

MP464: Solid State Physics

Problem Sheet

(1) Write down primitive lattice vectors for the 2-dimensional rectangular lattice, with sides a and b in the x and y -directions respectively, and a face-centred rectangular lattice, with a conventional cell of the same dimensions. Determine what happens to the primitive lattice vectors in each case under reflections in the x and y -axes. The results are different because the space groups are different.

(2) A two dimensional lattice has primitive lattice vectors \mathbf{a}_1 and \mathbf{a}_2 . A different choice of primitive lattice vectors \mathbf{a}'_1 and \mathbf{a}'_2 can always be written as a linear combination of the first choice,

$$\begin{aligned} \mathbf{a}'_1 &= \alpha_{11}\mathbf{a}_1 + \alpha_{12}\mathbf{a}_2 \\ \mathbf{a}'_2 &= \alpha_{21}\mathbf{a}_1 + \alpha_{22}\mathbf{a}_2 \end{aligned} \quad \Rightarrow \quad \begin{pmatrix} \mathbf{a}'_1 \\ \mathbf{a}'_2 \end{pmatrix} \begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \end{pmatrix},$$

with integer co-efficients α_{11} , α_{12} , α_{21} and α_{22} . Show that this requires that

$$\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21} = \pm 1$$

(hint: all primitive cells have the same volume).

Which of the following are legitimate primitive lattice pairs

- $i)$ $\mathbf{a}'_1 = \mathbf{a}_1 + 2\mathbf{a}_2, \quad \mathbf{a}'_2 = \mathbf{a}_2;$
- $ii)$ $\mathbf{a}'_1 = 2\mathbf{a}_1 - \mathbf{a}_2, \quad \mathbf{a}'_2 = \mathbf{a}_1 + \mathbf{a}_2;$
- $iii)$ $\mathbf{a}'_1 = 2\mathbf{a}_1 + 5\mathbf{a}_2, \quad \mathbf{a}'_2 = \mathbf{a}_1 + 3\mathbf{a}_2?$

A three dimensional lattice has primitive lattice vectors \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 . Is

$$\begin{aligned} \mathbf{a}'_1 &= 3\mathbf{a}_1 + \mathbf{a}_2 + 2\mathbf{a}_3 \\ \mathbf{a}'_2 &= 3\mathbf{a}_1 + 2\mathbf{a}_2 + 5\mathbf{a}_3 \\ \mathbf{a}'_3 &= \mathbf{a}_1 + \mathbf{a}_2 + 3\mathbf{a}_3 \end{aligned}$$

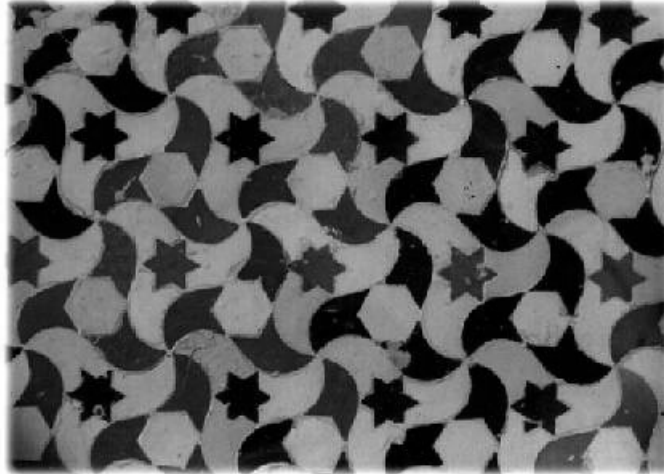
a primitive set?

(3) A two-dimensional centred rectangular lattice has a conventional cell with sides a and b . Show that the special case $b = a$ corresponds to a square lattice.

(4) A two-dimensional centred rectangular lattice has a conventional cell with sides a and b . Show that the special case $b = \sqrt{3}a$ corresponds to a hexagonal lattice.

Identify the 2-d lattice type, all the point group symmetries of the lattice and all the point group symmetries of the tiling below, found in the Alhambara palace in Andalusia, Spain.

Which symmetries of the lattice are absent in the tiling?



(5) Derive the ratio $\frac{c}{a} = \sqrt{\frac{8}{3}}$ quoted in the lectures for the hexagonal close packed (HCP) structure (hint: find the height of a tetrahedron with a base consisting of an equilateral triangle of side a).

