1. In class, we studied thermal lattice vibrations for a monatomic three-dimensional Bravais lattice, and calculated the thermal average \( \langle u(0)^2 \rangle \). We found this to be proportional to temperature, vanishing at \( T = 0 \). This cannot be entirely correct, because at zero temperature there will be quantum fluctuations. In this problem you will calculate the same average, but at zero temperature, where it becomes an expectation value in the quantum ground state.

We start with the Hamiltonian in the form
\[
H = \frac{1}{2M} \sum_k \sum_\lambda p_k \cdot p_k + \frac{M}{2} \sum_k \sum_\lambda [\omega_\lambda(k)]^2 u_k \cdot u_k.
\] (1)

The sums are over the entire Brillouin zone. The coordinates and momenta satisfy \( u_{-k} = u^\dagger_k \) and \( p_{-k} = p^\dagger_k \). Here we haven’t quite completed the job of going to normal mode coordinates (i.e. \( u^R \) and \( u^I \)), etc), because we won’t have to for the present purposes. The commutation relations of the coordinates and momenta are:
\[
\begin{align*}
[u_{k\lambda}, p^\dagger_{k'\lambda'}] &= \delta_{\lambda\lambda'} \delta_{kk'} \\
[u_{k\lambda}, u_{k'\lambda'}] &= [p_{k\lambda}, p_{k'\lambda'}] = 0.
\end{align*}
\] (2)(3)

To proceed, we will need to find a set of harmonic oscillator raising and lowering operators. We’ll do this by making a guess and checking that it works. We guess:
\[
a_{k\lambda} = \sqrt{\frac{M\omega_\lambda(k)}{2\hbar}} u_{k\lambda} + \frac{i}{\sqrt{2\hbar M\omega_\lambda(k)}} p_{k\lambda},
\] (4)
\[
a^\dagger_{k\lambda} = \sqrt{\frac{M\omega_\lambda(k)}{2\hbar}} u_{-k\lambda} - \frac{i}{\sqrt{2\hbar M\omega_\lambda(k)}} p_{-k\lambda}.
\] (5)

(a) Show that \([a_{k\lambda}, a^\dagger_{k'\lambda'}] = \delta_{\lambda\lambda'} \delta_{kk'}\) and also \([a_{k\lambda}, a_{k'\lambda'}] = 0\).

(b) Show that
\[
H = \sum_k \sum_\lambda \hbar \omega_\lambda(k) (a^\dagger_{k\lambda} a_{k\lambda} + 1/2).
\] (6)

So far, you have shown that \(a_{k\lambda}\) and \(a^\dagger_{k\lambda}\) form a set of harmonic oscillator raising and lowering operators. Let’s call \(|\psi_0\rangle\) the ground state of the system. Then it is true that
\[
a_{k\lambda}|\psi_0\rangle = \langle \psi_0|a^\dagger_{k\lambda} = 0.
\] (7)

You will need to use this fact to calculate the expectation values in the next part. You will also need
\[
u^\mu(R) = \frac{1}{\sqrt{N}} \sum_k \sum_\lambda e^{iR \cdot k} S_{\mu\lambda}(k) u_{k\lambda},
\] (8)

where \(S_{\mu\lambda}(k)\) is a \(3 \times 3\) orthogonal matrix as discussed in class.

(c) Using the results above, calculate \(\langle \psi_0|u(0)^2|\psi_0\rangle\). You should express your answer as an integral over the Brillouin zone that depends only on the frequencies \(\omega_\lambda(k)\), the atomic mass \(M\), the volume \(a^3\) of a primitive unit cell, and fundamental constants.

(d) Is \(\langle \psi_0|u(0)^2|\psi_0\rangle\) finite or infinite? What about for \(d = 1\) and \(d = 2\)? Discuss any differences in your result from the classical, finite-temperature calculation we did in class, and give a physical interpretation.

2. Ashcroft & Mermin 2.1.
3. Consider a nearly free Fermi gas (in three dimensions) confined by an isotropic trapping potential $V(r) = (1/2)m\omega^2 r^2$, as is now routinely done in JILA. Let $N \gg 1$ be the number of fermions in this Fermi gas. For this problem, we consider fermions that don’t have any spin.

This problem is a generalization of the box with periodic boundary conditions discussed in class and in Ashcroft & Mermin, with the important difference that the single particle states are no longer labeled by momentum $p$. Instead they are $d = 3$ harmonic oscillator states labeled by the discrete quantum numbers $\{n_x, n_y, n_z\}$, where $n_x = 0, 1, 2, \ldots$, and so on. You will need to evaluate sums over $n_x, n_y$ and $n_z$ – for $N \gg 1$ it is legitimate to replace these sums by integrals, which makes them much easier to evaluate. Also, for convenience you should ignore the zero-point energy – its only role here is to shift the zero of the chemical potential.

(a) Calculate the Fermi energy $\epsilon_F$, as a function of $\omega t$ and $N$.

(b) Calculate the density of states $D(\epsilon)$. You should not calculate the density of states per unit volume, as we did in class, but the density of states for the whole system. So, here, $D(\epsilon)$ should have units of (Energy)$^{-1}$.

Useful hint: You should be able to do the remaining parts of the problem using only $D(\epsilon)$ and $\epsilon_F$ as input.

(c) Calculate the chemical potential $\mu(T)$ as a function of temperature, to leading nontrivial order in $T$. That is, calculate the leading correction to the $T = 0$ value, $\mu(T = 0) = \epsilon_F$.

(d) Calculate the total energy of the system $E(T, N)$. Keep terms up through the leading temperature-dependent term.

(e) Calculate the heat capacity $C(T, N)$. (Not the heat capacity per unit volume, but the total heat capacity.) Again, keep only the leading temperature-dependent term.