Department of physics, NTNU
TFY4340 Mesoscopic Physics
Spring 2010

Exercise 2

Assistance: Tuesday February 2.

Question 1

Find the nearest–neighbour tight–binding band structure $E(\boldsymbol{k})$ for the 2D triangular lattice (nearest neighbour distance a). Assume one atomic orbital pr atom and choose the energy of this orbital so that $E(\boldsymbol{k}=0)=0$. Overlap integrals are $\delta_{\boldsymbol{R},0}$ and transfer integrals are γ for (the six) nearest neighbours. Plot $E(\boldsymbol{k})$ along lines from the Γ–point to the edge(s) and corner(s) of the (hexagonal) 1BZ, the socalled M– and K–point(s), respectively. What is the band width in this model? Hint: Remember that the reciprocal lattice $(\boldsymbol{b}_1, \boldsymbol{b}_2)$ can be constructed from $\boldsymbol{b}_i \cdot \boldsymbol{a}_j = 2\pi\delta_{ij}$, see Exercise 1. Use Matlab, gnuplot, or any other favorite program for plotting.

Question 2

A similar approach as in the previous question, to the hexagonal graphene lattice, yields the *two* bands

$$E^{\pm}(\boldsymbol{k}) = E_0 \mp \gamma\sqrt{1 + 4\cos\frac{3k_x a}{2}\cos\frac{\sqrt{3}k_y a}{2} + 4\cos^2\frac{\sqrt{3}k_y a}{2}}$$

$(\gamma < 0)$, due to the two–atomic primitive unit cell. (Carbon atoms at the origin and in $a\hat{x}$; primitive lattice vectors $\boldsymbol{a}_1 = (3a/2)\hat{x} - (\sqrt{3}a/2)\hat{y}$ and $\boldsymbol{a}_2 = (3a/2)\hat{x} + (\sqrt{3}a/2)\hat{y}$). Show that the valence band E^- and the conduction band E^+ touch at the K–point(s) (i.e. the corners of the 1BZ), hence, the band gap is $E_g = 0$. Investigate the band structure more closely by playing around with your favorite software for 2D and 3D plotting.