Reciprocal Space and Fourier Analysis

Additional reading

- Any book in solid state physics, in particular
  - Ashcroft and Mermin, chapters 4 and 5.
  - the oxford solid state basics, Simon, chapters 12 and 13.
- The books will cover this material in much more detail than these notes. But you don't need to know everything. In this course we will, luckily, only need the basics

Contents

Reciprocal space and Fourier analysis

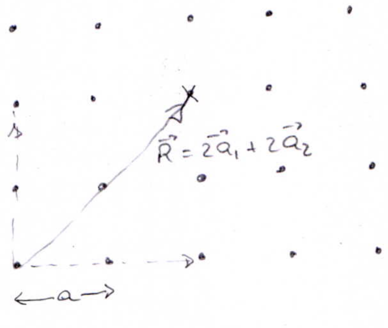
In these notes you will learn how to deal with crystalline systems. Funny enough, 99% of our work will not be in real space, but in an abstract mathematical space called reciprocal space (it look a bit like the upside-down of Stranger things).

We begin by defining a crystal and discussing some important crystal structures. this discussion will not be the most complete, since we will only need some basic facts for our course. If you want a more detailed analysis I recommend the book by Ashcroft and Mermin.

A crystal has 2 parts

$$\boxed{\text{Crystal} = \text{Bravais lattice} + \text{Basis}} \qquad (1)$$

A Bravais lattice is an infinite collection of equivalent points. One example is the square lattice



The word "equivalent" is very important: in a Bravais lattice, if an Allien moves you from one point to another, you won't even know you moved. Your surroundings are absolutely identical no matter in which point you sit.

For every lattice we may define a set of independent primitive vectors $\vec{a}_i$, such that any point in the lattice may be reached by an integer combination of the $\vec{a}_i$. that is, starting at any point you may reach any other point as

$$\boxed{\begin{array}{c} \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \\ n_i = \text{integers.} \end{array}} \tag{2}$$

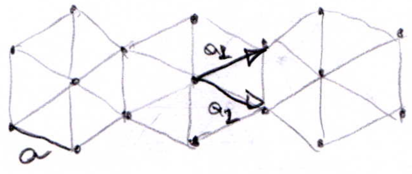
[I wrote the result as if the lattice is 3D. If your lattice is 2D simply set $n_3 = 0$].

For the square lattice the obvious choice of basis vectors are

$$\vec{a}_1 = a(1,0) \qquad \vec{a}_2 = a(0,1) \tag{3}$$

where a is the lattice spacing

Another important Bravais lattice is the hexagonal/triangular lattice



$$\vec{a}_1 = a(1,0) \tag{4}$$

$$\vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$

(NOT UNIQUE)

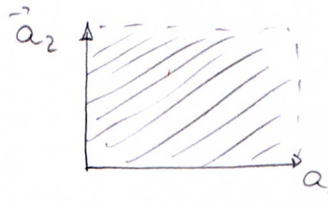
or

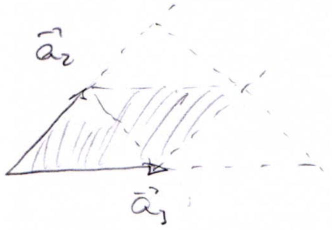
$$\vec{a}_1 = \frac{a}{2}(\sqrt{3}, 1) \tag{5}$$

$$\vec{a}_2 = \frac{a}{2}(\sqrt{3}, -1)$$

This lattice has 120° rotation symmetry, whereas the square lattice has 90°.

the primitive vectors $\vec{a_i}$ define a unit cell. In a bravais lattice a unit cell contains always a single point and is such that, if you copy and paste the unit cell in all of space, you create the whole crystal.

