SFI5711 - Solid State Physics (2020)
List of exercises #5

1. Van Hove singularities in phonon dispersion

A van Hove singularity takes place when the phonon density of states $D(\omega)$ (or its first derivative) diverges at a frequency ω.

(a) For the monoatomic 1D lattice, the phonon dispersion relation is given by $\omega(k) = 2\Omega_0 \left|\sin\frac{ka}{2}\right|$, with $\Omega_0 = \sqrt{K/M}$ being the natural frequency of a single oscillator. Show that the phonon density of states becomes

$$D(\omega) = \frac{2}{\pi a\sqrt{4\Omega_0^2 - \omega^2}}.$$

(b) Consider a 3D lattice in which the phonon dispersion $\omega_s(\mathbf{k})$ displays an isotropic maximum $\omega_{\max}$ at a certain momentum $\mathbf{k} = \mathbf{k}_{\max}$ for a certain polarization $s = s_{\max}$. Show that although $D(\omega)$ vanishes at $\omega_{\max}$, its first derivative diverges at this point.

2. Lindemann theory of melting

A simple criterion for the melting of a solid is when the mean square displacement of an ion $\langle u^2\rangle$ becomes comparable to the lattice parameter square a^2. Of course, as $\langle u^2\rangle$ becomes larger, the harmonic approximation might not be the most appropriate one. Nevertheless, this simple model offers a good starting point to tackle the problem.

(a) Using the Debye model and considering the high-temperature limit $T \gg \Theta_D$, find the Lindemann melting temperature as function of Θ_D, M, and a.

(*Hint*: use the fact that $\langle u^2\rangle = \frac{1}{N}\sum_{\mathbf{k}}\langle\tilde{\mathbf{u}}(\mathbf{k})\cdot\tilde{\mathbf{u}}(-\mathbf{k})\rangle$ and express $\mathbf{u}$ in terms of the phonon creation and annihilation operators.)

(b) Using the Debye model and approximating the average velocity by $c = a\sqrt{K/M}$, determine the minimum mass M of the ion necessary for the crystal to remain solid at $T = 0$. Express your answer only in terms of a, the effective spring constant K, and the ionic density n.

(c) Show that $\langle u^2\rangle$ diverges in a 1D lattice at any non-zero temperature. What does it imply? (*Hint*: you do not need to evaluate the integral, just show that it diverges).

3. Thermal expansion

The thermal expansion coefficient of a cubic solid is defined as $\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P$. By introducing the bulk modulus $B = -V\left(\frac{\partial P}{\partial V}\right)_T$ the thermal expansion coefficient can be rewritten as: $\alpha = \frac{1}{B}\left(\frac{\partial P}{\partial T}\right)_V$.

(a) Briefly explain why $\alpha = 0$ in the harmonic lattice approximation.

(b) The previous item implies that the thermal expansion of solids is a result of anharmonic terms in the ionic potential energy expansion. Ultimately, they cause the phonon frequencies $\omega_s(\mathbf{k})$ to depend on the volume V. We can nevertheless approximate the total internal energy $\langle E\rangle$ of the system by the harmonic expression

$$\langle E\rangle = E_0 + \sum_{\mathbf{k},s}\hbar\omega_s(\mathbf{k})\left(\langle n_s(\mathbf{k})\rangle + \frac{1}{2}\right),$$

where it is understood that $\omega_s(\mathbf{k})$ is a function of V. Now, from thermodynamic relationships, we can express P in terms of the internal energy $\langle E\rangle$

$$P = -\frac{\partial}{\partial V}\left[\langle E\rangle - T\int_0^T \frac{\mathrm{d}T'}{T'}\frac{\partial\langle E\rangle}{\partial T'}\right].$$

Using these expressions, show that

$$P = -\frac{\partial}{\partial V}\left[E_0 + \frac{1}{2}\sum_{\mathbf{k},s}\hbar\omega_s(\mathbf{k})\right] - \hbar\sum_{\mathbf{k},s}\frac{\partial\omega_s(\mathbf{k})}{\partial V}\left(\frac{1}{e^{\beta\hbar\omega_s(\mathbf{k})} - 1}\right).$$

(c) Show that the thermal expansion is given by $\alpha = \gamma C/B$ where C is the specific heat (per unit volume), γ is the so-called Grüneisen parameter, defined by

$$\gamma = \frac{\sum_{\mathbf{k},s}\gamma_s(\mathbf{k})C_s(\mathbf{k})}{\sum_{\mathbf{k},s}C_s(\mathbf{k})},$$

with $C_s(\mathbf{k})$ denoting the specific heat contribution of mode $\mathbf{k}, s$ and

$$\gamma_s(\mathbf{k}) = -\frac{\partial \ln \omega_s(\mathbf{k})}{\partial \ln V}.$$

4. Phonons in graphene

Consider the graphene honeycomb lattice (see Fig. 1). There are two identical carbon atoms per hexagonal unit cell belonging to sublattices A and B. Therefore, we expect two phonon modes and two optical modes. To obtain them, assume that ion A is connected via springs of constant K to its three B-ions nearest neighbors. Write down the total potential energy and derive the equations of motion for *small* displacements $\mathbf{u}^{\mathrm{A}} = \left(u_x^{\mathrm{A}}, u_y^{\mathrm{A}}\right)$ and $\mathbf{u}^{\mathrm{B}} = \left(u_x^{\mathrm{B}}, u_y^{\mathrm{B}}\right)$. Express the 4 equations in terms of a 4×4 matrix and diagonalize it to find the phonon frequencies. Identify the acoustic and optical modes. Plot the dispersions in the directions $\Gamma M K \Gamma$.

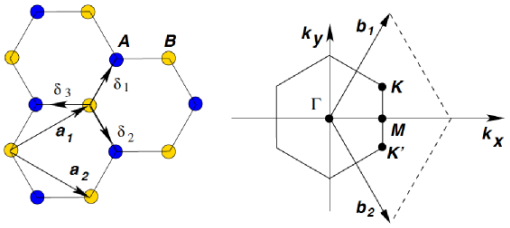

Figure 1: Graphene.