HOMEWORK SET 07

Theory of Condensed Matter
UFV/TKL1/99 lecture by Martin Gmitra
Winter Semester 2021, room KNKTFA(Pa9-PKn)

1. Prove the following properties of the dynamical matrix and its spectrum
   a) [*1 point*] D is hermitian: $D_{a\mu,b\nu}(\mathbf{q}) = D^*_{b\nu,a\mu}(\mathbf{q}) = D^*_{a\mu,b\nu}(-\mathbf{q})$
   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 $f_{\rm BE} = 1/[\exp(\hbar\omega/k_B T) - 1]$ 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 5.90×10^{28} m^{-3}.

7. [*2 extra points*] Use the data of the figure below to estimate the Debye temperature of diamond.