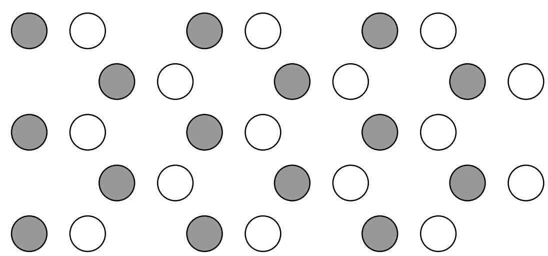
Physics 601 **Homework Set 2** **Fall, 2007**

Due date: Monday, Oct. 8.

Reading: Kaxiras Chs. 3.1-7, 5.1

1) (20 points.)
A layer of graphite is known as a "graphene sheet" and has carbon atoms arranged in a 2D hexagonal lattice. We consider a modified version in which the two sublattices instead contain boron atoms (filled circles) and nitrogen atoms (open circles) as shown below, so that this is a "boron nitride" version of the graphitic sheet. We treat this as a purely 2D problem, and assume that all 3-fold and mirror symmetries that appear to be present are really present.



   a) Choose a coordinate system, write down a pair of primitive lattice vectors, find the corresponding primitive reciprocal lattice vectors, and sketch the (Wigner-Seitz) Brillouin zone.
   b) Find all the elements of the point group and of the extended point group, and indicate the irreducible Brillouin zone (IBZ) on the sketch.
   c) Would the IBZ have been smaller if the two atoms were identical, e.g., a true graphene layer?

2) (20 points.) Plot the first few free-electron bands for an fcc crystal along the (001) direction from $\Gamma = \frac{2\pi}{a}(0,0,0)$ to $X = \frac{2\pi}{a}(0,0,1)$, and along the (111) direction from Γ to $L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Specify the degeneracy of each band along each of these lines, and also at the meeting points at Γ, X, and L. Don't forget to consider all short reciprocal lattice vectors, not just those belonging to one sublattice of the bcc reciprocal lattice, or lying in one plane. (Hint: You should see some crude resemblance to the plot shown for Al in Kaxiras Fig. 4.11, since the nearly-free electron approximation is not bad for Al. However, of course, the real Al bandstructure has splittings and broken degeneracies that will not occur in your plot.)

(Continued on reverse...)

3) (20 points.)

a) Show that the periodic part $u_{n\mathbf{k}}(\mathbf{r})$ of the Bloch solution to $H = -\hbar^2\nabla^2/2m + V(\mathbf{r})$ is an eigenfunction of the effective Hamiltonian

$$H_{\text{eff}}^{(\mathbf{k})} = -\frac{\hbar^2}{2m}(\nabla + i\mathbf{k})^2 + V(\mathbf{r}) \ .$$

b) Show that if the periodic part of the Bloch function is written in terms of its Fourier components,

$$u_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} u_{n\mathbf{k}}(\mathbf{G})\, e^{i\mathbf{G}\cdot\mathbf{r}} \ ,$$

then the Fourier components obey the matrix equation

$$\sum_{\mathbf{G}'} H_{\text{eff}}^{(\mathbf{k})}(\mathbf{G},\mathbf{G}')\, u_{n\mathbf{k}}(\mathbf{G}') = \epsilon_{n\mathbf{k}}\, u_{n\mathbf{k}}(\mathbf{G})$$

where

$$H_{\text{eff}}^{(\mathbf{k})}(\mathbf{G},\mathbf{G}') = \frac{\hbar^2}{2m}(\mathbf{G}+\mathbf{k})^2\,\delta_{\mathbf{G},\mathbf{G}'} + V(\mathbf{G}-\mathbf{G}') \ .$$

4) (20 points)

a) Calculate analytically the density of states $n(E) = \int dk\,\delta(E - \varepsilon(k))$ for a 1D electron band whose energy is given by $\varepsilon(k) = \varepsilon_0 + t\cos(ka)$ (with the BZ running from $k = -\pi/a$ to π/a).

b) Find and make a plot or sketch of the density of states $n(E) = \int d^2k\,\delta(E - \varepsilon(\mathbf{k}))$ for a 2D system having energy bands $\varepsilon(k_x, k_y) = \varepsilon_0 + t\cos(k_x a) + s\cos(k_y b)$, with the BZ extending over $k_x \in [-\pi/a, \pi/a]$, $k_y \in [-\pi/b, \pi/b]$. For consistency of results, let's all take $\varepsilon_0 = 2.0$, $t = -1.0$, and $s = -0.7$. (I don't much care about the scale of the vertical axis, so you can scale away a and b however you like.) To do this problem, you are free to take any of the following approaches, as you prefer: (i) make as much progress analytically by hand as you can; (ii) use a tool like Matlab, Mathematica, or Maple to help solve the problem analytically or numerically as far as possible; or (iii), write a program (in Fortran or C or Pascal or ...) to let k_x and k_y run over a dense mesh of $\mathbf{k}$-points, collect a histogram of the energies, and use these to make a rough density-of-states plot. (This problem is deliberately somewhat ill-defined and open-ended. See what you can do...)