Why is the HCP structure not a Bravais lattice?

(6) Find primitive lattice vectors for the 3-dimensional hexagonal lattice and calculate the volume of a primitive cell in terms of a and b .

(7) Calculate the angle between the primitive lattice vectors given in the lectures for the BCC lattice.

(8) Show that a FCC lattice with an extra point in the centre of a conventional cell, *i.e.* a chimera of a FCC and a BCC lattice, is not a Bravais lattice.

(9) Show that a BCC lattice with conventional cell spacing a is equivalent to a face-centred orthorhombic lattice with $b = c = \sqrt{2}a$ (hint: rotate the BCC lattice through 45° about a conventional cell edge).

(10) Why is there no face-centred tetragonal lattice in the Bravais list of 3-dimensional lattices?

(11) Derive the following packing fractions:

i) 2-dimensional hexagonal lattice: $\frac{\pi}{2\sqrt{3}}$;

ii) Diamond: $\frac{\sqrt{3}\pi}{16}$.

(12) Calculate the packing fraction for a face centred cubic crystal with a monatomic basis consisting of spherical atoms.

Given that lead crystallises in a face centred cubic structure with a monatomic basis, calculate the density of lead.

Note: Lead has atomic mass 207.2 and spherical atoms with radius 1.75×10^{-10} m.

(13) The lattice plane defined by any three Miller indices (h, k, l) is always a 2-dimensional Bravais lattice. Identify which 2-dimensional Bravais lattice is associated with the (111), (110) and (100) planes of a simple cubic lattice.

(14) Show that the reciprocal of the BCC lattice is a FCC lattice and calculate the volume of a primitive cell of the reciprocal lattice in terms of the lattice constant a of a conventional cell of the direct lattice.

Show that in general the reciprocal of a reciprocal lattice is the original direct lattice.

(15) Sketch the first three Brillouin zones for a 2-dimensional hexagonal lattice.

(16) A crystal with FCC lattice and a monatomic basis can be viewed as a simple cubic lattice with a basis consisting of four identical atoms. Calculate the structure factor for a FCC lattice in the latter picture.

(17) A crystal consisting of simple cubic lattice, with lattice spacing a and primitive lattice vectors $\mathbf{a}_1 = a\hat{\mathbf{x}}$, $\mathbf{a}_2 = a\hat{\mathbf{y}}$ and $\mathbf{a}_3 = a\hat{\mathbf{z}}$, has a diatomic basis of two identical atoms, one at the origin and one at $\frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$. In the lectures it was shown that the structure factor eliminates all Bragg reflections associated with reciprocal lattice vectors \mathbf{G}_{hkl} with $h + k + l$ an odd integer.

The same crystal can be viewed as a body centred cubic lattice with a monatomic basis. All reciprocal lattice vectors then give Bragg peaks. How are these two pictures reconciled?

(18) A two-dimensional square lattice has lattice spacing a . How many Bragg peaks will be present for incoming X-rays with wavelength $\sqrt{2}a \leq \lambda \leq 2a$?

(19) The Lennard-Jones potential for Neon is

$$U(r) = 4\epsilon \left\{ \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right\}$$

with $\epsilon = 5.0 \times 10^{-22}$ J and $\sigma = 2.74 \times 10^{-10}$ m. Calculate the ratio of the cohesive energies for Neon in BCC and FCC structures.

Note: in the notation used in the lectures the lattice sums for a BCC lattice are $A_{12} = 9.11418$ and $A_6 = 12.2533$.

(20) For any physical system exhibiting oscillatory behaviour of the form $e^{i(Kx-\omega t)}$, the phase of the oscillation is the same for points satisfying $\frac{x}{t} = \frac{\omega}{K}$. The velocity $v_P = \frac{\omega}{K}$ is called the *phase* velocity. The phase velocity is only physically relevant if the dispersion relation is such that $\omega(K)$ is a linear function of K , more generally it is the *group* velocity, $v_g = \frac{d\omega(K)}{dK}$, which is physically relevant. Calculate the group and phase velocities for the dispersion relation derived in the lectures for a one-dimensional crystal with a basis consisting of two ions with masses M_1 and M_2 and identical spring constants.

Show that the group velocity is zero for K at a Brillouin zone boundary.

