or an insulator?
   Explain why.

4. In the case of identical atoms, where the on-site energies are equal ($\epsilon_{\nu\bullet} = \epsilon_{\nu\circ}$), the model studied here reduces to the one in Problem 1.2 in the limit $t' = 0$. Prove that the band structures calculated in the two exercises coincide.
   Hint: How do the different Brillouin zones map into each other?

Frohes Schaffen!