

# Solid State Physics: Midterm 2 Review

November 6, 2018

## 1 One-dimensional Monatomic Chain

Consider a chain of identical atoms of mass  $m$  and lattice spacing  $a$ . The position of the  $n$ th atom is  $x_n$  and the equilibrium position of the  $n$ th atom is  $x_n^{eq} = na$ . Deviations from the equilibrium position are expressed as  $\delta x_n$  where

$$\delta x_n = x_n - x_n^{eq}$$

The total potential energy of the chain is

$$V = \sum_i \frac{1}{2} \kappa (x_{i+1} - x_i - a)^2 = \sum_i \frac{1}{2} \kappa (\delta x_{i+1} - \delta x_i)^2$$

The force on the  $n$ th mass of the chain is

$$F_n = -\frac{\partial V}{\partial x_n} = \kappa(\delta x_{n+1} - \delta x_n) + \kappa(\delta x_{n-1} - \delta x_n)$$

From this we obtain Newton's equation of motion

$$m(\delta \ddot{x}_n) = F_n = \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n)$$

- A *normal mode* is defined to be a collective oscillation where all particles move at the same frequency.
- Ansatz solution to equation of motion:

$$\delta x_n = A e^{i\omega t - i k x_n^{eq}} = A e^{i\omega t - i k n a}$$

where  $A$  is the amplitude of oscillation, and  $k$  and  $\omega$  are the wavevector and frequency of the proposed wave.

- Even though the solution is complex, we are implicitly meant to take the real part. We only need to consider  $\omega \geq 0$  but  $k$  can be positive or negative.

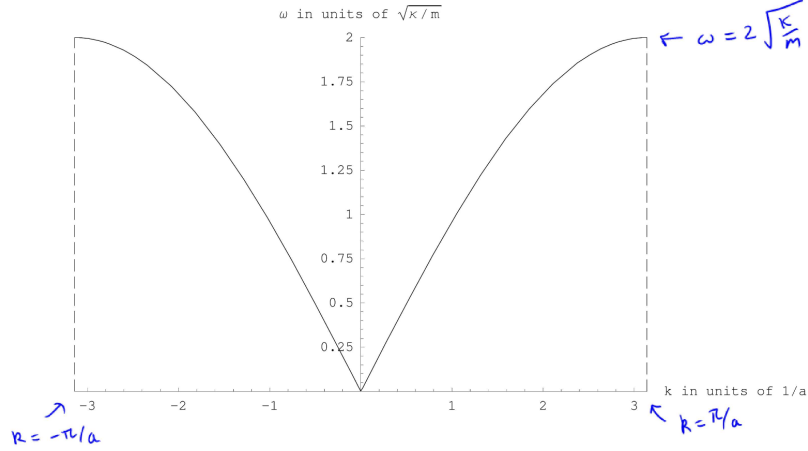


Figure 1: Dispersion relation for 1D monatomic chain.

Plugging the ansatz into the equation of motion yields

$$m\omega^2 = 2\kappa [1 - \cos(ka)] = 4\kappa \sin^2(ka/2)$$

and therefore

$$\omega = 2\sqrt{\frac{\kappa}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

which is the *dispersion relation* - defined as the relationship between frequency (or energy) and a wavevector (or momentum).

## 1.1 Reciprocal Lattice

The dispersion relation in Fig. 1 is periodic in  $k \rightarrow k + 2\pi/a$ . An important general principle is the following: *A system which is periodic in real space with a periodicity  $a$  will be periodic in reciprocal space with periodicity  $2\pi/a$ .* In other words, if the system "looks the same" when  $x \rightarrow x + a$ , then the dispersion will look the same when  $k \rightarrow k + 2\pi/a$ .

The periodic unit in  $k$ -space is known as the *Brillouin zone*. The *first Brillouin zone* is centered about  $k = 0$ . The points  $k = \pm\pi/a$  in Fig. 1 are known as the *Brillouin zone boundary*.

