Physics 861 { Fall 01
Problem set 8 - Due Tuesday, Nov 6

1.

Problem 4, page 586, of Ashcroft - Mermin

2.

At zero temperature (and neglecting the zero-point motion of the nuclei) the electron density ρ_0 of a perfect crystal can be expanded as a Fourier series

$$\rho_0(r) = \sum_G \rho_{0G} \exp(iG \cdot r) \tag{1}$$

where G are the reciprocal lattice vectors. Assume the electron density of a single atom is given by a function $F(r)$, the so-called atomic form factor. Now imagine building a monatomic crystal by placing these atoms at the sites of a Bravais lattice. Given the Fourier transform of the atomic form factor

$$F_G = \int F(r) \exp(-iG \cdot r)\, dV \tag{2}$$

and the volume of the primitive cell v, compute ρ_{0G}. Neglect overlaps of the electronic shells of the atoms forming the crystal.

3.

Identical point particles of mass m are placed at the sites of a very long one-dimensional lattice of period a. The corresponding mass density $\rho(x)$ is a periodic function that can be expanded in the Fourier series

$$\rho(x) = \sum_{n=-\infty}^{+\infty} \rho_n e^{iG_n x} \tag{3}$$

- What are the values of G_n and ρ_n?
- If the atoms are replaced by diatomic molecules (if each point mass is replaced by two point masses, m and M, separated by a distance $b < a/2$ along x), what are then the values of G_n and ρ_n?

For problems 2 and 3, consult the lecture notes in the Physics Library