Let's begin our discussion of lattices by talking about the Bravais lattice...

A fundamental concept in the description of crystalline solids is that of a "Bravais lattice". A Bravais lattice is an infinite arrangement of points (or atoms) in space that has the following property:

**The lattice looks exactly the same when viewed from any lattice point**

A 1D Bravais lattice:

![1D Bravais lattice diagram]

A 2D Bravais lattice:

![2D Bravais lattice diagram]
We may continue to construct higher dimensional Bravais lattices:

A 2D Bravais lattice:

A 3D Bravais lattice:

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A Bravais lattice has the following property:
The position vector of all points (or atoms) in the lattice can be written as follows:

\[ \mathbf{R} = n \mathbf{a}_1 \]

\[ \mathbf{R} = n \mathbf{a}_1 + m \mathbf{a}_2 \]

\[ \mathbf{R} = n \mathbf{a}_1 + m \mathbf{a}_2 + p \mathbf{a}_3 \]

Where \( n, m, p = 0, \pm 1, \pm 2, \pm 3, \ldots \).

And the vectors, \( \mathbf{a}_1, \mathbf{a}_2, \) and \( \mathbf{a}_3 \)

are called the "primitive lattice vectors" and are said to span the lattice. These vectors are not parallel.

Example (1D):

Example (2D):
Consider a 2D example...

Example (2D):

All lattices are not Bravais lattices:

The honeycomb lattice
Let's move on to discuss the primitive cell...

- A primitive cell of a Bravais lattice is the smallest region which when translated by all different lattice vectors can “tile” or “cover” the entire lattice without overlapping.

Two different choices of primitive cell
- The primitive cell is not unique.

The volume (3D), area (2D), or length (1D) of a primitive cell can be given in terms of the primitive vectors, and is independent of the choice of the primitive vectors or of the primitive cells:

1D: \( \Omega_1 = |\mathbf{a}_1| \)

2D: \( \Omega_2 = |\mathbf{a}_1 \times \mathbf{a}_2| \)

3D: \( \Omega_3 = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| \)

Example, for the 2D lattice above:
\[
\begin{align*}
\mathbf{a}_1 &= b \mathbf{x} \\
\mathbf{a}_2 &= c \mathbf{y}
\end{align*}
\]

or
\[
\begin{align*}
\mathbf{a}_1 &= b \mathbf{x} + c \mathbf{y}
\end{align*}
\]

The Wigner-Seitz (WS) primitive cell of a Bravais lattice is a special kind of a primitive cell and consists of region in space around a lattice point that consists of all points in space that are closer to this lattice point than to any other lattice point.

- The Wigner-Seitz primitive cell is unique.

The volume (3D), area (2D), or length (1D) of a WS primitive cell can be given in terms of the primitive vectors, and is independent of the choice of the primitive vectors:

1D: \( \Omega_1 = |\mathbf{a}_1| \)

2D: \( \Omega_2 = |\mathbf{a}_1 \times \mathbf{a}_2| \)

3D: \( \Omega_3 = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| \)

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or
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\begin{align*}
\mathbf{a}_1 &= b \mathbf{x} + c \mathbf{y}
\end{align*}
\]

\( \Omega_3 = |\mathbf{a}_1 \times \mathbf{a}_2| = bc \)

\( \Omega_2 = |\mathbf{a}_1 \times \mathbf{a}_2| = bc \)
Let's examine another example of a Wigner-Seitz Cell...

Example (2D):

\[ \vec{a}_1 = b \hat{x} \]
\[ \vec{a}_2 = \frac{b}{2} \hat{x} + \frac{b}{2} \hat{y} \]
\[ \Omega_2 = |\vec{a}_1 \times \vec{a}_2| = \frac{b^2}{2} \]

Example (3D):

\[ \Omega_3 = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| = bcd \]

Now let's add in a basis...

Consider the following lattice:

- Clearly it is not a Bravais lattice (in a Bravais lattice, the lattice must look exactly the same when viewed from any lattice point).

- It can be thought of as a Bravais lattice with a basis consisting of more than just one atom per lattice point—two atoms in this case. So associated with each point of the underlying Bravais lattice there are two atoms. Consequently, each primitive cell of the underlying Bravais lattice also has two atoms.