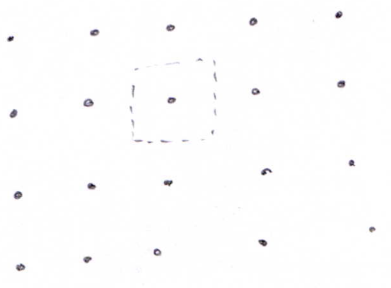


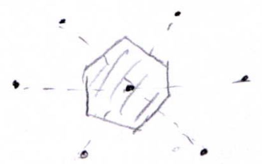


the volume of the unit cell is

$$V_c = |(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3|. \tag{6}$$

The choice of unit cell is not unique. the most convenient one is the Wigner Seitz cell: fill the part of space closest to a given point



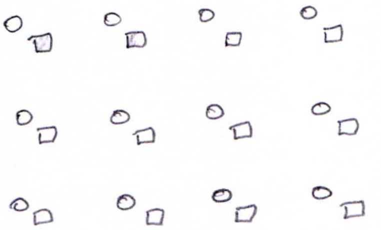


the Wigner Seitz cell reflects the symmetry of the lattice. Even though the unit cell is not unique, all unit cells have the same volume.

As mentioned in Eq (1), the Bravais lattice is only one part of a crystal. The 2^{nd} part is the Basis. The name basis is due to historical reasons. What it means is

Basis = number of atoms in a unit cell (and their positions) (7)

For instance, consider the lattice



This is a rectangular lattice with 2 atoms in the basis. The position of the atoms are denoted by vectors. For instance

$$\vec{S}_\circ = (0,0) \qquad \vec{S}_\square = \delta(1,-1) \tag{8}$$

where $\delta < a$, in the above example

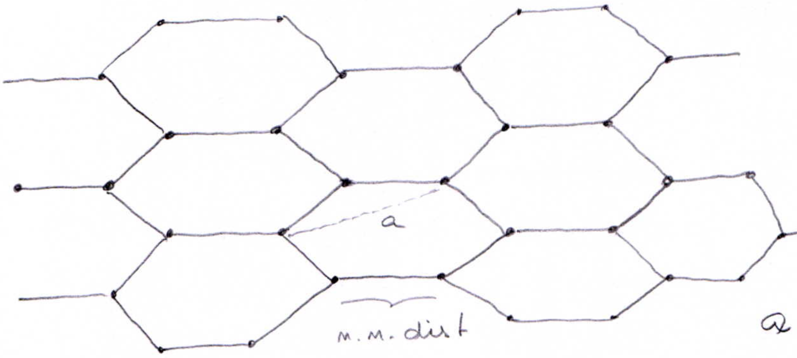
Thus

Every atom in a crystal can be located by a particular Bravais lattice vector $\mathbb{R}$ and a basis vector $\vec{S}_m$, $m = 1, \dots, B$. (9)

B is the number of atoms in a basis, which is the same as the number of atoms in a unit cell.

Example: honeycomb lattice

Graphene crystallizes in the Honeycomb lattice, which is a hexagonal/triangular lattice with 2 atoms in its basis.



← This drawing is stretched in one dimension. Sorry!

$a = 2.46$ Å

The primitive vectors are given by (4) and the two atoms are located at

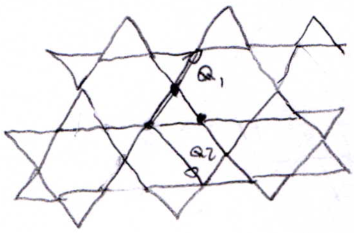
$$\vec{S}_1 = (0,0) \qquad \vec{S}_2 = a\left(\frac{1}{\sqrt{3}}, 0\right) \tag{10}$$

Note that a is not the nearest neighbor distance, which is

$$\text{carbon-carbon dist} = \frac{a}{\sqrt{3}} \simeq 1.42 \text{ Å} \quad (\text{for graphene}). \tag{11}$$

Example: Kagome lattice: hexagonal with 3 atoms in the basis

$$s_1 = (0,0)$$



$$s_2 = \frac{a_1}{2} \qquad s_3 = \frac{a_2}{2}.$$

Periodic boundary conditions

An infinite lattice is both a blessing and a curse:

$$\boxed{\text{Infinite lattice} \begin{cases} \nearrow \text{Translation invariance (GOOD)} \\ \searrow \text{An infinite number of atoms (BAD)} \end{cases}} \qquad (12)$$

Translation invariance is, by far, the most important property of crystalline systems. It is the reason behind most advances in solid state physics. We use an infinite lattice to ensure translation invariance. But the downside is that now we have an infinite number of atoms. this means that the energy, the volume and other things will be infinite, which is a pain.

