Fakultät für Physik
Prof. Christian Back, Prof. Milena Grifoni

WS 12/13

Übungen zu Integrierter Kurs II - Festkörper und Statistische Physik

Blatt 10

Übungsleiter:

Dr. Andrea Donarini (3.1.24, phone 2040) (theory, Tue 12h-14h c.t., Phy 7.3.14)
Sebastian Putz (4.1.36, phone 2032) (experiment, Thu 10h-12h c.t., Phy 7.3.14)

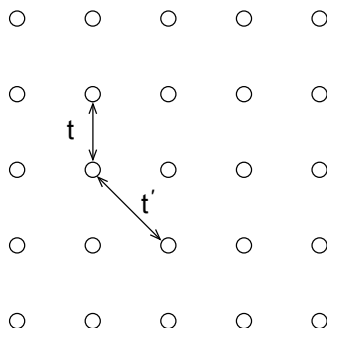
Part I: Theory

10.1 Fermi surface in 2D: square lattice

Consider a two-dimensional square crystal (see figure below), 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. Let us assume one atomic orbital per atom. The Hamilton operator in Wannier basis is given by

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

where for both tunnelling amplitudes $t, t' < 0$.



1. What is the first Brillouin zone of the system? Calculate the band structure for this Hamiltonian (use the secular equation). How many bands do you find? (2 points)

2. Prove that in the case $t' = 0$ 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. (2 points)

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

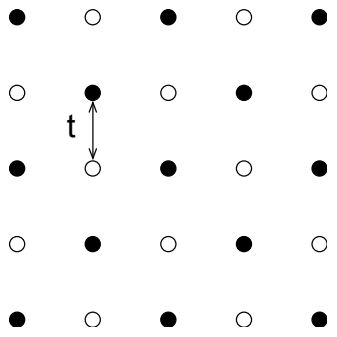
4. Sketch the Fermi surface in the following 3 cases (you can use e.g. Maple, Mathematica, Matlab...) i) $t' = 0$, $\epsilon_F = 0$ (just a check of the analytics!), ii) $t' = 0$, $\epsilon_F = 0.2t$, iii) $t' = 0.1t$, $\epsilon_F = -0.2t$. (2 points)

10.2 Diatomic square lattice

Consider now the crystal shown below, with the following Hamiltonian:

$$\hat{h} = \sum_{\vec{R}_\bullet} \epsilon_\bullet |\vec{R}_\bullet\rangle \langle \vec{R}_\bullet| + \sum_{\vec{R}_\circ} \epsilon_\circ |\vec{R}_\circ\rangle \langle \vec{R}_\circ| - t \sum_{\substack{\vec{R}\vec{R}' \\ \text{nearest} \\ \text{neighbours}}} |\vec{R}\rangle \langle \vec{R}'|,$$

where the $\bullet$ and $\circ$ are the indices denoting the two sublattices.



1. How many atoms are there in the unit cell? Draw the first Brillouin zone for the system. (1 point)

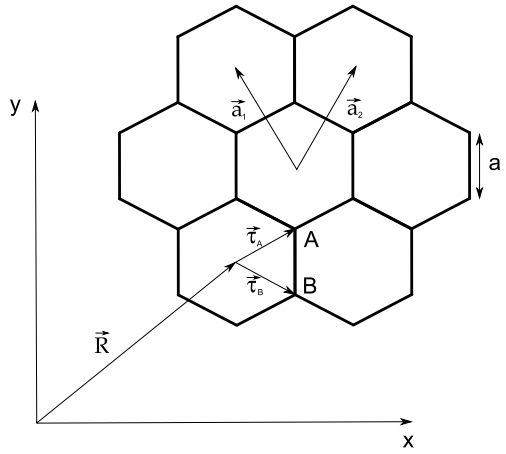
2. Write the secular equation for this system and by solving it find the band structure. How many bands do you find? (2 points)

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? (2 points)

4. In the case of identical atoms $\epsilon_\bullet = \epsilon_\circ$ the model studied here reduces to the one in Problem 10.1 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. (2 points)

10.3 Electronic structure of non-interacting graphene

A graphene sheet is a honeycomb lattice of carbon atoms, as shown on the right. Let the distance between carbon atoms be $a = 1.42$ 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. 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 2×2 matrix eigenvalue problem - the time-independent Schrödinger equation written in the basis of extended states. (2 points)

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. 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. 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. (2 points)

Part II: Experiment

10.4 Periodische Randbedingungen für ebenes quadratisches Gitter

Betrachten Sie ein endliches ebenes quadratisches Gitter mit der Gitterkonstanten a, bestehend aus $N = 6 \cdot 6 = 36$ Atomen.

1. Was sind, unter Annahme von periodischen Randbedingungen, die erlaubten Werte für die Wellenvektoren $\vec{k} = (k_x, k_y)$ von Phononen? Zeichnen Sie die erlaubten Werte in der k_x-k_y-Ebene. (1 Punkt)

2. Tragen Sie in der Zeichnung die Grenze der ersten Brillouinzone ein – unter der Annahme von periodischen Randbedingungen. Wie ändert sich die Grenze der Brillouinzone, wenn das Gitter aus 100 Atomen mit gleicher Gitterkonstanten a besteht? (1 Punkt)

10.5 Singularität in der Zustandsdichte für Phononen

Die Dispersionsrelation einer linearen Kette mit ausschlielicher nächster-Nachbar Wechselwirkung lautet

$$\omega(k) = \sqrt{\frac{4C_1}{M}} |\sin(\frac{ka}{2})|,$$

wobei M die Massen der Atome sind und C_1 die relevante Federkonstante. Verwenden Sie periodische Randbedingungen für eine endliche Kette der Länge $L = N \cdot a$ mit $N \gg 1$ Atomen und zeigen Sie, dass die Zustandsdichte $D(\omega)$ der akustischen Phononen eine Singularität bei der Maximalfrequenz der Phononen hat. (2 Punkte)

10.6 Unstetigkeit in der Zustandsdichte optischer Phononen

Angenommen, ein optischer Phononenast habe im Dreidimensionalen nahe $k = 0$ die Form $\omega(k) = \omega_0 - Ak^2$. Berechnen Sie für $\omega < \omega_0$ die Zustandsdichte $D(\omega)$ und zeigen Sie, dass $D(\omega)$ bei $\omega = \omega_0$ unstetig ist. (2 Punkte)