Lecture 2. Direct Lattices, Wigner-Seitz Cell
Reciprocal Lattices, 1st Brillouin Zone

- Direct Lattices
  - Bravais Lattice
  - Wigner-Seitz cell

- Reciprocal Lattices
  - Scattering by lattices: Bragg Law and Laue Condition
  - 1st Brillouin zone
Recap of L1

Why is the melting $T$ so low in comparison with $E_{bond}$?
The main principle – to minimize the free energy of a system of atoms \((U - TS)\).

Assembly instructions:

- keep the charges of the same sign apart;
- keep electrons close to ions;
- reduce the electron kinetic energy by quantum mechanical spreading (delocalization) of electrons.

Minimum of energy corresponds to a regular (crystal) ordering of atoms in space.
A Bravais lattice is a discrete infinite regular arrangement of points in the \( \mathbb{R}^3 \) space. Translation of the whole lattice by any translation vector leaves the lattice unchanged, all lattice points are equivalent.

\[
\vec{R}_{n,m,p} = n\vec{a}_1 + m\vec{a}_2 + p\vec{a}_3
\]

The choice of **primitive lattice vectors** \( \vec{a}_i \) is not unique.

The Bravais lattice looks exactly the same when viewed from any lattice point.

Not all lattices are Bravais lattices. The honeycomb lattice is not a Bravais lattice: points A and B are not equivalent.
Lattice Cells

**Primitive unit cell** of a Bravais lattice is the **smallest** region which when translated by all different lattice vectors can “tile” the entire lattice **without overlapping**. Primitive unit cell contains only one lattice point.

**Non-primitive unit cell**: contains more than one lattice point.

For a certain lattice there are many different possible unit cells.

Arbitrarily chosen unit cell does not reflects the symmetry of the lattice.
- A, B, and C are primitive unit cells. Why?
- D, E, and F are not. Why?
The volume (3D), area (2D), or length (1D) of a primitive cell

\[ \Omega_1 = |\vec{a}_1| \quad \Omega_2 = |\vec{a}_1 \times \vec{a}_2| \quad \Omega_3 = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| \]

The “volume” is **independent** of the choice of the primitive vectors.

**Example**

\[ \Omega_2 = |\vec{a}_1 \times \vec{a}_2| = |b\hat{x} \times c\hat{y}| = bc \]

\[ \Omega_2 = |\vec{a}_1 \times \vec{a}_2| = |b\hat{x} \times (c\hat{y} + b\hat{x})| = bc \]
Lattice with a Basis

The repetitive element can be more complex than just a point-like atom (e.g., a molecule). The 2D “bear” crystal is not a Bravais lattice if each bear is considered as a lattice point. However, if two (red and green) bears are considered as a single entity (the basis), they form a Bravais lattice.

The location of all basis atoms, with respect to the underlying Bravais lattice point, is given by the basis vectors.

\[
\hat{d}_1 = 0 \quad \hat{d}_2 = h \hat{x}
\]

The honeycomb lattice can be considered as a Bravais lattice with a two-atom basis.

\[
\hat{d}_1 = -\frac{h}{2} \hat{x} \quad \hat{d}_2 = \frac{h}{2} \hat{x}
\]
The Wigner-Seitz cell is a special type of primitive cells: its volume encloses all points in space which are closer to this particular lattice point than to any other.

The Wigner-Seitz cell is unique; it reflects the symmetry of the lattice.

How to draw the Wigner-Seitz cell:
- draw lines connecting a given lattice point to all neighboring lattice points;
- draw bisecting lines (or planes) to the previous lines.

Can you draw the Wigner-Seitz cell for the hexagonal lattice?
**Wigner-Seitz Cell**

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**How to draw the Wigner-Seitz cell:**
- draw lines connecting a given lattice point to all neighboring lattice points;
- draw bisecting lines (or planes) to the previous lines.
**Solid State Physics** is all about propagation of waves in periodic structures.

Propagation of different kind of waves in periodic structures can be treated in a unified manner: (a) acoustic waves in crystals, (b) electrons in crystals, (c) EM waves in periodic LC circuits (filters: band-pass, notch, etc.), (d) EM waves in photonic crystals, etc.

Crystal lattice serves as a diffraction grating for the waves.

The (simplified) condition of strong scattering:

\[ n\lambda = 2a \ (n - \text{integer}) \]

\[ \lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{\hbar k} = \frac{\hbar}{p} \]

- \( \lambda \) – the wavelength
- \( a \) – the lattice period

Thus, there should be specific values of the wave vector for which the scattering is strong (constructive interference).