If we take  $k \rightarrow k + 2\pi p/a$ , where  $p$  is any integer, then our solution for  $\delta x_n$  will not change since it is a deep fact that

$$e^{i2\pi np} = 1$$

The *reciprocal lattice* is therefore defined as a set of point in  $k$ -space (*reciprocal space*) which are physically equivalent to the point  $k = 0$ . The set of points  $x_n$  are known as the *direct lattice* or *real-space lattice*.

As an example, the points in the direct lattice of the one-dimensional monatomic chain with lattice spacing  $a$  are

$$x_n = \dots, -2a, -a, 0, a, 2a, \dots$$

and the reciprocal lattice points are

$$G_n = \dots, -2\left(\frac{2\pi}{a}\right), -\left(\frac{2\pi}{a}\right), 0, \left(\frac{2\pi}{a}\right), 2\left(\frac{2\pi}{a}\right), \dots$$

And the defining property of the reciprocal lattice points are:

$$\boxed{e^{iG_m x_n} = 1} \quad (1)$$

That is, a point  $G_m$  is in the reciprocal lattice only if the above holds for all  $x_n$  in the direct lattice. An important note:  $k$  and  $k + G_m$  only describe the same wave when measured at direct lattice points  $x_n$ . If measured arbitrarily along the x-axis, they may differ.

## 1.2 Sound Waves

Sound waves are vibrations with a long wavelength compared to the interatomic spacing. That is,  $k = \frac{2\pi}{\lambda}$ , where  $\lambda \gg a$ . Therefore, the dispersion becomes

$$\omega = v_{sound}k = \left(a\sqrt{\frac{\kappa}{m}}\right)k$$

At larger  $k$  (shorter  $\lambda$ ), the dispersion is no longer linear and one typically defines two velocities.

- The group velocity  $v_{group} = d\omega/dk$ . The speed at which the wavepacket moves. The group velocity becomes 0 at the Brillouin zone boundary.
- The phase velocity  $v_{phase} = \omega/k$ . The speed at which individual minima/maxima move.

## 1.3 Counting Normal Modes

At first glance, it would appear that any choice of  $k$  in the first Brillouin zone yields a unique normal mode with frequency  $\omega(k)$ . But periodic boundary conditions imply that  $x_n = x_{n+N}$ . This yields the requirement in our solution that

$$e^{ikNa} = 1$$

From which we obtain the restriction on possible values of  $k$ :

$$k = \frac{2\pi m}{Na}$$

where  $m$  is some integer. So the full dispersion relation only contain several allowed  $k$  values, the spacing between which is  $2\pi/Na$ . The total number of normal modes is therefore given by the range of the Brillouin zone (e.g.  $[-\pi/a, \pi/a]$ ), divided by the spacing between allowed normal mode values of  $k$ . Be careful to only include one endpoint in the Brillouin zone.

## 1.4 Quantum Phonons

Quantum correspondance: If a classical harmonic system has a normal oscillation mode at frequency  $\omega$  the corresponding quantum system will have eigenstates with energy

$$E_n = \hbar\omega(n + \frac{1}{2})$$

- At a given wavevector  $k$  there are many possible eigenstates.
- The ground state is the  $n = 0$  state with zero point energy  $\hbar\omega(k)/2$ .
- All excitations occur in units of  $\hbar\omega(k)$ .

A *phonon* is a discrete quantum of vibration, and corresponds to an excitation of the normal mode by increasing the quantum number  $n$ .

