HOMEWORK SET 07

Theory of Condensed Matter

UFV/TKL1/99 lecture by Martin Gmitra

Winter Semester 2024, room KNKTFA

1. Prove the following properties of the dynamical matrix and its spectrum
   a) [*1 point*] D is hermitian: $\mathcal{D}_{a\mu,b\nu}(\mathbf{q}) = \mathcal{D}^*_{b\nu,a\mu}(\mathbf{q}) = \mathcal{D}^*_{a\mu,b\nu}(-\mathbf{q})$
   b) [*2 points*] the frequencies and polarizations satisfy: $\omega_\lambda(-\mathbf{q}) = \omega_\lambda(\mathbf{q})$, and $(e^\lambda_{a\mu}(-\mathbf{q}))^* = e^\lambda_{a\mu}(\mathbf{q})$; and use this to show that the normal coordinates satisfy $Q_\lambda(\mathbf{q}) = Q^*_\lambda(-\mathbf{q})$.
   c) [*2 points*] for $\mathbf{q} = 0$ in three dimensions there are always three degenerate states with zero frequency $\omega_\lambda(0) = 0, \lambda = 1, 2, 3$. These states are origin of the three acoustic modes. Guess the form of the eigenstate polarization vectors (*hint: use the orthonormality property of the polarization vectors*). What do these vectors correspond to physically? Why is their energy zero?

2. Consider a two dimensional square lattice with lattice constant a and a basis of three atoms per primitive cell.
   a) [*2 points*] What are the total number of phonon branches for each of the following: longitudinal acoustic, transverse acoustic, longitudinal optic, and transverse optic?
   b) [*2 extra points*] Assume that the acoustic modes are represented by the Debye model. What is the maximum acoustic phonon frequency in terms of the lattice constant a and the velocity of sound v_s ?
   c) [*2 extra points*] Find the contribution to the low-temperature heat capacity (within a dimensionless coupling constant) from the longitudinal acoustic phonon branch.

      Express your answer in terms of T, T_D , and N, where T is the temperature, T_D is the Debye temperature, and N is the number of cells in the crystal.

3. Real crystals are not constructed of ideal elastic springs for which the potential varies as $U(x) = cx^2$. The potential rather includes also anharmonic contributions, $U(x) = cx^2 - gx^3 - fx^4$. We can estimate the thermal expansion of a crystal by computing the thermal average equilibrium separation using Boltzmann statistics as
$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x e^{-U(x)/k_B T} dx}{\int_{-\infty}^{\infty} e^{-U(x)/k_B T} dx}$$
   a) [*2 points*] Show that for a crystal bound with ideal springs, there is no thermal expansion.
   b) [*2 extra points*] Show that for an anharmonic interaction, the thermal expansion is given approximately as $\langle x \rangle = 3gk_B T/4c^2$. Use expansion for the small x as $e^{-U(x)/k_B T} \approx e^{-cx^2/k_B T}(1 + gx^3/k_B T + fx^4/k_B T)$.

4. [*5 extra points*] Show that the potential energy of atomic vibrations in terms of the normal modes is $\sum_{\mathbf{q}\lambda} \omega^2(\mathbf{q})|Q_\lambda(\mathbf{q})|^2$.

5. [*1 extra points*] A crystal has a volume of 1 cm^3 and a sound velocity of 6000 m/s. At T = 300 K, what is the number of phonons between the frequencies 4.0 × 10^6 Hz and 4.1 × 10^6 Hz? (*hint: 4.0 × 10^6 Hz is much lower than the Debye frequency so the dispersion relation is linear at these frequencies and the crystal structure is not relevant. This is the long-wavelength limit. First calculate the number of the phonon modes in this frequency interval. Then use the Bose-Einstein factor $f_{\mathrm{BE}} = 1/[\exp(\hbar\omega/k_B T) - 1]$ to calculate the mean number of phonons in these modes.)*

6. [*1 extra points*] Calculate the density of gold from the phonon density of states. By numerically integrating over all frequencies it is possible to determine the number of phonon modes per m^3. This must be equal to number of vibrational degrees of freedom per m^3. The number of vibrational degrees of freedom is 3 times the number of atoms per m^3. Calculate the

concentration of atoms per m^3 and multiply by the mass of an atom to get the density. For the integral of the phonon density of states over all frequencies use 17.7×10^{28} m^{-3}.

7. [*2 extra points*] Use the data in the figure below to estimate the Debye temperature of the silicon in the diamond structure. The sound velocities for the acoustic modes estimate on the ΓX line.