But fear not, for there is a trick to extract the best of both worlds: periodic boundary conditions. We say that each direction determined by the $\vec{a}_i$ actually has only N_i atoms. And, when we reach the end, we get back to the beginning.

In 1D this means we wrap a line to form a ring

In 2D we wrap a plane to form a torus. In 3D there is no way of visualizing it. Maybe if we use LSD.

PBCs are not real. they are just a mathematical construct to help us keep translation invariance while having a finite number of atoms. Since the crystal is very large, what we do at the boundaries should have a negligible effect on the bulk. this is true in most cases, except when you are dealing with long range interactions.

To understand the consequences of PBC's, let us first consider a 1D crystal. Let $f(x)$ be any quantity of our system, such as a density or a wavefunction or whatever. If the system has PBC then we must necessarily have

$$f(x+Na) = f(x) \tag{13}$$

If you translate by $L = Na$ (the size of the crystal), we get back where we started.

We may now expand $f(x)$ in a Fourier series

$$f(x) = \frac{1}{\sqrt{L}} \sum_k f_k \, e^{ikx} \tag{14}$$

where the factor of $1/\sqrt{N}$ is placed for convenience and the allowed values of k are still to be determined. In fact, they are fixed when we impose PBCs: combining (13) and (14) we get

$$\boxed{e^{ikNa} = 1} \tag{15}$$

this means that

$$kNa = 2\pi l, \qquad l = 0, \pm 1, \pm 2, \ldots$$

or

$$\boxed{k = \frac{2\pi l}{Na}, \quad l = 0, \pm 1, \pm 2, \ldots} \tag{16}$$

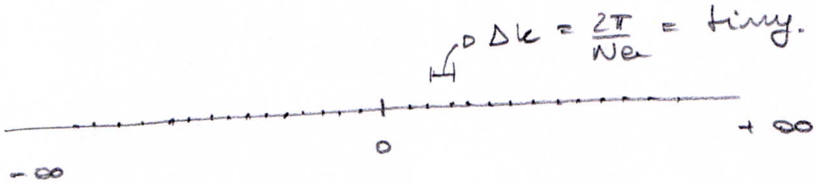
Thus, the sum over k in Eq (14) is actually a sum over $k(l)$, with $l = 0, \pm 1, \pm 2, \ldots$

For reasons that will only become clear later, this "k" has the interpretation of momentum. But if that sounds weird to you, don't worry: we will get there.

From Eq (16) we therefore conclude that the allowed values of k should be quantized. they may go from $-\infty$ to $+\infty$, but in steps of

$$\Delta k = \frac{2\pi}{Na} \qquad (17)$$

Since $N \sim 10^{23}$, these steps will be tiny. So it is as if k varied continuously:



Now I want you to consider a function f which is not defined for a continuous x, but rather is defined only at the lattice sites. In 1D we can label them as

$$x_m = am \quad , \quad m = \text{integer} \tag{18}$$

which is the 1D analog of (2). The Fourier expansion (14) will then look like

$$f(x_m) = \frac{1}{\sqrt{N}} \sum_k e^{ikx_m} f_k \tag{19}$$

In principle this looks the same as (14). But now a new symmetry has appeared; change k by $2\pi/a$.

$$k \to k + \frac{2\pi}{a}$$

then

$$e^{ikx_m} \to e^{ikx_m} \underbrace{e^{i\left(\frac{2\pi}{a}\right)(ma)}}_{e^{2\pi i m} = 1}$$

Thus, if we change k by $2\pi/a$ we get back the same term.

