Problem Set #1 (Part II)

September 29, 2016
(Due date: October 11, 2016)

1. Trigonal Bravais lattices

A trigonal Bravais lattice is generated by three primitive vectors (or, unit lattice vectors) of equal length a_0 and making equal angles θ with one another.

(a) Show that the reciprocal of a trigonal Bravais lattice is also trigonal, with an angle θ^* given by the relation $-\cos\theta^* = \cos\theta/(1+\cos\theta)$, and a primitive vector length a^* given by the expression $a^* = (2\pi/a_0)(1+2\cos\theta^*\cos\theta)^{-1/2}$.

(b) The simple cubic lattice structure may be considered as a special case of a trigonal Bravais lattice with $\theta = 90°$. Show that for $\theta = 60°$ or $\cos^{-1}(-1/3)$, the lattice becomes face-centered cubic or body-centered cubic.

(c) Show that the simple cubic structure can also be represented as a trigonal lattice with primitive lattice vectors $\mathbf{a}_i$ forming 60° angle relative to one another and a two-point basis at positions $\pm(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)/4$.

(d) Describe what structure results if the basis of the trigonal lattice described in (c) is replaced by $\pm(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)/8$.

2. The structure factor of a monatomic hexagonal close-packed crystal

(a) Show that the structure factor of a monatomic hexagonal close-packed crystal can take on any of the six values $(1+e^{in\pi/3})$, where $n = 1, 2, ..., 6$, for all reciprocal lattice vectors $\mathbf{K}$ of the simple hexagonal reciprocal lattice.

(b) Show that all reciprocal lattice points have non-vanishing structure factor in the plane perpendicular to the c-axis containing $\mathbf{K} = 0$.

(c) Show that points of zero structure factor are found in alternate planes in the family of reciprocal lattice planes perpendicular to the c-axis.

(d) Show that in such a plane the points that are displaced from $\mathbf{K} = 0$ by a vector parallel to the c-axis has zero structure factor.

(e) Show that the removal of all points of zero structure factor from such a plane reduces the triangular reciprocal lattice structure to a honeycomb reciprocal lattice structure.

3. Low-temperature specific heat of a harmonic crystal in *D*-dimensions

(a) Show that in a *D*-dimensional harmonic crystal, the phonon density $g(\omega)$ in the low-frequency limit ($\omega \to 0$) exhibits a power-law dependence on frequency, $g(\omega) \propto \omega^{D-1}$.

(b) Using the frequency dependence given in (a), show that the low-temperature specific heat of a *D*-dimensional harmonic crystal vanishes as T^D, where T denotes the temperature.

(c) Now consider a special case when the phonon frequencies exhibit non-linear dispersion relation so that $\omega(k) \propto k^{\nu}$ where k is the magnitude of the wave-vector. Show that in this case the low-temperature specific heat of a D-dimensional crystal vanishes as $T^{D/\nu}$.

4. van Hove singularities in various dimensions

(a) We have shown in Part II.5 that a one-dimensional lattice with only nearest-neighbor interactions and a lattice constant a_0 has a phonon dispersion relation $\omega(k) = \omega_0|\sin(ka_0/2)|$, where ω_0 denotes the maximum frequency for k on the zone boundary. Show that the density of phonons in this case is given by

$$g(\omega) = \frac{2}{\pi a_0 \sqrt{\omega_0^2 - \omega^2}}.$$

The singularity at $\omega = \omega_0$ is known as the van Hove singularity.

(b) Next we consider a three-dimensional harmonic crystal. Show that near the maximum of $\omega(\mathbf{k})$, the phonon density $g(\omega)$ varies as $(\omega_0 - \omega)^{1/2}$. Therefore, the van Hove singularities in three dimensions do not occur in $g(\omega)$. Rather, they appear in the derivatives of $g(\omega)$.

(c) Describe the frequency dependence of the phonon density $g(\omega)$ in two dimensions near the maximum of $\omega(\mathbf{k})$.

(d) If ω_0 is a saddle point rather than a maximum in two dimensions, describe the frequency dependence of the phonon density $g(\omega)$ near the maximum of $\omega(\mathbf{k})$.

5. The Debye-Waller factor in different spatial dimensions

We have derived the Debye-Waller factor e^{-2W} for thermal smearing of Bragg diffraction peaks in Part II.8 for a three-dimensional crystal, and we find that $W \propto T$ at high temperatures.

(a) Estimate the order of magnitude of the Debye-Waller factor for a three-dimensional crystal.

(b) Show that $e^{-2W} = 0$ for both two- and one-dimensional crystals. What is the physical implication of this finding for the possible existence of one- or two-dimensional crystalline order?