PHYSICS 320: Assignment No. 6
Due: November 4, 2009

1. Consider a three-dimensional system of electrons with a uniform neutralizing background of positive charge (Jellium model) at $T = 0$. Assume the electrons to be non-interacting in parts (a)-(d).

   (a) Express the total kinetic energy of the system as a function of the (uniform) density ρ of the electrons.

   (b) Let $V(\mathbf{r})$ be an external potential that makes the system inhomogeneous. Using the Thomas-Fermi approximation, relate the local density $\rho(\mathbf{r})$ to $V(\mathbf{r})$.

   (c) Use the result of part (a) to express the total kinetic energy as a functional of the (now inhomogeneous) local density $\rho(\mathbf{r})$. Assume that $V(\mathbf{r})$, and therefore, the local density $\rho(\mathbf{r})$ are slowly varying in space, so that gradient corrections can be neglected. Also, express the total potential energy in terms of $V(\mathbf{r})$ and $\rho(\mathbf{r})$.

   (d) Minimize the total energy with respect to $\rho(\mathbf{r})$ to obtain a relation between $\rho(\mathbf{r})$ and $V(\mathbf{r})$. Show that the result is the same as that obtained in part (b).

   (e) Generalize both the density functional and the Thomas-Fermi treatments to include the exchange energy. Use the Hartree-Fock form for the exchange energy. Compare the two resulting relations between $\rho(\mathbf{r})$ and $V(\mathbf{r})$.

2. Obtain the equations that determine the phonon frequencies and polarization vectors for a two-dimensional harmonically coupled crystal with one atom per unit cell of a triangular lattice. Evaluate the expressions you find for two special symmetry directions in the Brillouin zone. Assume only nearest-neighbor interactions of the form

$$V(\vec{R}_1, \vec{R}_2) = \frac{1}{2} K(|\vec{R}_1 - \vec{R}_2| - a)^2,$$

   where a is the lattice spacing.

3. According to Lindemann's law of melting, a solid melts if the root-mean-square displacement, $\sqrt{\langle |\mathbf{u}|^2 \rangle}$, of an atom from its equilibrium position exceeds a fraction, $1/\alpha$, of the interatomic distance ($\alpha \approx 10$). Consider a simple cubic lattice of spacing a. Each site is occupied by an atom of mass M. Assuming a Debye spectrum for the phonons, calculate the melting temperature of the solid in terms of the Debye temperature Θ_D, M, a, α and fundamental constants. You may assume that the values of M and a are such that the melting temperature $T_M \gg \Theta_D$.

4. The Debye-Waller factor appearing in the theory of the scattering of neutrons by a solid (see Ashcroft and Mermin, Appendix N) is defined as $e^{-2W(\mathbf{q})}$ where

$$2W(\mathbf{q}) = \langle [\mathbf{q} \cdot \mathbf{u}]^2 \rangle.$$

Here $\mathbf{u}$ is the displacement of an ion from its equilibrium position, and $\langle \ldots \rangle$ represents a thermal average.

   (a) Obtain an expression for $W(\mathbf{q})$ in terms of phonon frequencies and polarization vectors. This should involve an integral over all the phonon modes.

   (b) Show that $e^{-2W(\mathbf{q})} = 0$ in one and two dimensions. (Hint: consider the behaviour of the integrand of the $\mathbf{k}$-integral in part (a) for small values of k.) What are the implications of this result for the possible existence of one- or two-dimensional crystalline ordering?

5. Consider a linear monatomic chain with only nearest-neighbour interactions. First, assume that the interaction between nearest neighbours is purely harmonic.

   (a) Show that the phonon dispersion relation for this system is given by

$$\omega(k) = \omega_0 |\sin(ka/2)|,$$

   where the constant ω_0 is the maximum frequency (this occurs for k on the zone boundary) and a is the spacing between nearest neighbors.

   (b) Calculate the phonon density of states $g(\omega)$ for this system. In particular, show that $g(\omega)$ has a van Hove singularity at $\omega = \omega_0$. Find the form of this singularity.

   (c) Calculate the temperature-dependence of the phonon part of the specific heat of this system at low temperatures.

   (d) Now consider the more general situation where the interaction between nearest neighbors is no longer assumed to be purely harmonic. Let $\phi(r)$ be the pair potential that describes the interaction between nearest neighbors. Define the Grüneisen parameter for the phonon mode with wavenumber k as

$$\gamma(k) = -\frac{\partial \ln \omega(k)}{\partial \ln L}$$

   where $L = Na$ is the length of the chain [N is the number of atoms in the chain]. Show that $\gamma(k)$ is in fact independent of k, and is given by

$$\gamma = -\frac{a}{2}\frac{\phi'''(a)}{\phi''(a)}.$$