- Phonons are bosons. We may think of them as particles with energy  $\hbar\omega$  and *crystal* momentum  $\hbar k$ . We always describe momentum using  $k$  within the first Brillouin zone. Even though  $k$  is equivalent to  $k + G_m$ , they do not describe the same momentum.
- At finite temperature, there are non-zero number of phonons occupying a given mode, described by the Bose occupation factor:

$$n_B(\beta\hbar\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}$$

- The expectation value of energy of phonons at wavevector  $k$  is given by

$$E_k = \hbar\omega(k) \left( n_B(\beta\hbar\omega) + \frac{1}{2} \right)$$

- The total energy is given by

$$U_{tot} = \sum_k E_k$$

where the sum is over all possible normal modes (i.e.  $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$ , such that  $k = \frac{2\pi m}{Na}$ ). When the system is very large, the spacing between normal modes shrinks, and we may convert the sum into an integral.

$$\sum_k \rightarrow \frac{Na}{2\pi} \int_{-\pi/a}^{\pi/a} dk$$

- We also note that the total number of normal modes is given by

$$\frac{Na}{2\pi} \int_{-\pi/a}^{\pi/a} dk$$

- From the integral form of  $U_{tot}$ , we could calculate the heat capacity

$$C = \frac{dU}{dT}$$

- This approach is identical to the Debye model, except that Debye assumed  $\omega = vk$ , whereas our dispersion relation is much more complicated.
- We may also convert the integral over  $k$  to an integral over  $\omega$  by introducing a density of states  $g(\omega)$ .

$$\frac{Na}{2\pi} \int_{-\pi/a}^{\pi/a} dk = \int d\omega g(\omega)$$

$$g(\omega) = 2 \frac{Na}{2\pi} \left| \frac{dk}{d\omega} \right|$$

## 2 Vibrations of the One-Dimensional Diatomic Chain

Consider a one-dimensional chain of alternating masses  $m_1$  and  $m_2$  with alternating connecting spring constants  $\kappa_1$  and  $\kappa_2$ . The unit cell for the diatomic chain consists of both masses and is of length (lattice constant)  $a$ . It is useful to pick a reference point for each unit cell, the set of these reference points forms a simple lattice. Within each unit cell, the individual atoms in the cell are described relative to the reference point - this description forms the basis.

### 2.1 Normal Modes

Assume for now that  $m_1 = m_2 = m$ . The equations of motion follow from the monatomic case. But now, let  $x_n$  be the position of the  $n$ th  $m_1$  mass and  $y_n$  be the position of the  $n$ th  $m_2$  mass. Let  $\kappa_1$  connect  $y_n$  to  $x_{n+1}$ .

$$m\delta\ddot{x}_n = \kappa_2(\delta y_n - \delta x_n) + \kappa_1(\delta y_{n-1} - \delta x_n)$$

$$m\delta\ddot{y}_n = \kappa_1(\delta x_{n+1} - \delta y_n) + \kappa_2(\delta x_n - \delta y_n)$$

The ansatz solutions will be

$$\delta x_n = A_x e^{i\omega t - ikna}$$

$$\delta y_n = A_y e^{i\omega t - ikna}$$

- Because the lattice spacing is  $a$ ,  $k$  is physically equivalent to  $2\pi/a$ , so the first Brillouin zone is defined by

$$-\pi/a \geq k \leq \pi/a$$

- For  $N$  unit cells, such that the system length is  $L = Na$ , the allowed values of  $k$  are

$$k = \frac{2\pi m}{Na} = \frac{2\pi m}{L}$$

- The number of possible  $k$  values is  $N$  - one value of  $k$  per unit cell.
- Debye's intuition: there should be one mode per degree of freedom. We have  $2N$  degrees of freedom, but  $N$  values of  $k$ . Resolution: there are two modes per  $k$  value.