- The location of all the basis atoms, with respect to the underlying Bravais lattice point, within one primitive cell are given by the basis vectors:

\[ d_1 = 0 \]
\[ d_2 = h \hat{x} \]
Now let's consider a lattice made of two different atoms: red and black...

- It is clearly not a Bravais lattice since two different types of atoms occupy lattice positions.
- The lattice defined by the “red” atoms can be taken as the underlying Bravais lattice that has a two-atom basis: one “red” and one “black”.
- The lattice primitive vectors are:
  \[
  \mathbf{a}_1 = a \hat{x}, \quad \mathbf{a}_2 = \frac{a}{2} \hat{x} + \frac{a}{2} \hat{y}
  \]
- The two basis vectors are:
  \[
  \mathbf{d}_1 = 0, \\
  \mathbf{d}_2 = \frac{a}{2} \hat{x}
  \]
There are only 5 Bravais lattices in 2D:

1. Oblique
2. Rectangular
3. Centered Rectangular
4. Hexagonal
5. Square

Now let's look at lattices in 3D and the concept of the unit cell...

Simple Cubic Lattice:
\[ \hat{a}_1 = a \hat{x} \]
\[ \hat{a}_2 = a \hat{y} \]
\[ \hat{a}_3 = a \hat{z} \]

- It is unpleasant to draw entire lattices in 3D so some small portion of the lattice, that contains the fully symmetry of the lattice, is usually drawn.

- The small portion can be repeated to draw the entire lattice is the "unit cell" and it may be larger than the primitive cell.
There is a difference between unit cells and primitive cells.

- The primitive cell is the volume associated with one lattice point.
- Often it is more convenient to use a unit cell that is larger than the primitive cell since such a cell illustrates the crystal symmetry in a clearer way.

\[ V_{\text{unit}} = a_3 \cdot a_1 \cdot a_2 = a^3 \]

THE GRAY REGION DENOTES THE PRIMITIVE CELL FOR THIS LATTICE WHOSE VOLUME CAN BE DETERMINED FROM THE PRIMITIVE VECTORS INTRODUCED IN Eqs. 2.7 - 2.9

\[ V_{\text{primitive}} = a_3 \cdot (a_1 \times a_2) = \frac{a^3}{4} \]

In 3D there are 14 different Bravais lattices that are classified into 7 different crystal systems. Below we show the unit cells:

1) Triclinic:

2) Monoclinic:

3) Orthorhombic:

4) Tetragonal:

5) Rhombohedral:

6) Hexagonal:

7) Cubic:
Of these, the most important are the Body Centered Cubic (BCC) and the Face Centered Cubic (FCC)...

Body Centered Cubic (BCC)
Lattice:

\[ \mathbf{a}_1 = a \hat{x} \quad \mathbf{a}_2 = a \hat{y} \quad \mathbf{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} + \hat{z}) \]

Or a more symmetric choice is:

\[ \mathbf{a}_1 = \frac{a}{2} (-\hat{x} + \hat{y} + \hat{z}) \quad \mathbf{a}_2 = \frac{a}{2} (\hat{x} - \hat{y} + \hat{z}) \quad \mathbf{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z}) \]

Face Centered Cubic (FCC)
Lattice:

\[ \mathbf{a}_1 = \frac{a}{2} (\hat{y} + \hat{z}) \quad \mathbf{a}_2 = \frac{a}{2} (\hat{x} + \hat{z}) \quad \mathbf{a}_3 = \frac{a}{2} (\hat{x} + \hat{y}) \]

We need to be clear that the choice of the unit cell is not a unique one...

Shown are two different unit cells for the FCC lattice

FCC Unit Cell

FCC Unit Cell
The Wigner-Seitz primitive cells for FCC and BCC lattices are shown:

Materials with FCC lattices:
Aluminum, Nickel, Copper, Platinum, Gold, Lead, Silver, Silicon, Germanium, Diamond, Gallium Arsenide, Indium Phosphide

Materials with BCC lattices:
Lithium, Sodium, Potassium, Chromium, Iron, Molybdenum, Tungsten, Manganese

The lattices of silicon, germanium and diamond...