Conclusion: in the Fourier expansion (19), k is still quantized like in (16), but we only need to take k-values in an interval of length $2\pi/a$.

The choice of interval is arbitrary, but the most common choice is

$$\boxed{k \in \left[-\frac{\pi}{a}, \frac{\pi}{a} \right]} \qquad (20)$$

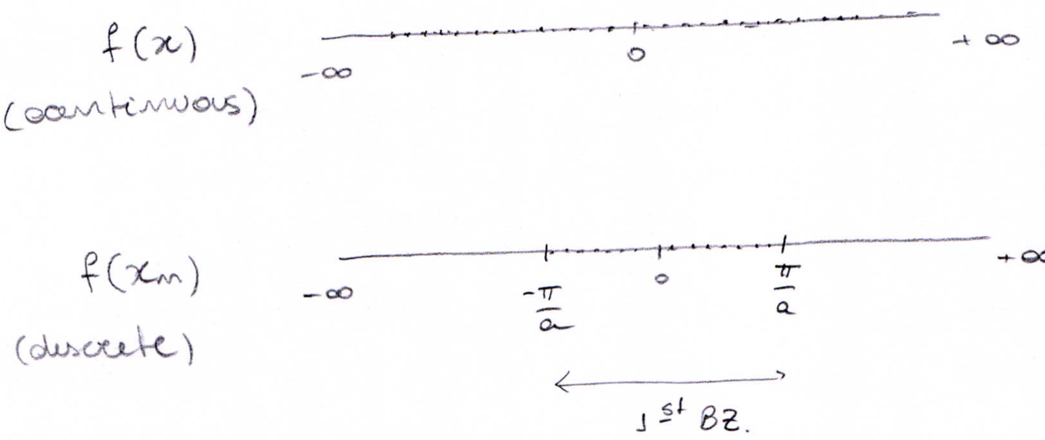
↳ 1st BZ

For historical reasons this is called the <u>1st Brillouin zone</u>.

The quantization (16) may then be written as

$$\boxed{k = \frac{2\pi l}{Na}, \quad l = -\frac{N}{2}, \dots, \frac{N}{2}} \qquad (21)$$

Let us then compare our two results



$$\boxed{k = \frac{2\pi l}{Na} \quad \text{(always)}}$$

The concepts we just discussed will be used literally <u>all the time</u> from now on. So make sure you understand them. What I will do next is extend them to an arbitrary lattice in arbitrary dimension. And in order to do that we need the concept of a <u>reciprocal lattice</u>

Some comments

1) Look back at the 2 figures in page 10. If we take the lattice spacing a and make it smaller and smaller, we will push the 1st BZ further and further into infinity. In the limit $a \to 0$ we recover the continuous case $f(x_n) \to f(x)$.

2) We see two basic measures of wave-vectors

$$1/a = \text{large} = \text{size of first BZ}$$
$$= \text{"ultraviolet (UV) cutoff"}$$

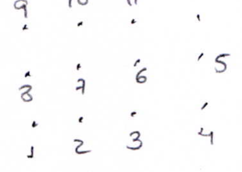
$$1/L = \text{small} = \text{magnitude of } \Delta k$$
$$= \text{"Infrared (IR) cutoff"}$$

these names are borrowed from quantum field theory

3) Lattice labelling in arbitrary D.

In 1D we label the sites by n and denote their positions by $x_n = an$. In arbitrary D it is convenient to continue to label them by n and denote the positions by R_n.