(21) In the lectures the dispersion relation for a one-dimensional crystal, with a monatomic basis of atoms with mass M and lattice spacing a , was derived using a simple model using Hooke's law with spring constants C ,

$$\omega(K) = \omega_0 \sin\left(\frac{|K|a}{2}\right),$$

where $\omega_0 = 2\sqrt{C/M}$.

Show that this dispersion relation gives a density of states

$$D(\omega) = \frac{2\mathcal{N}}{\pi} \frac{1}{\sqrt{\omega_0^2 - \omega^2}},$$

where \mathcal{N} is the number of lattice points in the crystal.

This diverges at the zone boundary as $K \rightarrow \frac{\pi}{a}$ and $\omega \rightarrow \omega_0$. A divergence like this in the dispersion relation is not uncommon and is called a **van Hove singularity**.

(22) A one-dimensional lattice with lattice spacing a has a diatomic basis consisting of two ions with identical masses m and equilibrium positions na and $na+d$, with $0 < d < a/2$. Assume that each ion only interacts with its nearest neighbours on either side and model the force using Hooke's law with spring constant D on the left and C on the right of the ions at equilibrium positions na . Derive the dynamical equations that govern the displacement $u_n(t)$ away from equilibrium of ions at equilibrium positions na and the displacement $v_n(t)$ away from equilibrium of ions at equilibrium positions $na+d$. Using plane-wave solutions of the form

$$u_n = \epsilon_1 e^{i(Kna-\omega t)}, \quad v_n = \epsilon_2 e^{i(Kna-\omega t)}$$

derive the coupled equations

$$\begin{aligned} (m\omega^2 - (C + D)) \epsilon_1 + (C + De^{-iKa}) \epsilon_2 &= 0 \\ (C + De^{iKa}) \epsilon_1 + (m\omega^2 - (C + D)) \epsilon_2 &= 0 \end{aligned}$$

for ϵ_1 and ϵ_2 . Derive the dispersion relation

$$\omega^2 = \frac{C + D}{m} \pm \frac{1}{m} \sqrt{C^2 + D^2 + 2CD \cos(Ka)}$$

and show that the eigenvectors are given by

$$\epsilon_2 = \mp \frac{C + De^{iKa}}{|C + De^{iKa}|} \epsilon_1.$$

Show that the group velocity of the two branches is

$$v_g = \mp \frac{CDa \sin(Ka)}{\omega \sqrt{C^2 + D^2 + 2CD \cos(Ka)}}.$$

Calculate the group velocity near a Brillouin zone boundary.

(23) Consider a monatomic one-dimensional crystal of unit cell dimension a in which atoms separated by pa interact with a force constant C_p . Show that the dispersion relation is

$$\omega^2(K) = \frac{4}{M} \sum_p C_p \sin^2 \left(\frac{p|K|a}{2} \right).$$

Show that, in the long-wavelength (small $|K|$) limit,

$$\omega(|K|) = \frac{a}{\sqrt{M}} \left(\sum_p p^2 C_p \right)^{\frac{1}{2}} |K|,$$

provided the sum is finite.

(24) Show that the heat capacity for a gas of phonons in the Debye approximation, without assuming low temperature, is

$$C_V = 9\mathcal{N}k_B \left(\frac{T}{\Theta_D} \right)^3 \int_0^{x_D} \frac{x^4 dx}{(e^x - 1)^2}.$$

(25) The thermal energy of a collection of harmonic oscillators with frequency $\omega(|K|)$ is

$$U(T, V) = \hbar \int_0^{\omega_{Max}} \omega \left(\langle n \rangle + \frac{1}{2} \right) D(\omega) d\omega.$$

In the lectures the zero point energy of the oscillators $\frac{\hbar\omega}{2}$ was ignored in the calculation of the specific heat, as it is independent of temperature, but does it depend on the volume? Including this term in the Debye approximation show that the thermal energy at low temperature, assuming 3 acoustic modes, is

$$U(V, T) = \frac{\pi^2 V (k_B T)^4}{10v^3 \hbar^3} + 3\hbar v \left(\frac{3\mathcal{N}}{4} \right)^{\frac{4}{3}} \left(\frac{\pi^2}{V} \right)^{\frac{1}{3}},$$

where v is the speed of sound.

For a monatomic one-dimensional crystal, with atoms of mass M and spring constant C , we saw that $v = \sqrt{\frac{C}{M}} a$. Express v in terms of V to find how U above depends on V .