

Problem Set #1 (Part II)

October 3, 2017
(Due date: October 12, 2017)

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 $\theta = 90^\circ$. Show that for $\theta = 60^\circ$ 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 structural factors of the sodium chloride and the zincblende structures

- (a) The sodium chloride structure may be regarded as an *fcc* Bravais of cube side a_0 , with a basis consisting of a positively charged ion at the origin and a negatively charged ion at the position $(a_0/2)\hat{\mathbf{x}}$. Show that the reciprocal lattice is *bcc*, and that the general reciprocal lattice vector \mathbf{G} has the following form

$$\mathbf{G} \equiv \frac{4\pi}{a_0} (v_1\hat{\mathbf{x}} + v_2\hat{\mathbf{y}} + v_3\hat{\mathbf{z}}),$$

where the coefficients v_i ($i = 1, 2, 3$) are either integers or integers plus $1/2$.

- (b) If the atomic form factor for the positive ion is f_+ and that for the negative ion is f_- , show that the structure factor is $S_{\mathbf{G}} = f_+ + f_-$ if the coefficients v_i are integers, and becomes $S_{\mathbf{G}} = f_+ - f_-$ if the coefficients v_i are integers plus $1/2$. Can you explain the physical reason (not mathematical) why $S_{\mathbf{G}} = 0$ in the latter case when $f_+ = f_-$?
- (c) The zincblende structure is also an *fcc* Bravais of cube side a_0 , with a basis consisting of a positively charged ion at the origin and a negatively charged ion at the position $(a_0/4)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$. Show that the structural factor is $S_{\mathbf{G}} = f_+ + f_-$ if v_i are integers and $(v_1+v_2+v_3)$ is even, $S_{\mathbf{G}} = f_+ - f_-$ if v_i are integers and $(v_1+v_2+v_3)$ is odd, and $S_{\mathbf{G}} = f_+ \pm i f_-$ if v_i are integers plus $1/2$.
- (d) Suppose that the structural factors f_{\pm} of a known *fcc* cubic crystal depend only on the magnitude of the reciprocal lattice vector. Discuss how one may be able to determine whether the crystalline structure is the sodium chloride type or the zincblende type from the structural factors associated with the Bragg peaks.

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 ($\omega \rightarrow 0$) 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?