Example:



Reciprocal lattices

Consider an arbitrary lattice defined by the primitive vectors $\vec{a}_i$. Recall that an arbitrary point in this lattice may be reached by the vectors

$$\mathbb{R}_m = m_1 a_1 + m_2 a_2 + m_3 a_3 , \quad m_i = \text{integers} \tag{22}$$

We now define the reciprocal lattice as the set of points $\mathbb{G}$ which satisfy

$$\boxed{e^{i \mathbb{G} \cdot \mathbb{R}_m} = 1} \quad \text{for every } \mathbb{R}_m \tag{23}$$

To determine the allowed values of $\mathbb{G}$, define a new set of vectors $\mathbb{b}_i$ which satisfy

$$\boxed{a_i \cdot \mathbb{b}_j = 2\pi \delta_{ij}} \tag{24}$$

then $\mathbb{G}$ may be written as

$$\boxed{\mathbb{G} = m_1 \mathbb{b}_1 + m_2 \mathbb{b}_2 + m_3 \mathbb{b}_3} , \quad m_i = \text{integers} \tag{25}$$

This looks exactly like (22), but with basis vectors $\mathbb{b}_i$. These $\mathbb{G}$ points therefore define a Bravais lattice. This is the reciprocal lattice. Every lattice has a reciprocal lattice (like your evil twin in a parallel universe).

To check that this works, multiply

$$\mathbf{G}\cdot\mathbf{R}_n = \sum_{ij} m_i n_j \, \mathbf{b}_i\cdot\mathbf{a}_j \quad = 2\pi \sum_i m_i n_i$$

this has the form $2\pi \times$ integers so $e^{i\mathbf{G}\cdot\mathbf{R}_n} = 1$ for any $\mathbf{R}_n$

qed.

To find the actual $\mathbf{b}_i$ we can use the following formulas

$$\mathbf{b}_1 = \frac{2\pi}{V_c}\,\mathbf{a}_2\times\mathbf{a}_3 \qquad \mathbf{b}_2 = \frac{2\pi}{V_c}\,\mathbf{a}_3\times\mathbf{a}_1 \qquad \mathbf{b}_3 = \frac{2\pi}{V_c}\,\mathbf{a}_1\times\mathbf{a}_2 \qquad (26)$$

where $V_c = |(\mathbf{a}_1\times\mathbf{a}_2)\cdot\mathbf{a}_3|$. For instance, in a square lattice we have

$$\mathbf{a}_1 = a(1,0,0) \qquad \mathbf{a}_2 = a(0,1,0) \qquad \underbrace{\mathbf{a}_3 = (0,0,1)}_{\text{we don't care about } \mathbf{a}_3.}$$

then the volume of the unit cell will actually be an area

$$V_c = A_c = |(\mathbf{a}_1\times\mathbf{a}_2)\cdot\mathbf{a}_3| = a^2$$

and we get

$$\mathbf{b}_1 = \frac{2\pi}{a}(1,0) \qquad \mathbf{b}_2 = \frac{2\pi}{a}(0,1) \qquad (27)$$

[we don't care about $\mathbf{b}_3$]. We thus see that the reciprocal lattice of the square lattice is also a square lattice, but with lattice constant $2\pi/a$. Note how this has the dimensions of wave number (1/length), which is also the units of momentum when $\hbar = 1$.

We are now ready to give a general definition of the 1st Brillouin zone:

1st BZ = Wigner - Seitz cell of the reciprocal lattice (28)

Volume = $\frac{2\pi}{V_c}$

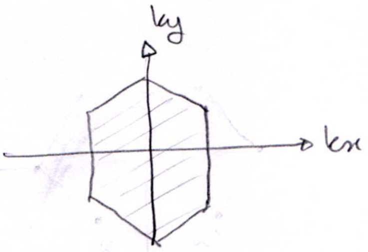
Example: hexagonal lattice

$$a_1 = \frac{a}{2}(\sqrt{3}, 1) \qquad a_2 = \frac{a}{2}(\sqrt{3}, -1) \tag{29}$$

$$V_c = \frac{\sqrt{3}\,a^2}{2} \qquad V_{BZ} = \frac{2\pi}{V_c} = \frac{4\pi}{\sqrt{3}\,a^2} \tag{30}$$

$$b_1 = \frac{-2\pi}{\sqrt{3}\,a}(1, \sqrt{3}) \qquad b_2 = -\frac{2\pi}{\sqrt{3}\,a}(1, -\sqrt{3}) \tag{31}$$

the reciprocal lattice of the hexagonal is therefore also hexagonal, but rotated by 90°. the 1st BZ is therefore a hexagon



Fourier analysis for an arbitrary lattice

Now consider an arbitrary lattice defined by its primitive vectors $\vec{a}_i$. We assume that each direction $\vec{a}_i$ has a total of N_i sites so that, in total, the crystal has

$$N = N_1 N_2 N_3 \tag{32}$$

Bravais sites.

