1. In class, we considered a model for phonons in a simple cubic lattice, with the Hamiltonian

\[ H = \frac{1}{2M} \sum_k p(k) \cdot p(-k) + \frac{K}{2} \sum_k f(k) u(k) \cdot u(-k). \]  

(1)

Here, the sums over \( k \) range over the Brillouin zone of the cubic lattice, and \( f(k) = 6 - 2[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)] \). The Fourier components of the ion positions and momenta satisfy the commutation relations

\[ [u_i(k), p_j(k')] = i\hbar \delta_{ij} \delta_{k,-k'}, \]  

(2)

and, because \( u(k) \) and \( p(k) \) are Fourier transforms of real-valued variables, we also have

\[ u(-k) = [u(k)]^\dag, \]  
\[ p(-k) = [p(k)]^\dag. \]  

(3)

(4)

By writing \( u(k) \) and \( p(k) \) in terms of their real and imaginary parts, show that \( H \) can be written as a sum of decoupled harmonic oscillators. That is, show that \( H \) can be put in the form

\[ H = \sum_i \left[ \frac{1}{2m_i} p_i^2 + \frac{1}{2}m\omega_i^2 q_i^2 \right], \]  

(5)

where \( q_i \) and \( p_i \) are Hermitian operators, and \([q_i, p_j] = i\hbar \delta_{ij}\). Note that, here, \( i \) is a label that distinguishes the various different harmonic oscillators. **Hint:** You will want to work out the implications of Eq. (3) and Eq. (4) for the real and imaginary parts of \( u \) and \( p \).

2. Consider the cubic lattice Hamiltonian from class, but with an extra term added:

\[ H = \frac{1}{2M} \sum_R \left[ p(R) \right]^2 + \frac{K}{2} \sum_{RR'} \left[ u(R) - u(R') \right]^2 + \frac{V}{2} \sum_R \left[ u(R) \right]^2. \]  

(6)

What is the physical meaning of the last term? Could it occur in a real crystal? Solve for the phonon frequency \( \omega(k) \). What happens to \( \omega(k) \) at small \( |k| \)? Give a physical interpretation of this result.

3. In this problem, we will show that the zero- and one-phonon contributions to \( S(q, \omega) \) calculated in class really do correspond to processes where a neutron emits/absorbs zero and one phonons, respectively. For simplicity, we focus on the case of zero temperature, where the initial state in the scattering process is \(|i\rangle = |0\rangle \). The starting point is the expression

\[ S(q, \omega) = \frac{1}{N} \sum_f \int \frac{dt}{2\pi} e^{i\omega t} \sum_{R, R'} e^{-iq \cdot (R-R')} \langle 0|e^{iq \cdot u(R')}|f\rangle \langle f|e^{-iq \cdot u(R, t)}|0\rangle. \]  

(7)

(a) Zero-phonon processes correspond to the single final state \(|f\rangle = |0\rangle \). Starting from Eq. (7), evaluate \( S(q, \omega) \) for a zero-phonon process, and show that it reduces to the same expression we obtained in class. That is, show

\[ S_0(q, \omega) = e^{-2W} \int \frac{dt}{2\pi} e^{i\omega t} \sum_R e^{-iq \cdot R}. \]  

(8)
(b) Single-phonon processes correspond to

\[ |f\rangle = a_i^\dagger(k)|0\rangle, \]  

and

\[ \sum_f \rightarrow \sum_{k,i}. \]  

This corresponds to the neutron emitting a phonon. (At zero temperature, the neutron cannot absorb a phonon, and such processes are not included.) Again, starting from Eq. (7), evaluate \( S(q, \omega) \) by summing over all single-phonon processes, and show that it reduces to the form obtained in class (for zero temperature). That is, show

\[ S_1(q, \omega) = e^{-2W} \int \frac{dt}{2\pi} e^{i\omega t} \sum_R e^{-iq\cdot R} \langle 0|q\cdot u(0)||q\cdot u(R, t)||0\rangle. \]  

\[ \] 

\textit{Hint.} You will find the following identity helpful in evaluating the object \( \langle 0|a_i(k)e^{-iq\cdot u(R, t)}|0\rangle \). Suppose \( a \) and \( a^\dagger \) are the lowering/raising operators for a single harmonic oscillator. Then

\[ [a, f(a^\dagger)] = f'(a^\dagger). \]  

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