University of Regensburg Summer Term 2014

Quantum Theory of Condensed Matter I

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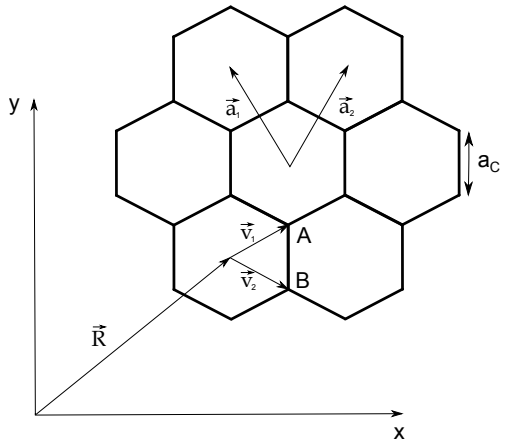
5.1.01 Mondays 10:15
9.2.01 Tuesdays 12:15

Sheet 4

1. Electronic structure of non-interacting graphene



A graphene sheet is a honeycomb lattice of carbon atoms, as shown above. Let the distance between carbon atoms be $a_C = 1.42$ Å. A good model for graphene is to consider a plane in which there is one valence electron per carbon atom. To calculate the electronic bands of the non-interacting problem we will use the LCAO method with a single p_z orbital at each carbon site. Let $\vec{R}$ denote the centers od the hexagons in the honeycomb: these form the underlying Bravais lattice. (Note that it is different from the graphene hexagonal lattice.) The unit cell spanned by $\vec{a}_1$ and $\vec{a}_2$ contains two carbon atoms conventionally labelled as A and B atoms, located at $\vec{R}+\vec{\tau}_A$, $\vec{R}+\vec{\tau}_B$ as shown in the figure. The tight-binding amplitude connecting these sites is denoted by $-t$. We can choose the zero of energy so that the energy of an isolated p_z orbital is zero. Then the entire Hamiltonian consists only of the nearest-neighbour hopping.

1. Find the reciprocal lattice and construct the first Brillouin zone. **(1 Point)**

2. Write the Hamiltonian in the basis of the extended states

$$\begin{aligned} \left|\phi_{A\vec{k}}\right\rangle &= \frac{1}{\sqrt{N_{cell}}}\sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \left|p_z, \vec{R}+\vec{\tau}_A\right\rangle \\ \left|\phi_{B\vec{k}}\right\rangle &= \frac{1}{\sqrt{N_{cell}}}\sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \left|p_z, \vec{R}+\vec{\tau}_B\right\rangle, \end{aligned}$$

where N_{cell} is the number of the unit cells of the crystal and $\left|p_z, \vec{S}\right\rangle$ is the state of the p_z orbital localized in the position $\vec{S}$. Hint: make use of the relation

$$\frac{1}{N_{cell}}\sum_{\vec{R}} \exp\left\{i(\vec{k}-\vec{k}')\cdot\vec{R}\right\} = \delta_{\vec{k}\vec{k}'},$$

where the sum is intended over the Bravais lattice and $\vec{k}$ and $\vec{k}'$ belong to the reciprocal lattice.
(2 Points)

3. The generic extended states of the graphene sheet have the form:
   $|\psi\rangle = \sum_{\vec{k}} c_{A\vec{k}}|\phi_{A\vec{k}}\rangle + c_{B\vec{k}}|\phi_{B\vec{k}}\rangle$, where $c_{A\vec{k}}$ and $c_{B\vec{k}}$ are complex numbers. Find the eigenstates of the system and the corresponding eigenvalues. How many bands do you find? What are the energy-wavevector relations? **(2 Points)**
   Hint: You will need to solve a 2×2 matrix eigenvalue problem - the time-independent Schrödinger equation written in the basis of extended states.

4. Show that the Fermi energy is equal to zero by verifying that this gives the correct electron density. Find the set of $\vec{k}$ points for which $\epsilon(\vec{k}) = 0$. Show that these correspond to the corners of the first Brillouin zone. **(2 Points)**

5. Plot the complete dispersion relation of graphene. **(1 Point)**

6. **(Oral)** Show that near to a (first) Brillouin zone corner with wavevector $\vec{K}$ (note that $\vec{K}$ is the location of a BZ corner, not a reciprocal lattice vector), the spectrum is approximately

$$\epsilon(\vec{k}) \approx \pm\hbar v\sqrt{(k_x - K_x)^2 + (k_y - K_y)^2}.$$

   Determine the velocity v in terms of t and a_C. This behaviour is intermediate between that of a metal (with a Fermi surface instead of Fermi points $\vec{K}$) and an insulator (with a band gap). Indeed, graphene behaves like a semi-metal, with poor conductivity yet significantly higher than in an insulator.

Frohes Schaffen!