Now let $f(\mathbb{r})$ be an arbitrary function. Periodic boundary conditions (PBC) imply that

$$f(\mathbb{r} + N_i \vec{a}_i) = f(\mathbb{r}) \quad \text{for every } i \tag{33}$$

As before, we expand f in a Fourier series, as

$$f(\mathbb{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbb{k}} f_{\mathbb{k}} \, e^{i \mathbb{k} \cdot \mathbb{r}} \tag{34}$$

Eq (33) then imposes the restraints

$$e^{i \mathbb{k} \cdot a_i N_i} = 1 \qquad \text{for all } i \tag{35}$$

To figure out what to do with this, we write $\mathbb{k}$ in terms of the reciprocal lattice vectors

$$\mathbb{k} = \frac{a}{2\pi} (k_1 \mathbb{b}_1 + k_2 \mathbb{b}_2 + k_3 \mathbb{b}_3) \tag{36}$$

Please note that $k_1 \neq k_x$ and so on since, in general, the $\mathbb{b}_i$ are not cartesian coordinates. By the way: the factor of $a/2\pi$ is inserted simply so that the k_i has units of momentum (wave vector)

Eq (35) then gives

$$\mathbf{k} \cdot \mathbf{a}_i = \frac{a}{2\pi}\left(\sum_j k_j \mathbf{b}_j\right) \cdot \mathbf{a}_i = a k_i$$

so we get

$$e^{i a k_i N_i} = 1 \qquad (37)$$

which is the same as

$$\boxed{k_i = \frac{2\pi l_i}{N_i a}, \quad l_i = 0, \pm 1, \pm 2, \ldots} \qquad (38)$$

this is identical to the 1D case, Eq (16), but now holds for each direction k_i. Thus, everything we did in the 1D case carries over to an arbitrary lattice, provided we take the $\mathbf{k}$ as a linear combination of the $\mathbf{b}_i$.

Referring back to (36), if you want to know the components (k_x, k_y, k_z), they will be given as linear combinations of k_1, k_2, k_3.

As before, we may now consider what happens when $f(\mathbf{r})$ is only defined at the lattice sites $\mathbf{R}$. In this case it is convenient to label them as $\mathbf{R}_m$. We then expand

$$f(\mathbf{R}_m) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} f_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{R}_m} \tag{39}$$

Now translate $\mathbf{k}$ by any reciprocal lattice vector $\mathbf{G}$. We get

$$e^{i\mathbf{k}\cdot\mathbf{R}_m} \to e^{i\mathbf{k}\cdot\mathbf{R}_m}\, e^{i\mathbf{G}\cdot\mathbf{R}_m}$$

But, by the definition of the reciprocal lattice, Eq (23), the last term is 1.

Thus we conclude that if $f(\mathbf{R}_m)$ is defined only at the lattice sites, translating $\mathbf{k}$ by any reciprocal lattice vector $\mathbf{G}$ changes nothing. This means that we only need to take $\mathbf{k}$ inside a unit cell: after all, $\mathbf{G}$ is the vector connecting unit cells. Again, the most common choice is the 1st BZ, but any unit cell of the reciprocal lattice will do. This therefore constraint the k_i in (38) to the interval

$$k_i \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right] \tag{40}$$

This defines a unit cell but, unlike in the 1D case, this will not necessarily be the first BZ. If you want the 1st BZ you will in general need a more complicated constraint. In any case,

$$\boxed{\text{Each } k_i \text{ takes on } N_i \text{ values inside a unit cell}} \tag{41}$$

