Physics 212 – Final Exam

The exam is worth a total of 100 points. The distribution of points is indicated below.

This is an open-book exam. However, I strongly advise you that it will be easier for you to work these problems on your own than to parse answers that you may find in the literature. If you do make strong use of a reference other than the class textbook and notes, please cite the reference in your solutions.

1. (50 points) Here is a very crude model of a chain of flexible molecules that stack into helicies: Let each molecule be in one of two states, (R) a right-handed loop or (L) a left-handed loop. If consecutive molecules are either both right-handed or both left-handed, there is a stabilizing interaction, with energy $(-J)$. For a mismatched pair, the interaction energy is zero.

   (a) Write the partition function for a chain of N molecules. It might be convenient to write $w = e^{\beta J}$.

   (b) Compute the free energy. It suffices to find the extensive term proportional to N as $N \to \infty$.

   (c) Compute $\langle R_n \rangle$, the probability that the nth link is an R, for n in the middle of a long chain.

   (d) Compute the correlation function

   $$\langle R_n R_{n+m} \rangle \tag{1}$$

   for a long chain.

   (e) At low temperature, $w \gg 1$, the correlation function becomes long-ranged. From the average R, what is the typical number of steps until we encounter an L?

   (f) Let each R correspond to a twist by an angle ϕ and each L correspond to a twist by an angle $-\phi$. Show how to insert factors of $e^{\pm\phi\tau}$ into the partition function so that differentiating with respect to τ gives the expectation value of the macroscopic twist Φ over the whole chain.

   (g) It is tempting to guess that τ is the torque on the chain. Justify or correct this statement. Compute the extension due to a small torque,

   $$\frac{\partial \Phi}{\partial \tau}\Big|_{\text{torque}=0}$$

   (h) If the chain is torqued adiabatically (in the direction of its twist) does it heat up or cool down? Give a reasoned answer, *e.g.*, making use of a Maxwell relation.

2. (50 points)

Consider a material made up of a bundle of one-dimensional conducting chains of N atoms each. Model each chain as a periodic one-dimensional array of atoms with lattice spacing a.

(a) Electrons in this lattice have wavefunctions that depend on the lattice site n and obey the Schödinger equation

$$H\psi_n = -\frac{\hbar^2}{2ma^2}[(\psi_{n+1} - \psi_n) - (\psi_n - \psi_{n-1})] \tag{2}$$

This is a discrete version of the second derivative. Use the ansatz

$$\psi_n = Ae^{ikna}$$

to find the energy spectrum of electrons on a chain.

(b) Now imagine distorting the chain so that every other atom moves a small distance $\alpha/2$, with positive α a motion to the right. This changes the Schr̈dinger equation to

$$H\psi_n = \begin{cases} -\frac{\hbar^2}{2ma^2}[(1+\alpha)(\psi_{n+1} - \psi_n) - (1-\alpha)(\psi_n - \psi_{n-1})] & \text{even } n \\ -\frac{\hbar^2}{2ma^2}[(1-\alpha)(\psi_{n+1} - \psi_n) - (1+\alpha)(\psi_n - \psi_{n-1})] & \text{odd } n \end{cases} \tag{3}$$

Use the ansatz

$$\psi_{2m} = Ae^{ik2ma} \quad \psi_{2m+1} = Be^{ik(2m+1)a}$$

to find the energy spectrum of electrons on the distorted chain. The spectrum that you find will be very similar to that in (a) except near $k = \pm\pi/2a$. You will find it useful to to set $\kappa = k - \pi/2a$. Then you can work in the leading approximation for small α and κ.

(c) In the undistorted lattice, at $T = 0$, what value of the electron chemical potential $\mu = \mu_0$ corresponds to filling of the levels up to $|k| = \pi/2a$? What is the density of electrons at this value of μ? What is the difference in the total energy of the electrons between the distorted and undistorted lattices? (Your answer should be proportional to $\alpha^2 \log(1/\alpha)$.)

(d) Distorting the lattice requires energy. Model this with a Landau expression

$$\mathcal{E}(\alpha) = \frac{1}{2}A\alpha^2 + \frac{1}{4}B\alpha^4 \tag{4}$$

where $\mathcal{E}$ is the energy per site (so that $E = N\mathcal{E}$). Show that, for any finite value of A, the lattice will distort when the electron chemical potential is equal to μ_0. Find the lattice distortion α for $\mu = \mu_0$, assuming that A and B are such that the minimum occurs at a small value of α.

(e) Show that, as the electron chemical potential is decreased, there is a phase transition where the lattice returns to its original periodic form. Estimate this critical value of μ. Show that, as μ is increased from μ_0, there is another critical value.

(f) Suggest a way to vary μ in a real material to map these transitions experimentally.

(g) Now consider effects of temperature. First, what is the form of the specific heat of this material at low temperature for $\mu = \mu_0$? For μ below the critical value? For μ just at the critical value? (Giving the T-dependence will suffice; you do not need to find the order-1 coefficient.)

(h) Finally, what happens to the phase transitions when T increases from zero? Is there a T at which the lattice distortion goes away? If so, estimate it. Sketch the phase diagram in the plane of μ vs. T.