Plugging in the ansatz solutions to the equations of motion yields

$$-\omega^2 m A_x = \kappa_2 A_y + \kappa_1 A_y e^{ika} - (\kappa_1 + \kappa_2) A_x$$

$$-\omega^2 m A_y = \kappa_1 A_x e^{-ika} + \kappa_2 A_x - (\kappa_1 + \kappa_2) A_y$$

This can be written as

$$m\omega^2 \begin{bmatrix} A_x \\ A_y \end{bmatrix} = \begin{bmatrix} (\kappa_1 + \kappa_2) & -\kappa_2 - \kappa_1 e^{ika} \\ -\kappa_2 - \kappa_1 e^{-ika} & (\kappa_1 + \kappa_2) \end{bmatrix} \begin{bmatrix} A_x \\ A_y \end{bmatrix}$$

The solutions are obtained by finding the zeroes of the characteristic determinant.

$$0 = \begin{vmatrix} (\kappa_1 + \kappa_2) - m\omega^2 & -\kappa_2 - \kappa_1 e^{ika} \\ -\kappa_2 - \kappa_1 e^{-ika} & (\kappa_1 + \kappa_2) - m\omega^2 \end{vmatrix}$$

The roots are given by

$$m\omega^2 = (\kappa_1 + \kappa_2) \pm |\kappa_1 + \kappa_2 e^{ika}|$$

which can be written as

$$\omega^2 = \frac{(\kappa_1 + \kappa_2)}{m} \pm \frac{\sqrt{\kappa_1^2 + \kappa_2^2 + 2\kappa_1\kappa_2 \cos(ka)}}{m}$$

The  $\pm$  in the dispersion indicates that there are two branches of the dispersion for each  $k$  value - and therefore  $2N$  normal modes in total.

The long-wavelength, low-energy branch of excitations with linear dispersion (corresponding to  $\omega_-$  as  $k \rightarrow 0$ ) is the *acoustic mode*. In this linear region, we expect

$$\omega_- = v_{sound} k$$

Therefore,

$$v_{sound} = \frac{d\omega_-}{dk} = \sqrt{\frac{a^2 \kappa_1 \kappa_2}{2m(\kappa_1 + \kappa_2)}}$$

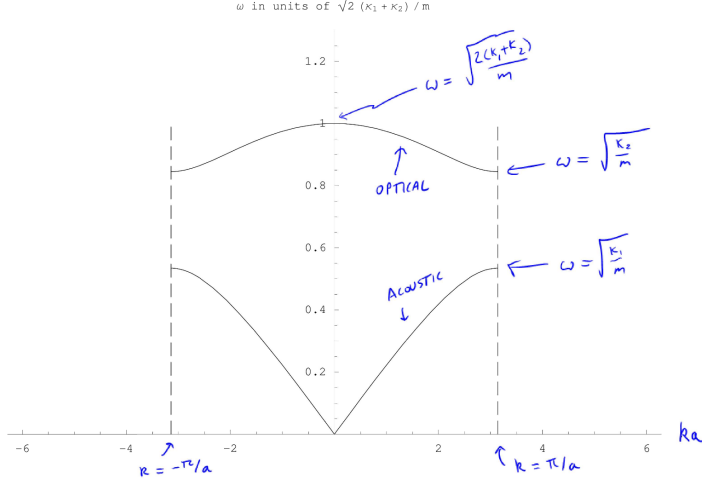


Figure 2: Dispersion relation for 1D diatomic chain.

The higher-energy branch is the *optical mode*. At  $k = 0$ , the optical frequency is

$$\omega_+(k=0) = \sqrt{\frac{2(\kappa_1 + \kappa_2)}{m}}$$

and  $v_{group} = \omega'_+ = 0$ . Side note: optical modes are so-named because photons can only be absorbed by solids for very small  $k$  (since photon energy is given by  $\omega = ck$ ). But at very small  $k$ , only the optical modes have enough energy to absorb a photon and conserve energy.

### 2.1.1 The Long Wavelength Limit

In the long wavelength limit ( $k \rightarrow 0$ ), the eigenvalue equation becomes

$$\omega^2 \begin{bmatrix} A_x \\ A_y \end{bmatrix} = \frac{\kappa_1 + \kappa_2}{m} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} A_x \\ A_y \end{bmatrix}$$

- As  $k \rightarrow 0$ ,  $\omega_- \rightarrow 0$ , and we obtain

$$A_x = A_y = 1$$

which indicates that the two masses in the unit cell move together (in-phase) in the long wavelength limit of the acoustic mode.