- Each atom is covalently bonded to four other atoms via sp3 bonds in a tetrahedral configuration
- The lattice defined by the position of the atoms is not a Bravais lattice
- The underlying lattice is an FCC lattice with a two-point (or two-atom) basis
- The lattice constant “a” usually found in the literature is the size of the unit cell, as shown. The primitive lattice vectors are:
  \[ \vec{a}_1 = \frac{a}{2} (y + z), \quad \vec{a}_2 = \frac{a}{2} (x + z) \]
  \[ \vec{a}_3 = \frac{a}{2} (x + y) \] (Same as for a FCC lattice)
- The two basis vectors are:
  \[ d_1 = 0, \quad d_2 = \frac{a}{4} (x + y + z) \]
What about the lattices of III-V binary compounds...

- Each Group III atom is covalently bonded to four other group V atoms (and vice versa) via sp³ bonds in a tetrahedral configuration.
- The underlying lattice is an FCC lattice with a two-point (or two-atom) basis. In contrast to the diamond lattice, the two atoms in the basis of zincblende lattice are different.

What is the Fourier transform of a 1D lattice...

Consider a 1D Bravais lattice:

Now consider a function consisting of a “lattice” of delta functions – in which a delta function is placed at each lattice point:

\[ f(x) = \sum_{n=\infty}^{\infty} \delta(x - n a) \]

The FT of this function is (as you found in your homework):

\[ f(k_x) = \int_{-\infty}^{\infty} dx \sum_{n=\infty}^{\infty} \delta(x - n a) e^{-i k_x x} = \sum_{n=\infty}^{\infty} e^{i k_x n a} = \frac{2\pi}{a} \sum_{m=\infty}^{\infty} \delta(k_x - \frac{2\pi m}{a}) \]

The FT of a train of delta functions is also a train of delta functions in k-space.
The reciprocal lattice is the Fourier transform of a 1D lattice. Consider the 1D Bravais lattice...

For the 1D Bravais lattice,

\[ f(x) = \sum_{n=-\infty}^{\infty} \delta(x - R_n) \]

The FT of this function is:

\[ f(k_x) = \int_{-\infty}^{\infty} f(x) e^{-i k_x x} \, dx = \sum_{n=-\infty}^{\infty} e^{i k_x R_n} \]

The reciprocal lattice in k-space is defined by the set of all points for which the k-vector satisfies,

\[ e^{i k \cdot \vec{R}_n} = 1 \]

for all \( \vec{R}_n \) of the direct lattice.

For the points in k-space belonging to the reciprocal lattice the summation becomes very large!
There are some constraints on the reciprocal lattice of a 1D lattice...

For the 1D Bravais lattice,

\[ \vec{a}_1 = a \hat{x} \]

The position vector \( \vec{R}_n \) of any lattice point is given by: \( \vec{R}_n = n \vec{a}_1 \)

The reciprocal lattice in k-space is defined by the set of all points for which the \( k \) vector satisfies,

\[ e^{i \vec{k} \cdot \vec{R}_n} = 1 \]

for all \( \vec{R}_n \) of the direct lattice

For \( \vec{k} \) to satisfy \( e^{i \vec{k} \cdot \vec{R}_n} = 1 \), it must be that for all \( \vec{R}_n \):

\[ \vec{k} \cdot \vec{R}_n = 2\pi \times \{ \text{integer} \} \]

\[ \Rightarrow k_x n a = 2\pi \times \{ \text{integer} \} \]

\[ \Rightarrow k_x = \frac{m 2\pi}{a} \]

where \( m \) is any integer

\[ \vec{b}_1 = \frac{2\pi}{a} \hat{x} \]

What about in 2D? Consider the 2D rectangular Bravais lattice...

If we place a 2D delta function at each lattice point we get the function:

\[ f(x, y) = \sum_{n=\infty}^{\infty} \sum_{m=\infty}^{\infty} \delta(x - n a) \delta(y - m c) \]

The above notation is too cumbersome, so we write it in a simpler way as:

\[ f(r) = \sum_j \delta^2(r - \vec{R}_j) \]

The summation over \( \vec{R}_j \) is over all the lattice points.

