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Physics 731 HOMEWORK ASSIGNMENT #8 Due: Thursday, Nov. 2, 2006
Deadline: Tuesday, Nov. 7

Read about tight-binding: A&M chapters 10, F&J (correct initials for D&G): 2.2.4; also read the Schönenberger tutorial on graphene and nanotube bandstructure available on the class webpage of web resources.

Problems to turn in (read the rest):

1. 10–1, parts a-i, a-iv, and c.
2. Consider a single-band tight-binding model for a square lattice of side a. Neglect overlap. Then $\varepsilon(\mathbf{k}) = \varepsilon_s - \beta - 2\gamma\,[\cos(k_x a) + \cos(k_y a)]$.

   a) i) Find the equivalent of Eq. (10.24) for small $|\mathbf{k}|a$.

   ii) If one writes this as a free-electron dispersion relation, what is the "mass"?

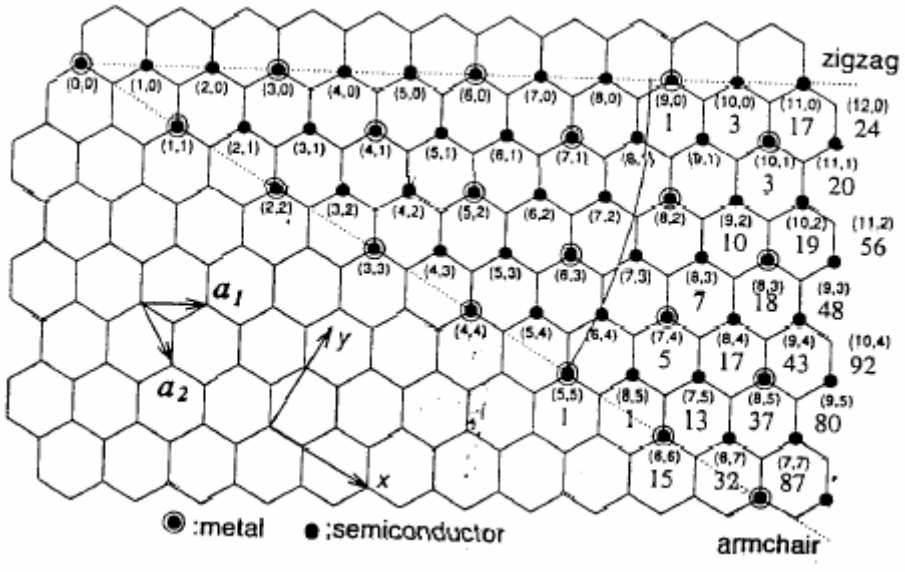
   b) Note that the constant-energy "surfaces" (i.e. curves in 2D) are not circular for larger values of $|\mathbf{k}|a$. In which directions is the curve elongated? Specifically, find the ratio of $|\mathbf{k}|$ in the {11} directions to $|\mathbf{k}|$ in the {10} directions on a curve with

   i) $\varepsilon(\mathbf{k}) - \varepsilon_s + \beta = -3\gamma/2$ ii) $\varepsilon(\mathbf{k}) - \varepsilon_s + \beta = -\gamma$ iii) $\varepsilon(\mathbf{k}) - \varepsilon_s + \beta = -\gamma/2$

   c) Find the shape of the constant-energy curve for $\varepsilon(\mathbf{k}) - \varepsilon_s + \beta = 0$.

   d) For general (not small) values of $|\mathbf{k}|a$, show that the electron velocity $\mathbf{v}(\mathbf{k}) \propto \nabla_{\mathbf{k}}\varepsilon$ parallel to $\mathbf{k}$ only in high-symmetry — {10} and {11}—directions

3 (20 points). CORRECTED Consider the band structure of carbon nanotubes. The figure from a Dresselhaus[2] review, pasted below, will be helpful



Recall that in the nearest-neighbor, single-band, tight-binding model, the energy of a honeycomb is given by

$$\varepsilon(k_x, k_y) = \pm\gamma\left[1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)\right]^{1/2}$$

in Schönenberger notation, with a the lattice constant of the hexagonal Bravais net, so $\sqrt{3}$ times the nearest-neighbor (NN) spacing a_0. This notation assumes that the points of the hexagons are in the x direction.

a) In the armchair orientation, the wrapping is by (n,n) in terms of the primitive vectors, with the unit-cell spacing (along the circumference of the tube) being the NN spacing plus the distance across a hexagon tip-to-tip. (Cf. Fig. 19.2.) i) Show then that this unit distance $|\boldsymbol{a}_1 + \boldsymbol{a}_2|$ is 3 times the NN spacing, or $a\sqrt{3}$. By analogy with finding the allowed values of k for periodic boundary conditions, find the n allowed values of k_x here and iii) write the dispersion relation for each as a function of k_y →- k, the 1D wavevector in the "infinite" direction. (Only one equation need be written, with k_x replaced by its discrete values.)

b) Draw the 2D Brillouin zone for graphene (making use of your results in earlier homework sets) and on it draw the lines corresponding to these solutions for n = 5 (solid lines) and n=6 (dashed lines).

c) Now consider the zigzag orientation, with periodicity(n,0). i) Show that the unit distance is a (so that the circumference of the tube is na) and that the wrapping can be viewed as being in the y direction. As above ii) find the allowed values of k_y and iii) write the dispersion relation.

d) Again draw the 2D Brillouin zone for graphene with solid and dashed lines for n= 5 and 6, respectively.

e) Comment on the difference between the two and why the figure says armchair tubes are always metallic but zig-zag ones are metallic only when n is a multiple of 3.