- As  $k \rightarrow 0$ ,  $\omega_+^2 \rightarrow \frac{2(\kappa_1 + \kappa_2)}{m}$ , and we obtain

$$A_x = -A_y$$

which indicates that the two masses in the unit cell move in opposite directions (180 degrees out of phase) in the long wavelength limit of the optical mode.

Note: in the case of  $M$  atoms per unit cell, there will be  $M$  modes per distinct value of  $k$  (i.e.  $M$  dispersion branches) and one branch will be acoustic ( $w(k) \rightarrow 0$  as  $k \rightarrow 0$ ) while the rest are optical. When higher degrees of freedom (e.g. transverse motion) are allowed, we must take them into account when determining number of modes. For example, 3D crystals with  $n$  atoms per unit cell have  $3n$  degrees of freedom per unit cell and  $3n$  total dispersion branches - 3 of these are acoustic, while  $3(n - 1)$  are optical.

### 2.1.2 The Brillouin Zone Boundary

At the Brillouin zone boundary,  $k = \pm \frac{\pi}{a}$ . The frequencies are (assuming  $\kappa_1 > \kappa_2$ )

$$\omega_- = \sqrt{\frac{2\kappa_2}{m}}$$

$$\omega_+ = \sqrt{\frac{2\kappa_1}{m}}$$

and, in both cases,  $v_{group} \rightarrow 0$ .

## 2.2 Brillouin Zone Schemes and Monoatomic Perturbations

- The *reduced zone scheme* is the plotting of all dispersion relations within the first Brillouin zone only. See Fig. 2.
- The *extended zone scheme* is the plotting of all dispersion relations across multiple Brillouin zones such that each  $k$  point is mapped to a single mode. See Fig. 3.

In the limit  $\kappa_1 \rightarrow \kappa_2$ , the two atoms in the unit cell become truly indistinguishable and we approach the simple monatomic chain situation with lattice constant  $a/2$ . We can see that the dispersion curve of the diatomic chain with lattice constant  $a$  will also approach that of a monatomic chain with lattice constant  $a/2$  (see Fig. 4).

When the atoms in the unit cell are slightly different, a small gap opens at the Brillouin zone boundary, but the dispersion will continue to mostly look like the monatomic case.

## 3 Crystal Structure

### 3.1 Basics of Crystal Structure

- A *lattice* is an infinite set of points defined by integer sums of a set of linearly independent *primitive lattice vectors*.



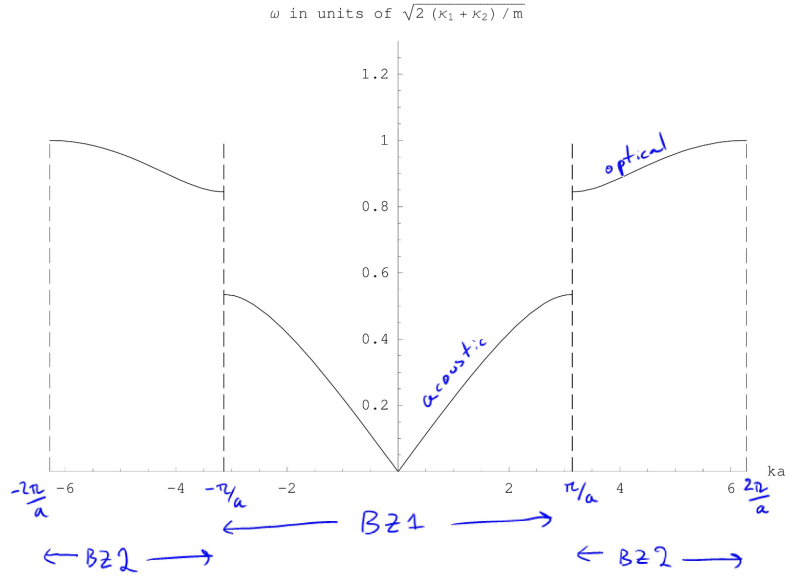


Figure 3: Dispersion relation for 1D diatomic chain.