A 2D delta function has the property:

\[ \int d^2 \vec{r} \delta^2(\vec{r} - \vec{r}_0) g(\vec{r}) = g(\vec{r}_0) \]

and it is just a product of two 1D delta functions corresponding to the \( x \) and \( y \) components of the vectors in its arguments:

\[ \delta^2(\vec{r} - \vec{r}_0) = \delta(x - r_{0x}) \delta(y - r_{0y}) \]

Now we Fourier transform the function \( f(r) \):

\[ f(\vec{k}) = \int d^2 \vec{r} \ f(r) \ e^{-i \vec{k} \cdot \vec{r}} = \int d^2 \vec{r} \ \sum_j \delta^2(\vec{r} - \vec{R}_j) \ e^{-i \vec{k} \cdot \vec{r}} \]

\[ = \sum_j e^{-i \vec{k} \cdot \vec{R}_j} = \sum_{n=\infty}^{\infty} \sum_{m=\infty}^{\infty} \delta(k_x - n \frac{2\pi}{a}) \delta(k_y - m \frac{2\pi}{c}) \]
Continuing to examine our Fourier transformed result...

\[ f(k) = \sum_j e^{-i \vec{k} \cdot \vec{R}_j} = \left(\frac{2\pi i}{ac}\right)^2 \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta\left(k_x - n \frac{2\pi}{a}\right) \delta\left(k_y - m \frac{2\pi}{c}\right) \]

• Note also that the reciprocal lattice in \( k \)-space is defined by the set of all points for which the \( k \)-vector satisfies,
\[ e^{i \vec{k} \cdot \vec{R}_j} = 1 \]
for all \( \vec{R}_j \) of the direct lattice.

• Reciprocal lattice as the FT of the direct lattice or as set of all points in \( k \)-space for which \( \exp(\vec{k} \cdot \vec{R}_j) = 1 \) for all \( \vec{R}_j \), are equivalent statements.

We can draw some interesting conclusions in 2D...

• The reciprocal lattice of a Bravais lattice is always a Bravais lattice and has its own primitive lattice vectors, for example, \( \vec{b}_1 \) and \( \vec{b}_2 \) in the above figure.

• The position vector \( \vec{G} \) of any point in the reciprocal lattice can be expressed in terms of the primitive lattice vectors:
\[ \vec{G} = n \vec{b}_1 + m \vec{b}_2 \]

So we can write the FT in a better way as:
\[ f(k) = \left(\frac{2\pi i}{ac}\right)^2 \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta\left(k_x - n \frac{2\pi}{a}\right) \delta\left(k_y - m \frac{2\pi}{c}\right) = \left(\frac{2\pi i}{ac}\right)^2 \sum_j \delta^2(\vec{k} - \vec{G}_j) \]

where \( \Omega_2 = ac \) is the area of the direct lattice primitive cell.
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What about the reciprocal lattice in 3D?

Consider an orthorhombic direct lattice:

$$ \mathbf{R} = n \mathbf{a}_1 + m \mathbf{a}_2 + p \mathbf{a}_3 $$

where $n$, $m$, and $p$ are integers.

Then the corresponding delta-function lattice is:

$$ f(\mathbf{r}) = \sum_j \delta^3(\mathbf{r} - \mathbf{R}_j) $$

A 3D delta function has the property:

$$ \int d^3 \mathbf{r} \delta^3(\mathbf{r} - \mathbf{r}_0) g(\mathbf{r}) = g(\mathbf{r}_0) $$

The reciprocal lattice in $k$-space is defined by the set of all points for which the $k$-vector satisfies: $\exp(i \mathbf{k} \cdot \mathbf{R}_j) = 1$ for all $\mathbf{R}_j$ of the direct lattice. The above relation will hold if $\mathbf{k}$ equals $\mathbf{G}$:

$$ \mathbf{G} = n \mathbf{b}_1 + m \mathbf{b}_2 + p \mathbf{b}_3 \quad \text{and} \quad \mathbf{b}_1 = \frac{2\pi}{a} \mathbf{x}, \quad \mathbf{b}_2 = \frac{2\pi}{c} \mathbf{y}, \quad \mathbf{b}_3 = \frac{2\pi}{d} \mathbf{z} $$

