Assignments to Condensed Matter Theory I
Sheet 7

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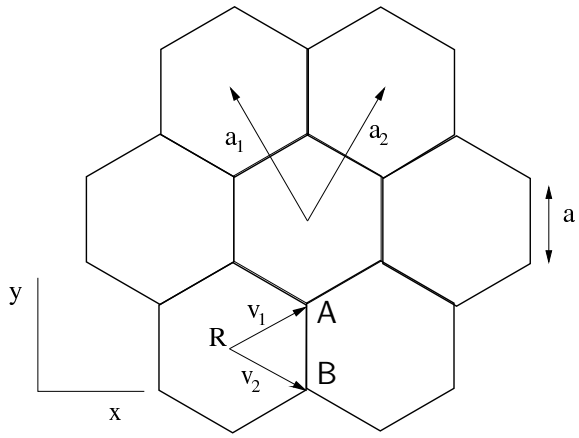
sheet online: `http://www-MCG.uni-R.de/teaching/`

Problem set: Band structure: graphene and carbon nanotubes

7.1. Electronic structure of graphene

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



between carbon atoms be a. A good model for graphene is to consider a single plane in which there is one valence electron per carbon atom. We will use the tight-binding approximation, in which this electron can occupy a single p_z orbital at each carbon site. Let $\mathbf{R}$ 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 $\mathbf{a}_1$ and $\mathbf{a}_2$ contains two carbon atoms conventionally labelled as A and B atom, located at $\mathbf{R}+\mathbf{v}_\mathrm{A}$, $\mathbf{R}+\mathbf{v}_\mathrm{B}$, 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 an isolated atomic orbital is zero. The entire Hamiltonian consists of the nearest-neighbor hopping.

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

(b) Write down the tight-binding equations governing the system. 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. This exercise was first attacked by Wallace in 1947.[1]

[1] You might want to read the original paper "P. R. Wallace, Phys. Rev. **71**, 622 (1947)". It is available online (when logged in the `uni-r.de` domain) under `http://link.aps.org/abstract/PR/v71/p622` . Alternatively you can refer to some more recent formulation as, e.g., in Section 2.4 "Band structure of graphene" of Dr. Hauptmann's PhD thesis (`http://www.nbi.dk/~nygard/JonasSpeciale2003.pdf`).

(c) Show that the Fermi energy is equal to zero, by verifying that this gives the correct electron density. Find the set of $\mathbf{k}$ points for which $\varepsilon(\mathbf{k}) = 0$. Show that these correspond to the corners of the first Brillouin zone.

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

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

Determine the velocity v in terms of t and a. This behavior is intermediate between a metal (with a Fermi surface instead of points $\mathbf{K}$) and an insulator (with a band gap). Indeed, graphite behaves as a semi-metal, with poor conductivity significantly higher than in an insulator.

(e) **[Kür]** Graphite is composed of a stack of graphene layers identically atop one another in the z direction (a distance d apart), and there is some small residual hopping $t_\perp$ between orbitals in neighboring layers at the same (x, y) position. Sketch the Fermi surface, assuming $t_\perp \ll t$.

7.2. Electronic structure of single wall carbon nanotubes

Carbon nanotubes Carbon nanotubes are made up of a section of the graphene lattice that has been wrapped up into a cylinder. You can specify the way the lattice is wound up by identifying the winding vector $\mathbf{W}$. The winding vector must be a Bravais lattice vector, and so can be specified by two integers:

$$\mathbf{W} = n\,\mathbf{a}_1 + m\,\mathbf{a}_2,$$

where n and m are integers. To construct a nanotube, take a graphene lattice and mark one atom (either A type or B type) as the origin. Shift the origin of the vector $\mathbf{W}$ on the chosen atom. The new vector $\tilde{\mathbf{W}}$ will point to another atom of the same type. Roll up the sheet perpendicular to $\tilde{\mathbf{W}}$ so that the second atom sits exactly on top of the first. You have constructed a (n, m) nanotube!
A bit of nomenclature. We can specify some special tubes said *achiral*: they are (n, n) tubes which are called *armchair* tubes, and $(n, 0)$ *zig-zag* tubes (Bruckmandl would be probably more appropriate, but there is no mention of this in the literature yet...). All other tubes are said *chiral*.

(a) Build a $(5, 5)$ armchair tube (*i.e.* with scissors and adhesive tape!) by making use of the provided transparencies.[2]

(b) Construct a $(8, 0)$ zig-zag tube.

(c) Build a chiral $(7, 3)$ tube.

[2] A pdf is also available under the following (clickable) link
http://www-MCG.uni-R.de/downloads/graphene.pdf .

(d) Let's determine the band structure of a nanotube. To do so, impose periodic boundary conditions on the wavefunction in the direction around the cylinder. Show that this means that $\mathbf{k} \cdot \mathbf{W} = 2\pi\ell$, where ℓ is an integer.

(e) Draw the graphene first Brillouin zone from the previous problem, indicating (a) the points $\mathbf{K}$ (where the energy of the graphene layer is zero, $E = E_{\mathrm{F}}$) and (b) the lines given by the quantization conditions –introduced in the previous point– for $(n, m) = (3, 3)$ and $(n, m) = (2, 0)$.

(f) Plot the energy versus k_x for the allowed values of k_y in the (3,3) tube above. Then plot the energy versus versus k_y for the allowed values of k_x in the $(2, 0)$ tube.
For each case, is the nanotube metallic or insulating according to band theory?

(g) For which n and m are the Brillouin zone corners allowed wavevectors for a nanotube? Show that the tubes satisfying this condition are metallic!

(h) **[Kür]** In reality, one expects that the curvature of the nanotube cylinder affects the tight-binding matrix elements slightly. Consider this effect for the special cases of armchair, and zig-zag tubes. In these cases, the curvature effect can be modeled by making the hopping matrix element slightly different ($= t'$) on transversal bonds (parallel to the winding vector in the case of the armchair tubes) than the other ones ($= t$). How does this affect the metallicity of the armchair and zig-zag tubes?