Physics 725: Assignment 4

(to be submitted by Thursday, March 21, 2019)

1. Suppose we have a single-element covalent crystal whose nearest neighbours are all equidistant. The equilibrium positions of the atoms are $\boldsymbol{R}_i^{(0)}$ and their dynamical positions are denoted $\boldsymbol{R}_i = \boldsymbol{R}_i^{(0)} + \boldsymbol{u}_i$. We'll let $\{\boldsymbol{\eta}\}$ be the set of nearest-neighbour vectors and employ a notational shorthand in which $j = i + \boldsymbol{\eta}$ labels the site at $\boldsymbol{R}_j^{(0)} = \boldsymbol{R}_i^{(0)} + \boldsymbol{\eta}$. In other words,

$$\begin{aligned} \boldsymbol{R}_{i+\boldsymbol{\eta}}^{(0)} &= \boldsymbol{R}_i^{(0)} + \boldsymbol{\eta}, \\ \boldsymbol{R}_{i+\boldsymbol{\eta}} &= \boldsymbol{R}_i^{(0)} + \boldsymbol{\eta} + \boldsymbol{u}_{i+\boldsymbol{\eta}}. \end{aligned}$$

Consider a model

$$H = \sum_i \left[\frac{P_i^2}{2M} + \frac{K}{4\eta^2} \sum_{\boldsymbol{\eta}} \left(|\boldsymbol{R}_{i+\boldsymbol{\eta}} - \boldsymbol{R}_i|^2 - \eta^2 \right)^2 + \frac{K'}{4\eta^2} \sum_{\langle \boldsymbol{\eta}, \boldsymbol{\eta}' \rangle} \left((\boldsymbol{R}_{i+\boldsymbol{\eta}} - \boldsymbol{R}_i) \cdot (\boldsymbol{R}_{i+\boldsymbol{\eta}'} - \boldsymbol{R}_i) - \boldsymbol{\eta} \cdot \boldsymbol{\eta}' \right)^2 \right]$$

that takes into account both bond stretching (K) and bond bending (K') processes.

   (a) Show that

$$-\frac{\partial H}{\partial \boldsymbol{u}_i} = K \sum_{\eta} (\hat{\boldsymbol{\eta}} \cdot \boldsymbol{\delta}) \hat{\boldsymbol{\eta}} + K' \sum_{\langle \boldsymbol{\eta}, \boldsymbol{\eta}' \rangle} (\hat{\boldsymbol{\eta}} \cdot \boldsymbol{\delta}' + \hat{\boldsymbol{\eta}}' \cdot \boldsymbol{\delta})(\hat{\boldsymbol{\eta}} + \hat{\boldsymbol{\eta}}') + O(\delta^2, \delta\delta', (\delta')^2),$$

   where $\boldsymbol{\delta}_i(\boldsymbol{\eta}) = \boldsymbol{u}_{i+\boldsymbol{\eta}} - \boldsymbol{u}_i = \boldsymbol{R}_{i+\boldsymbol{\eta}} - \boldsymbol{R}_i - \boldsymbol{\eta}$ and $\hat{\boldsymbol{\eta}} = \boldsymbol{\eta}/\eta$ is a unit vector.

   (b) Suppose this model applies to a honeycomb sheet of carbon (graphene). What is the dimension of the dynamical matrix, and what is its rank? Describe each of the harmonic degrees of freedom.

   (c) Imagine that the graphene sheet is lying in the x-y plane with all atoms sitting at their classical equilibrium positions except for one: a single atom is displaced in the z direction by a distance ϵ. What force does it feel? Argue that this disturbance cannot propagate outward as an acoustic wave (with transverse motion in the z direction).

   (d) Devise a term in the Hamiltonian that would give rise to such flexural modes.

2. For a crystal in d spatial dimensions having $b \geq d$ atoms per unit cell, there are exactly d acoustic modes and $(b-1)d$ optical modes. Explain why. (*Hint:* think about the long wavelength limit.)

3. The deviation $\boldsymbol{u}(\boldsymbol{R} + \boldsymbol{\tau}, t)$ of an atom at $\boldsymbol{R} + \boldsymbol{\tau} = \boldsymbol{R}^{(0)} + \boldsymbol{\tau} + \boldsymbol{u}$ from its equilibrium position at $\boldsymbol{R}^{(0)} + \boldsymbol{\tau}$ obeys the classical equation of motion

$$m_\tau \frac{\partial^2 \boldsymbol{u}(\boldsymbol{R} + \boldsymbol{\tau}, t)}{\partial t^2} = -\sum_{\boldsymbol{R}', \boldsymbol{\tau}'} \mathsf{K} \cdot \boldsymbol{u}(\boldsymbol{R}' + \boldsymbol{\tau}', t).$$

Here, $\boldsymbol{R}^{(0)}$ denotes a site in the Bravais lattice and τ an element of the basis; the restoring force is described by a Hooke's law tensor $\mathsf{K}(\boldsymbol{R} + \boldsymbol{\tau}, \boldsymbol{R}' + \boldsymbol{\tau}')$. Suppose that the crystal is in spatial dimension d and has basis elements $\{\tau_1, \tau_2, \ldots, \tau_b\}$. Define

$$\boldsymbol{\xi}_{a,j}(\boldsymbol{R}, t) = \sqrt{m_j} u_a(\boldsymbol{R} + \boldsymbol{\tau}, t) = \sum_{\boldsymbol{q}} \sum_{\lambda} e^{i(\boldsymbol{q} \cdot \boldsymbol{R} - \omega_{\boldsymbol{q}}^{(\lambda)} t)} \boldsymbol{\xi}_{a,j}^{(\lambda)}(\boldsymbol{q})$$

with $m_j \equiv m_{\tau_j}$ and the index j taking values from 1 to b. In the right hand side sums, $\boldsymbol{q}$ is a wavevector that ranges over the Brillouin Zone, and λ is a label that ranges over all the modes.

(a) Show that $\{(\omega_{\boldsymbol{q}}^{(\lambda)2}, \boldsymbol{\xi}_{\boldsymbol{q}}^{(\lambda)})\}$ constitutes a set of eigenvalue/eigenvector pairs with respect to a dynamical matrix that is the Fourier transform of

$$D_{a,j;b,l}(\boldsymbol{R}-\boldsymbol{R}') = \frac{1}{\sqrt{m_j}} K_{a,b}(\boldsymbol{R}+\boldsymbol{\tau}_j, \boldsymbol{R}'+\boldsymbol{\tau}_l) \frac{1}{\sqrt{m_l}}.$$

(b) How many distinct values of the mode label λ are there?

(c) What do $\omega_{\boldsymbol{q}}^{(\lambda)}$ and $\boldsymbol{\xi}_{\boldsymbol{q}}^{(\lambda)}$ represent physically?

(d) What do the three vectors $\boldsymbol{q}$, $\partial\omega_{\boldsymbol{q}}^{(\lambda)}/\partial\boldsymbol{q}$, and $\boldsymbol{\xi}_{\boldsymbol{q}}^{(\lambda)}$ represent and what is the relationship between them?