Finally, the FT of the direct lattice is:

$$ f(\mathbf{k}) = \int d^3 \mathbf{r} f(\mathbf{r}) e^{-i \mathbf{k} \cdot \mathbf{r}} = \int d^3 \mathbf{r} \sum_j \delta^3(\mathbf{r} - \mathbf{R}_j) e^{-i \mathbf{k} \cdot \mathbf{r}} $$

$$ = \sum_j e^{-i \mathbf{k} \cdot \mathbf{R}_j} \frac{2\pi}{acd} \sum_j \delta^3(\mathbf{k} - \mathbf{G}_j) = \frac{(2\pi)^3}{\Omega_3} \sum_j \delta^3(\mathbf{k} - \mathbf{G}_j) $$

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Let’s consider again the relationship between direct lattice vectors and reciprocal lattice vectors...

$$ \mathbf{R} = n \mathbf{a}_1 + m \mathbf{a}_2 $$

Remember that the reciprocal lattice in $k$-space is defined by the set of all points for which the $k$-vector satisfies,

$$ e^{i \mathbf{k} \cdot \mathbf{R}} = 1 $$

for all $\mathbf{R}$ of the direct lattice.

So for all direct lattice vectors $\mathbf{R}$ and all reciprocal lattice vectors $\mathbf{G}$ we must have:

$$ e^{i \mathbf{G} \cdot \mathbf{R}} = 1 $$
How do you find the reciprocal lattice vectors in a general case?

More often than not, the direct lattice primitive vectors, \( \mathbf{a}_1, \mathbf{a}_2, \) and \( \mathbf{a}_3 \), are not orthogonal.

**1D lattice:**

If the direct lattice primitive vector is: \( \mathbf{a}_1 = a \mathbf{\hat{x}} \)

and length of primitive cell is: \( \Omega_1 = a \)

Then the reciprocal lattice primitive vector is:

\[
\mathbf{b}_1 = \frac{2\pi}{a} \mathbf{\hat{x}}
\]

Note:

\( \mathbf{a}_1 \cdot \mathbf{b}_1 = 2\pi \)

\( e^{i \mathbf{G}_p \cdot \mathbf{R}_m} = 1 \)

**2D lattice:**

If the direct lattice is in the \( x-y \) plane and the primitive vectors are: \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \)

and area of primitive cell is: \( \Omega_2 = |\mathbf{a}_1 \times \mathbf{a}_2| \)

Then the reciprocal lattice primitive vectors are:

\[
\mathbf{b}_1 = \frac{2\pi}{\Omega_2} \mathbf{\hat{y}}
\]

\[
\mathbf{b}_2 = \frac{2\pi}{\Omega_2} \mathbf{\hat{x}}
\]

Note:

\( \mathbf{a}_j \cdot \mathbf{b}_k = 2\pi \delta_{jk} \) and \( e^{i \mathbf{G}_p \cdot \mathbf{R}_m} = 1 \)

What about the 3D case?

**3D lattice:**

If the direct lattice primitive vectors are: \( \mathbf{a}_1, \mathbf{a}_2, \) and \( \mathbf{a}_3 \)

and volume of primitive cell is: \( \Omega_3 = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| \)

Then the reciprocal lattice primitive vectors are:

\[
\mathbf{b}_1 = \frac{2\pi}{\Omega_3} \mathbf{\hat{z}}
\]

\[
\mathbf{b}_2 = \frac{2\pi}{\Omega_3} \mathbf{\hat{x}}
\]

\[
\mathbf{b}_3 = \frac{2\pi}{\Omega_3} \mathbf{\hat{y}}
\]

Note:

\( \mathbf{a}_j \cdot \mathbf{b}_k = 2\pi \delta_{jk} \)

\( e^{i \mathbf{G}_p \cdot \mathbf{R}_m} = 1 \)

Example 2D lattice: