University of Regensburg Summer Semester 2009

Quantum Theory of Condensed Matter

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Mo 10:15, 5.0.21
We 16:15, H33

Sheet 3

1. Dirac comb potential

Consider an electron confined to one-dimension and under the influence of the periodic potential given by the expression

$$V(x) = \lambda \sum_{n\in\mathbb{Z}} \delta(x - nL). \tag{1}$$

Calculate, step by step, the energy bands for such a periodic potential. Namely:

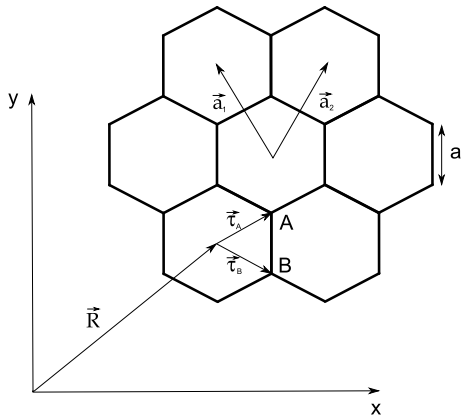
a) Solve the Schrödinger equation in the interval $(0, L)$.

b) Impose that the solution on the full x-axis with the periodic potential (**??**) is of the Bloch form (*i.e.* $\psi(x) = e^{ikx}u(x)$ where $u(x)$ is a periodic function with the same period of the potential), continuous and with a discontinuity in the first derivative proportional to the strength of the delta function in the points $x = nL$.

c) Prove that the conditions above can be fulfilled only by planewaves with specific values of the momentum. The corresposnding energies are the bands for the model.

2. 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.

a) Find the reciprocal lattice, and construct the first Brillouin zone.

b) 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.

c) Write the Hamiltonian also in the basis of the extended states

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

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

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

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

d) 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 .

e) 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.

f) (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 significantly higher than in an insulator.

Frohes Schaffen!