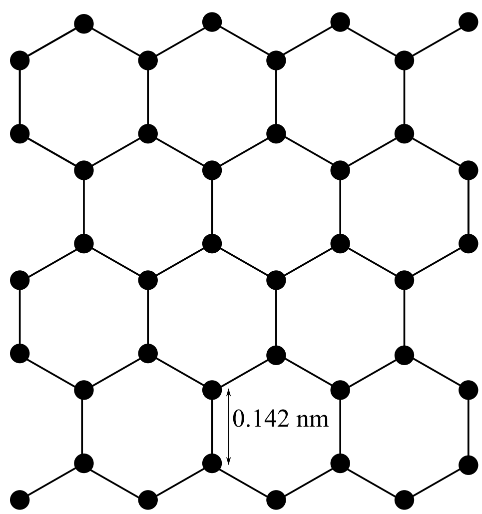
Assignment #1

Due : 3pm February 13th 2012 (before the lecture)

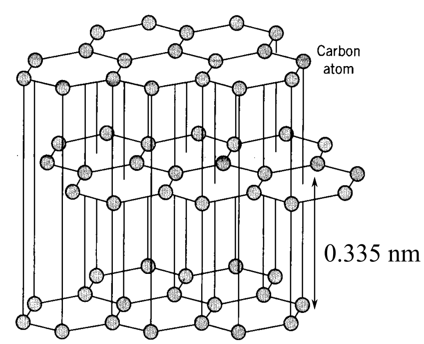
1. (C+L 2.1) In a one-dimensional model of an alloy, mass points are separated by a unit distance with probability p and by a longer distance $1+\rho$ with probability $1-p$. Show that the structure factor for this model is

$$S(q) = \frac{p(1-p)[1-\cos(\rho q)]}{1-p(1-p)-p\cos q-(1-p)\cos[(1+\rho)q]+p(1-p)\cos q\rho}.$$

2. The molecular form factor of CF_4 was calculated in the lecture. Let's consider a graphene as another example. Graphene is essentially a two-dimensional lattice of carbon atoms in a honeycomb lattice as shown in the figure.



graphene sheet



graphite

(a) For graphene, choose a two-dimensional unit cell. [Hint: the unit cell should contain two carbon atoms.] What kind of lattice does this unit cell (or "molecule") form? Define unit vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ accordingly. Using the definition (2.5.7), find reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$.

(b) For the basis of two carbon atoms, calculate molecular form factor for $\vec{q}$ along the directions parallel and perpendicular to the C-C bond. Note that $\vec{q}$ is expressed using reciprocal lattice vectors; e.g., $\vec{q} = h\mathbf{b}_1 + k\mathbf{b}_2$, and $\mathbf{a}_1$ is generally not parallel to $\mathbf{b}_1$. Plot this molecular form factor as a function of q.

(c) For $\vec{q} = \mathbf{G}$, h and k are integers, and we will observe Bragg peaks. However, real experiments are done in three dimensional world. What do you expect to see in this case of 2D crystal, if you actually do the experiment?

(d) Graphite is a three dimensional crystal made up of graphene sheets stacked as shown. Determine three dimensional unit cell. How many carbons are in your unit cell? Now, find the molecular form factor of this unit cell for $\vec{q}$ perpendicular to the graphene sheets, and plot this as a function of q.

3. (Cubic Crystal Field)

(a) Equal point charges are placed on each of the six corners of an octahedron. Taking the origin of a set of cartesian coordinates to be at the centre of the octahedron, there are point charges Q at $(\pm a, 0, 0)$, $(0, \pm a, 0)$, and $(0, 0, \pm a)$. Show that the potential energy of the electron at the centre due to the field of the point charges is given by

$$V(x, y, z) = \frac{Qe}{a}\left[6 + \frac{35}{4a^4}(x^4 + y^4 + z^4 - \frac{3}{5}r^4) + O(r^6)\right]. \tag{1}$$

Hint: Use the following generating function of Legendre polynomials.

$$\frac{1}{(1 - 2tu + t^2)^{\frac{1}{2}}} = \sum_{n=0}^{\infty} t^n P_n(u), \tag{2}$$

where $P_n(u)$'s are Legendre polynomials.

(b) The second term in Eq. (1) acts as a perturbation on the degenerate d levels. (The first term gives just a constant energy shift). We can choose the unperturbed wave functions in a variety of ways, so let us begin by picking eigenfunctions of $\hat{L}_z$, labelling them by their eigenvalues m_l. Thus

$$|\pm 2\rangle = R(r)\sin^2\theta e^{\pm 2i\phi} \tag{3}$$
$$|\pm 1\rangle = \mp 2R(r)\sin\theta\cos\theta e^{\pm i\phi} \tag{4}$$
$$|0\rangle = \sqrt{\frac{2}{3}}R(r)(3\cos^2\theta - 1), \tag{5}$$

where $R(r)$ is the radial part of the wave function which includes a normalization constant. A general state of the system can be written as $|\psi\rangle = \sum_{j=-2}^{2} a_j|j\rangle$ and then specified as a vector:

$$|\psi\rangle = \begin{pmatrix} a_2 \\ a_1 \\ a_0 \\ a_{-1} \\ a_{-2} \end{pmatrix}. \tag{6}$$

In this basis show that

$$V = \begin{pmatrix} Dq & 0 & 0 & 0 & 5Dq \\ 0 & -4Dq & 0 & 0 & 0 \\ 0 & 0 & 6Dq & 0 & 0 \\ 0 & 0 & 0 & -4Dq & 0 \\ 5Dq & 0 & 0 & 0 & Dq \end{pmatrix}, \tag{7}$$

where $D \equiv 35eQ/4a^5$ and $q \equiv (64\pi/1575) \int r^6 R(r)^2 dr$.

(c) Show that the eigenvalues and eigenfunctions are:

eigenvalues	eigenfunctions
6Dq	$\|0\rangle$
6Dq	$\frac{\|2\rangle+\|-2\rangle}{\sqrt{2}}$
-4Dq	$\|1\rangle$
-4Dq	$\|-1\rangle$
-4Dq	$\frac{\|2\rangle-\|-2\rangle}{\sqrt{2}}$.

4. Two-dimensional solid realized in rare gas on graphite played important role in developing our understanding of phase transitions and critical phenomena in two dimensions. Read the following article and discuss why synchrotron x-ray scattering was necessary for this study.

- Birgeneau and Horn, Science, 232, 329 (1986). (available for download at the course website)