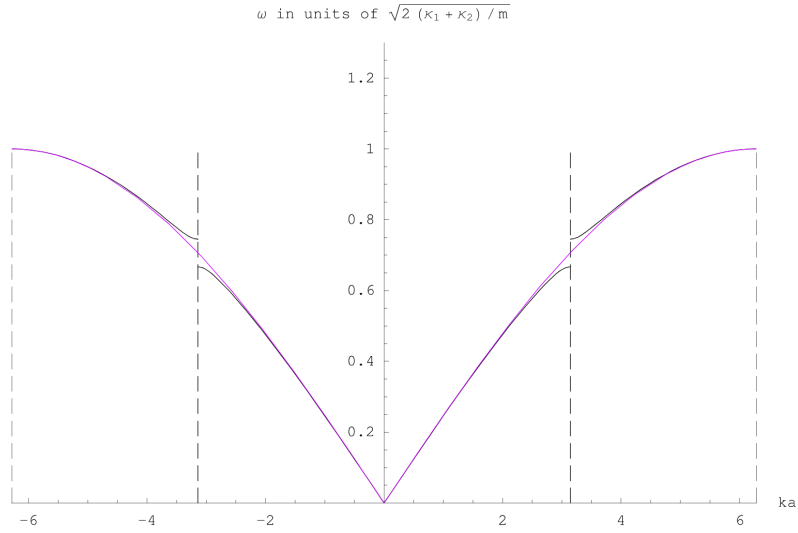


Figure 4: Dispersion relation for 1D diatomic chain as  $\kappa_1 \rightarrow \kappa_2$ .

- Alternatively: A *lattice* is an infinite discrete set of vectors where addition of any two vectors in the set gives a third vector in the set, or a *lattice* is an infinite discrete set of points where the environment of any given point is equivalent to the environment of any other point.
- Lattice points may be described in three dimensions as

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$$

- In 2+ dimensions, the choice of primitive lattice vectors is not unique.
- A *unit cell* is the repeated motif which is the elementary building block of any periodic structure. When many identical unit cells are tiled together, they completely fill all of space and reconstruct the full structure.
- A *primitive unit cell* is a unit cell containing exactly one lattice point.
- A *conventional unit cell* is a typically less-minimal unit cell, often with orthogonal axes, chosen due to ease of use.
- A *Wigner-Seitz cell* is constructed by including all points in space that are closer to a given lattice point than any other lattice point. Approach: choose a lattice cell and draw lines to all possible neighbors. Perpendicular bisectors of these lines bound the Wigner-Seitz cell.
- The description of the unit cell with respect to the associated lattice point is known as the *basis*.
- The positions of atoms can be described by

$$\mathbf{R} = \mathbf{R}_{lattice} + \mathbf{R}_{basis}$$

- The *coordination number* of a lattice is the number of nearest neighbors to any point of the lattice.

## 3.2 Three-Dimensional Lattices

The simplest example is the *simple cubic* lattice.

- The primitive unit cell is typically a cube, where each corner contributes 1/8 lattice point.
- *Tetragonal* and *orthorhombic* lattices have two and three different primitive lattice vector lengths, respectively.
- A point in the lattice may be written as  $[uvw]$  where

$$[uvw] = u\mathbf{a}_1 + v\mathbf{a}_2 + w\mathbf{a}_3$$

- In the case of orthogonal axes,  $\mathbf{a}_1$  is assumed to be in the  $\hat{x}$  direction, etc.

