Practice Problems for Physics 560A Midterm

Calculator and crib sheet (1-side 8.5"x11") allowed. Show work for full credit.

1) Reciprocal lattice

Consider a three-dimensional Bravais lattice $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, where $n_i \in Z$ and $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are noncoplanar vectors.

a) Any function with the periodicity of the Bravais lattice may be expressed as a Fourier sum over a set of *reciprocal lattice vectors*. State the condition(s) which must be satisfied by a reciprocal lattice vector.

b) Consider an *orthorhombic* Bravais lattice, with fundamental translation vectors $\mathbf{a}_1 = a\hat{x}$, $\mathbf{a}_2 = b\hat{y}$, and $\mathbf{a}_3 = c\hat{z}$, with a, b, and c all different. What are the fundamental translation vectors of the reciprocal lattice?

c) What is the first Brillouin zone for the orthorhombic lattice in (b)?

2) Zero-point fluctuations of a harmonic chain

Consider a one-dimensional Bravais lattice of atoms with lattice spacing a. The Hamiltonian is

$$H = \sum_{n=1}^{L} \left[\frac{p_n^2}{2m} + \frac{C}{2}(x_n - x_{n-1})^2 \right].$$

Calculate the mean-squared deviation $\langle 0|x_n^2|0\rangle$ of the nth atom from its equilibrium position at zero temperature.

Hint: the displacement operator for the nth atom may be expressed as

$$x_n = L^{-1/2} \sum_k \sqrt{\frac{\hbar}{2m\omega_k}} (a_k e^{ikna} + a_k^\dagger e^{-ikna}),$$

where $\omega_k = \sqrt{4C/m} |\sin(ka/2)|$. Also, in the limit $L \to \infty$ (which you may utilize) the sum over k may be replaced by an integral, $L^{-1}\sum_k \to (a/2\pi)\int dk$. (In evaluating the sum over normal modes, the mode with $k = 0$ should be omitted. This corresponds to displacements of the center of mass, and we are only interested in the displacement of the atom relative to a frame in which the center of mass of the crystal is fixed.)

What does your result imply about the possible existence of crystalline order in one dimension?

3) Two-body interaction

Verify that the expectation value of the 2-fermion interaction

$$H^{(2)} = \frac{1}{2} \sum_{ij\ell m} V_{ij\ell m} c_j^\dagger c_m^\dagger c_\ell c_i$$

in the state $|\mu\nu\rangle = c_\mu^\dagger c_\nu^\dagger |0\rangle$ is

$$\langle \mu\nu | H^{(2)} | \mu\nu \rangle = V_{\mu\mu\nu\nu} - V_{\mu\nu\nu\mu}.$$

Here use has been made of the symmetry $V_{ij\ell m} = V_{\ell m ij}$.