University of Regensburg Summer Term 2010

Quantum Theory of Condensed Matter I

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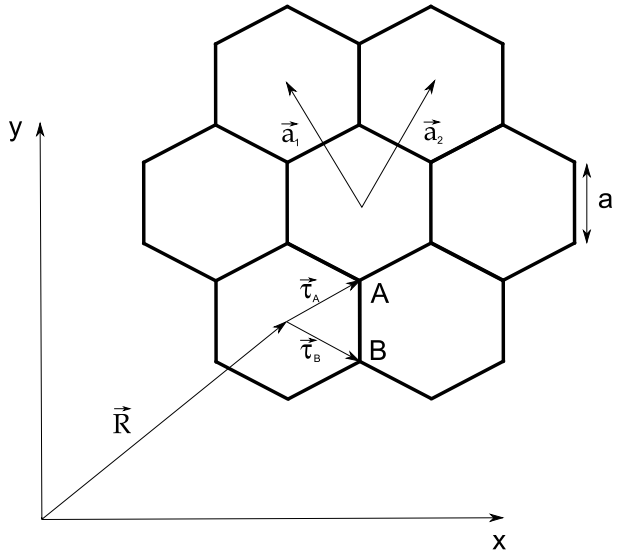
Sheet 10

1. Electronic structure of non interacting graphene

A graphene sheet is a honeycomb lattice of carbon atoms (see figure below). Let the distance between car-



bon atoms be $a = 1.42$Å.

1. Find the reciprocal lattice, and construct the first Brillouin zone.

(2 points)

2. 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 tight-binding approximation, in which this electron can occupy a single p_z orbital at each carbon site. Let $\vec{R}$ denote the centers of the hexagons in the honeycomb: these form the underlying hexagonal Bravais lattice. Please notice that the latter is indeed a Bravais lattice differently from the graphene honeycomb lattice. The unit cell spanned by $\vec{a}_1$ and $\vec{a}_2$ contains two carbon atoms conventionally labelled as A and B atom, located at $\vec{R} + \vec{\tau}_{\rm A}$, $\vec{R} + \vec{\tau}_{\rm B}$, as shown in the figure. Denote the tight-binding hopping amplitude connecting these sites by t. Choose the zero of energy so that the energy of the p_z isolated atomic orbital is zero. In the tight binding approximation only such matrix element is retained, so that in the p_z basis the entire Hamiltonian consists of the nearest-neighbour hopping. Write the Hamiltonian in second quantization in the basis of the (localized) p_z orbitals.

(2 points)

3. Write the Hamiltonian also in the basis of the extended states

$$|\phi_{A\vec{k}}\rangle = \frac{1}{\sqrt{N_{cel}}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} |p_z, \vec{R} + \vec{\tau}_A\rangle$$

$$|\phi_{B\vec{k}}\rangle = \frac{1}{\sqrt{N_{cel}}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} |p_z, \vec{R} + \vec{\tau}_B\rangle$$

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

$$\frac{1}{N_{cel}} \sum_{\vec{R}} \exp[-\mathrm{i}(\vec{k} - \vec{k}') \cdot \vec{R}] = \delta_{\vec{k}\vec{k}'} \,,$$

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

(2 points)

4. The generic extended state 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. Look for the eigenstates of the system and find also the corresponding eigenvalues. How many bands do you find? What are the energy-wavevector relations?

   Hint: You will need to solve a two-by-two matrix eigenvalue problem: Namely the time independent Schödinger equation written in the basis of extended states .

   (2 points)

5. 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 $\varepsilon(\vec{k}) = 0$. Show that these correspond to the corners of the first Brillouin zone.

   (2 points)

6. (Optional) 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

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

   Determine the velocity v in terms of t and a. This behavior 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 as a semi-metal, with poor conductivity yet significantly higher than in an insulator.

Frohes Schaffen!