The *body-centered cubic* lattice is identical to the simple cubic lattice, but with an additional lattice point in the center of the cube.

- The conventional unit cell contains  $8(1/8) + 1 = 2$  lattice points.
- The points of the BCC lattice can be written as

$$\mathbf{R}_{corner} = [n_1, n_2, n_3]$$

$$\mathbf{R}_{center} = [n_1, n_2, n_3] + [1/2, 1/2, 1/2]$$

- We can also think of the BCC as two interpenetrating SC lattices, displaced by  $[1/2, 1/2, 1/2]$ .
- The coordination number  $Z = 8$ .
- One choice of primitive lattice vectors:

$$\mathbf{a}_1 = [1, 0, 0]$$

$$\mathbf{a}_2 = [0, 1, 0]$$

$$\mathbf{a}_3 = [1/2, 1/2, 1/2]$$

The *face-centered cubic* lattice is similar to the simple cubic lattice, but with the addition of a lattice point on every cube face.

- The conventional unit cell contains  $8(1/8) + 6(1/2) = 4$  lattice points.
- The points of the FCC lattice can be written as

$$\mathbf{R}_{corner} = [n_1, n_2, n_3]$$

$$\mathbf{R}_{xy} = [n_1, n_2, n_3] + [1/2, 1/2, 0]$$

$$\mathbf{R}_{yz} = [n_1, n_2, n_3] + [0, 1/2, 1/2]$$

$$\mathbf{R}_{zx} = [n_1, n_2, n_3] + [1/2, 0, 1/2]$$

- We can also think of the FCC as four interpenetrating SC lattices, displaced as described above.
- One choice of primitive lattice vectors:

$$\mathbf{a}_1 = [1/2, 1/2, 0]$$

$$\mathbf{a}_2 = [1/2, 0, 1/2]$$

$$\mathbf{a}_3 = [0, 1/2, 1/2]$$

## 4 Reciprocal Lattice, Brillouin Zone, Waves in Crystals

### 4.1 General Reciprocal Lattice Definition

Given a direct lattice of points  $\mathbf{R}$ , a point  $\mathbf{G}$  is a point in the reciprocal lattice if and only if

$$\boxed{e^{i\mathbf{G}\cdot\mathbf{R}} = 1} \quad (2)$$

for all points  $\mathbf{R}$  of the direct lattice. If we write the points of the direct lattice in the form

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

where  $\mathbf{a}_i$  are the primitive lattice vectors, then the points of the reciprocal lattice can be written in the form

$$\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$$

where  $\mathbf{b}_i$  are the primitive reciprocal lattice vectors and

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

Note: one such choice of  $\mathbf{b}_i$  is

$$\mathbf{b}_1 = \frac{2\pi\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = \frac{2\pi\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_3 = \frac{2\pi\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

### 4.2 Reciprocal Lattice as a Fourier Transform

In one-dimension, the direct lattice is given by  $R_n = an$ . The density could then be written as

$$\rho(r) = \sum_n \delta(r - an)$$

The Fourier tranform is then

$$\mathcal{F}[\rho(r)] = \int dr e^{ikr} \rho(r) = \sum_n \int dr e^{ikr} \delta(r - an) = \sum_n e^{ikan}$$

Since  $e^{ikan} = 1$  if  $k = 2\pi m/a$  (that is, if  $k$  is a point on the reciprocal lattice) the sum will accumulate infinitely. If  $k$  does not meet this condition, the sum terms will oscillate and converge to 0. We obtain

$$\mathcal{F}[\rho(r)] = \sum_n e^{ikan} = \frac{2\pi}{|a|} \sum_m \delta(k - 2\pi m/a)$$

## 5 Misc

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$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i}$$

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$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2}$$

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$$\sin^2(x) = \frac{1 - \cos(2x)}{2}$$

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$$\cos^2(x) = \frac{1 + \cos(2x)}{2}$$