Lattice sums and k-sums

I know you are probably getting tired of all this mathematical formalism, but there are two more things I need to teach you: we will often encounter sums of the form

$$\sum_{n} g(\mathbf{R}_n) \qquad \text{or} \qquad \sum_{\mathbf{k}} h(\mathbf{k})$$

The first is a lattice sum (a sum over all lattice points) and the second is a $\mathbf{k}$ sum. Here g and h are arbitrary functions. The $\mathbf{k}$ sum is assumed to be over the N values in the unit cell.

To work with these sums, there are two tricks which appear all the time and are worth remembering: (1) δ-function identities and (2) converting a sum to an integral.

As for the first, the two identities are

$$\boxed{\begin{aligned} \frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_n-\mathbf{R}_m)} &= \delta_{nm} \qquad (42) \\ \frac{1}{N}\sum_{n} e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{R}_n} &= \delta_{\mathbf{k},\mathbf{q}} \qquad (43) \end{aligned}}$$

The logic is simple. Take (42) as an example. If $n \neq m$ we have a sum of oscillating stuff, which cancel out. If $n = m$ we are summing "1", N times, which cancels with the N below.

what I need to convince you is that the cancelation is perfect. I will do that in 1D. The general proof is analogous. I will also do it for (43). Again, (42) is analogous.

Eq (43) in 1D reads

$$\frac{1}{N} \sum_{M=1}^{N} e^{ikaM}$$

We may use the formula for the truncated geometric series

$$\sum_{M=1}^{N} x^M = \frac{x}{x-1}\left(x^N - 1\right)$$

with $x = e^{ika}$. But $k = \frac{2\pi l}{Na}$, with l = integer, so

$$x^N = e^{ikNa} = e^{i\frac{2\pi l}{Na}Na} = e^{i2\pi l} = 1$$

Thus the sum gives zero. The only exception is when $k = 0$ (or $k = g_1$). Then we get $\frac{N}{N} = 1$.

Finally I will show you how to convert from a sum to an integral. this happens for k sums and is justified due to the fact that, from (38)

$$\Delta k_i = \frac{2\pi}{N_i a} \qquad (44)$$

In the limit $N_i \to \infty$ these spacings become infinitesimal.

To convert from sums to integrals, you should always remember one of the first formulas you saw in calculus 1:

$$\boxed{\sum_{x_n} f(x_n)\,\Delta x \approx \int f(x)\,\Delta x} \qquad (45)$$

what is essential here is the Δx guy. In a sum such as $\sum_{k} h(k)$ there is no Δk, so we need to put it there. the trick is to multiply the sum by 1, where, from (44), we choose

$$1 = \left(\frac{N_1 a}{2\pi}\right)\left(\frac{N_2 a}{2\pi}\right)\left(\frac{N_3 a}{2\pi}\right)\Delta k_1 \Delta k_2 \Delta k_3$$

Note the appearance of

$$N_1 N_2 N_3 a^3 = N a^3 = V$$

this is the volume of the crystal. we then write

$$\sum_{k} h(k) = \frac{V}{(2\pi)^3} \sum_{k} h(k)\,\Delta k_1 \Delta k_2 \Delta k_3$$

Now this has the shape of a Riemann sum, Eq (45), so we may finally write

$$\boxed{\sum_{\mathbb{k}} h(\mathbb{k}) = \frac{V}{(2\pi)^3} \int_{1^{st}BZ} d^3\mathbb{k}\; h(\mathbb{k})} \qquad (46)$$

All you need to remember is the factor $V/(2\pi)^3$.

You may wonder: if in the end we want $\mathbb{k}$ to be continuous, why not take this limit before, the answer is: <u>convenience</u>. working with discrete $\mathbb{k}$ is useful because you avoid divergences. The longer you can postpone the continuum limit, the better.