**The arrangement of ions in “real” space shapes the “geometry” of relevant momentum space.**
Example: Electron Waves in Periodic Structures

The “free” waves in periodic structures are not entirely free – they interact with the periodic potential of the lattice, and, thus, they are “modulated” by the lattice.

Electron waves in a periodic potential:  
\[ -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = \varepsilon \psi(\vec{r}) \]

periodic  \( V(\vec{r}) = V(\vec{r} + \vec{R}) \)  \( \vec{R} \) is any lattice vector:  
\[ \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \]

Bloch’s Theorem states that the electron wave functions in a crystal have a basis consisting entirely of Bloch wave energy eigenstates.

\[ \psi_k(\vec{r}) = u_k(\vec{r})e^{i\vec{k} \cdot \vec{r}} \quad (“modulated plane wave”) \]

\[ u_k(\vec{r}) = u_k(\vec{r} + \vec{R}) \text{ is periodic in the unit cell} \]

and \( \vec{k} \) can be chosen within the 1st Brillouin zone.

Though the wave function is not periodic in the real space - the wavefunction at positions \( \vec{r} \) and \( \vec{r} + \vec{R} \) differs by the phase factor \( e^{i\vec{k} \cdot \vec{R}} \), but all measurable properties depend only on \( |\psi_k(\vec{r})|^2 = |u_k(\vec{r})|^2 \), which is periodic in the real space.

The real part of a Bloch wave in 1D (solid line). It is a product of the dotted line, which represents \( e^{i\vec{k} \cdot \vec{r}} \), and \( u_k(\vec{r}) \) has the same periodicity as the lattice.
Reciprocal Lattice in the $k$ (or Momentum) Space

Consider a plane wave (mechanical, electrical, etc.) in a crystal:

$$\Psi_k(\vec{r}) = u_k(\vec{r})e^{i\vec{k} \cdot \vec{r}} \quad \vec{k} - \text{an arbitrary wave vector}$$

Waves $\Psi_k(r)$ should have the periodicity of the Bravais lattice:

$$\Psi_k(\vec{r}) = \Psi_k(\vec{r} + \vec{R}) \quad e^{i\vec{k} \cdot \vec{r}} = e^{i\vec{k} \cdot (\vec{r} + \vec{R})}$$

$$\vec{k} = q\vec{b}_1 + s\vec{b}_2 + t\vec{b}_3$$

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

$$e^{i\vec{k} \cdot \vec{R}} = 1 \quad \vec{k} \cdot \vec{R} = 2\pi j \quad j = 0,1,2 \ldots$$

The equation must be fulfilled for every possible combination of integer $m, n, p$. This implies that $q, s, t$ must also be integers, and the set of vectors $\vec{k}$ (the reciprocal lattice) forms a Bravais lattice as well!

The reciprocal lattice in the $k$ (momentum) space is the set of all $\vec{k}$ for which the corresponding plane waves $\Psi_k(r)$ have the periodicity of the Bravais lattice in “real” space.
Example: Elastic Scattering of Waves by 1D Lattice

The incoming plane wave induces at all lattice sites the emission of secondary spherical waves, whereas the further scattering of spherical waves is neglected. The power reflected from each atom is a small fraction of the incident power, and many atom are involved in scattering. The scattered wave is the result of interference of all secondary waves.

**Constructive** interference of reflected waves: 

\[ e^{i\vec{k} \cdot \vec{r}} = 1 \quad \Delta \varphi = 2\pi j \]

\[ k \cdot R = 2\pi j \quad k \cdot n a = 2\pi j \quad k = \frac{j 2\pi}{n a} \]

For \( n = 1 \):

The length of the reciprocal lattice vectors is proportional to the reciprocal of the length of the direct lattice vectors. This is where the term reciprocal lattice comes from.
Reciprocal Lattices in 1D and 2D

Direct lattice (or the actual lattice):

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

Reciprocal lattice:

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

Real space

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

K space

\[ \vec{G} = n \vec{b}_1 + m \vec{b}_2 \]

Alternative definition of the reciprocal lattice:

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

- for all \( \vec{G} \) and \( \vec{R} \).
Formal Way to Introduce Reciprocal Lattice

Let’s choose a basis \{\vec{b}\}:

\[
\vec{b}_1 \cdot \vec{a}_2 = \vec{b}_1 \cdot \vec{a}_3 = 0 \quad \vec{b}_1 = c\vec{a}_2 \times \vec{a}_3 \quad \text{(if the basis \{\vec{a}\} is orthogonal, } \vec{b}_1 \parallel \vec{a}_1) \\
\vec{b}_1 \cdot \vec{a}_1 = c\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = 2\pi \quad c = \frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{\Omega_3} \quad \Omega_3 - \text{the volume of the parallelepiped spanned by } \vec{a}_i
\]

\[
\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\Omega_3} \quad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\Omega_3} \quad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\Omega_3}
\]

