EP431: Semicondcutor Physics (20 August 2016): Problem Set 2

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1. Show that the wavefunction $\frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}.\boldsymbol{R}}\phi(\boldsymbol{r}-\boldsymbol{R})$

   (a) satisfies the Bloch criteria $\psi(\boldsymbol{r}) = e^{i\boldsymbol{k}.\boldsymbol{r}}u_{\boldsymbol{k}}(\boldsymbol{r})$, where $u_k(\boldsymbol{r}+\boldsymbol{R}_n) = u_{\boldsymbol{k}}(\boldsymbol{r})$

   (b) is correctly normalized provided a certain assumption is made. What is the assumption?

2. Calculate the group velocity of a particle at the bottom of the band

$$E(k) = E_0 - 2|t|\cos ka$$

   and at the corner ($k = \pm\pi/a$). Show that there is a point of inflection (where the second derivative changes sign) somewhere between $k = 0$ and $k = \pm\pi/a$. Make a plot of the effective mass as a function of the wave vector k.

3. Consider a rectangular lattice with unit cell dimensions a and b. Show that the bandstructure would be of the form

$$E(k_x, k_y) = E_0 - 2t_1\cos(ak_x) - 2t_2\cos(bk_y)$$

   (a) What is the reciprocal lattice? Draw the first Brillouin zone.

   (b) Plot the constant energy contours, assuming $t_1 > t_2 > 0$ and $a < b$. Why is this physically reasonable?

   (c) Plot some constant energy contours. How do the contours look for small k? How do the shapes change at slightly larger k? Do all constant energy contours close within the first Brillouin zone?

   (d) Suppose $a = b$, *i.e.* it is a square lattice. What will be the shape of the Fermi level when the band is half full?

4. Tight-binding bandstructure with a single orbital per site on BCC and FCC lattice: Take the side of the conventional cube to be a units in length.

   (a) For Body Centered Cubic lattice write down the co-ordinates of the nearest neighbours of $(0, 0, 0)$

   (b) Then show, with 8 nearest neighbour hopping terms and a as the side of the cube

$$E(k_x, k_y, k_z) = E_0 + 8t\cos\frac{k_x a}{2}\cos\frac{k_y a}{2}\cos\frac{k_x a}{2}$$

   (c) For Face Centered Cubic lattice write down the co-ordinates of the nearest neighbours of $(0, 0, 0)$

   (d) Then show, with 12 nearest neighbour hopping terms and a as the side of the cube:

$$E(k_x, k_y, k_z) = E_0 + 4t\left[\cos\frac{k_x a}{2}\cos\frac{k_y a}{2} + \cos\frac{k_y a}{2}\cos\frac{k_z a}{2} + \cos\frac{k_z a}{2}\cos\frac{k_x a}{2}\right]$$

5. For the graphene lattice with nearest neighbour interaction only, Show that:

(a) the eigenvalues of the Hamiltonian are given by

$$
\begin{aligned}
E(k_x, k_y) &= \tilde{E}_0 \pm t|F(k_x, k_y)| \\
\text{where} \qquad |F|^2 &= 1 + 4\cos^2\frac{k_x a}{2} + 4\cos\frac{k_x a}{2}\cos\frac{\sqrt{3}}{2}k_y a
\end{aligned}
$$

(b) The reciprocal lattice vectors of the graphene lattice are given by:

$$
\begin{aligned}
\boldsymbol{b_1} &= \frac{2\pi}{a}\left(1, \frac{1}{\sqrt{3}}\right) \\
\boldsymbol{b_2} &= \frac{2\pi}{a}\left(-1, \frac{1}{\sqrt{3}}\right)
\end{aligned}
$$

(c) Calculate the co-ordinates of the six points where the two bands touch.

6. Consider the motion of the electrons in a cyclotron orbit induced by a magnetic field (as in the lecture notes). Show that

$$
\begin{vmatrix}
M_{xx} & M_{xy} + i\frac{eB_0}{\omega} & M_{xz} \\
M_{xy} - i\frac{eB_0}{\omega} & M_{yy} & M_{yz} \\
M_{zx} & M_{zy} & M_{zz}
\end{vmatrix} = 0
$$

Show that expanding the determinant gives

$$
\frac{\text{det}M}{M_{zz}} = \frac{e^2 B_0^2}{\omega^2}
$$