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Exercise Set 5
(Due date: Tuesday, November 24, 2009)

Exercise 11 (**Commutation relations**) (10 points)

Verify the the commutation relations

(1) $$\left[a_s(\vec{q}), a^\dagger_{s'}(\vec{q}\,')\right] = \delta_{ss'}\delta_{\vec{q}\vec{q}\,'}\,, \quad \left[a_s(\vec{q}), a_{s'}(\vec{q}\,')\right] = \left[a^\dagger_s(\vec{q}), a^\dagger_{s'}(\vec{q}\,')\right] = 0$$

for the phonon creation and annihilation operators $a^\dagger_s(\vec{q})$ and $a_s(\vec{q})$ by making use of those for the normal coordinates $Q_s(\vec{q})$ and momenta $P_s(\vec{q})$.

Exercise 12 (**Diatomic Linear Chain**) (20 points)

Consider a linear chain with two ions per primitive cell, with equilibrium positions na and $na + d$. The two ions have the same mass M. However, the force between neighboring ions depends on whether their separation is d or $a - d$. Assume that these atoms are connected by alternating springs with different spring constants K and G (where $K \geqslant G$).

(a) Taking into account the fact that only nearest neighbors interact, show that the dispersion relation for the normal modes is given by ($s = 1, 2$)

$$\omega_s(q)^2 = \frac{K+G}{M} \pm \frac{1}{M}\sqrt{K^2 + G^2 + 2KG\cos qa}\,,$$

where the ratio of the amplitudes of oscillation A_1 and A_2 of each atom in a primitive cell is given by

$$\frac{A_1}{A_2} = \mp \frac{K + G\,e^{iqa}}{|K + G\,e^{iqa}|}\,.$$

(b) Draw $\omega_s(q)$ for both the acoustic and optical branches.

(c) It is instructive to examine the dispersion relation obtained above for the diatomic linear chain in the limit in which the coupling constants K and G become very close:

$$K = K_0 + \Delta, \quad G = K_0 - \Delta, \quad \Delta \ll K_0\,.$$

Show that when $\Delta = 0$, the dispersion relation obtained in (a) reduces to that for a monoatomic linear chain with nearest-neighbor coupling. (*Warning*: If the length of the unit cell in the diatomic chain is a, then when $K = G$ it will reduce to a monoatomic chain with lattice constant $a/2$. Futhermore, the Brillouin zone $(-\pi/a < q < \pi/a)$ for the atomic chain will be only half the Brillouin zone $(-\pi/(2a) < q < \pi/(2a))$ of the monoatomic chain. You must therefore explain how two branches (acoustic and optical) in half the zone reduce back to one branch in the full zone. To demonstrate the reduction convincingly you should examine the behavior of the amplitude ratio A_1/A_2, when $\Delta = 0$.)

(d) Show that when $\Delta \neq 0$, but $\Delta \ll K_0$, then the dispersion relation differs from that of the monoatomic chain only by terms of order $(\Delta/K_0)^2$, except when $|\pi - qa|$ is of the order Δ/K_0. Show that when this happens the distortion of the dispersion relation for the monoatomic chain is linear in Δ/K_0.