The main features of the reciprocal lattice:

- the reciprocal lattice vectors are normal to \((nmp)\) planes of direct lattice;
- every symmetry property of the lattice is also a symmetry property of the reciprocal lattice;
- The Bravais lattices in real and \(k\)-spaces may be different (e.g. \(fcc\) becomes \(bcc\)).
The reciprocal lattice of a \( fcc \) lattice with edge length \( a \) is a \( bcc \) lattice with edge length \( 4\pi/a \). Accordingly, the reciprocal-lattice of a \( bcc \) lattice is a \( fcc \) lattice.

The direct and reciprocal lattices do not necessarily resemble each other.
Diffraction Conditions

Scattering of incident waves (diffraction) is observed if their wave vectors satisfy the condition of constructive interference.

**2D,3D**

**Bragg**: the reflected beams interfere constructively if

\[ 2a \sin \theta = n\lambda \]

**Laue**: the wave vectors of the incident and scattered waves are different by a vector of the reciprocal lattice.

\[ \vec{k} - \vec{k}' = \vec{G} \]
Equivalence of Bragg and Laue Conditions

\( \vec{k}' = \vec{k} - \vec{G} \quad |\vec{k}| = |\vec{k}'| \) - elastic scattering

\[(k')^2 = k^2 - 2\vec{k} \cdot \vec{G} + G^2\]

\[
\vec{k} \cdot \vec{G} = \left( \frac{G}{2} \right)^2
\]

2a cos \( \theta \) = \( m \lambda \)

\[
\frac{2\pi}{\lambda} \left( \frac{m \cdot 2\pi}{a} \right) \cos \theta = \frac{1}{2} \left( \frac{m \cdot 2\pi}{a} \right)^2
\]

\[
\vec{k} \cdot \vec{G} = \frac{G^2}{2} \quad \text{or} \quad \frac{\vec{k} \cdot \vec{G}}{2} = \left( \frac{G}{2} \right)^2
\]

1D

\[
\vec{k} \cdot \vec{G} = kG = \frac{G^2}{2} \quad k = \frac{b}{2} \rightarrow \lambda = 2a
\]
The Brillouin Zones are confined by the planes that are the perpendicular bisectors of the reciprocal vectors. A wave whose wave vector drawn from the origin terminates on any of the planes will satisfy the condition of diffraction.

\[ \vec{k} \cdot \frac{\vec{G}}{2} = \left( \frac{\vec{G}}{2} \right)^2 \] - diffraction condition
How to Draw Brillouin Zones

Reciprocal Lattice

- Bragg plane
Brillouin Zones for a Square 2D Lattice
**The First Brillouin Zone**

The first Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice centered at the origin $\mathbf{G} = 0$.

Waves with the periodicity of the crystal lattice (phonons, electrons, etc.) are unchanged if their wave vector is shifted by a reciprocal vector $\mathbf{k} \to \mathbf{k} + \mathbf{G}$

\[
e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{R}} = e^{i \mathbf{k} \cdot \mathbf{R}} e^{i \mathbf{G} \cdot \mathbf{R}} = e^{i \mathbf{k} \cdot \mathbf{R}}
\]

Thus, any primitive cell in the reciprocal space includes all physically different $\mathbf{k}$.

1D

![1D direct lattice](image1)

2D

![2D direct lattice](image2)
Significance of the first Brillouin Zone

At the next lecture, we’ll consider elastic waves in crystal lattices. What is the shortest wavelength (or the largest wavevector) the lattice wave can have?

Phase difference between oscillations of two neighboring atoms is meaningful only within \( \pm \pi \). The shortest wavelength = 2a. So allowed values of \( k \) are between \(-\frac{\pi}{a}\) and \(\frac{\pi}{a}\), which is the first Brillouin zone in 1D.

Example of the transverse sound wave:

**Aliasing**: example of the transverse sound wave:

\[
k_1 = \frac{2\pi}{10a}
\]

\[
k_2 = \frac{2\pi}{10a} + \frac{2\pi}{a} = 2\pi \frac{11}{10a}
\]

All physically distinct values of \( k \) for the waves with the periodicity of a Bravais lattice are within the first Brillouin zone.
Volume of the First Brillouin Zone

The volume (3D), area (2D), or length (1D) of the first Brillouin zone:

\[
\Pi_1 = |\vec{b}_1| \quad \Pi_2 = |\vec{b}_1 \times \vec{b}_2| \quad \Pi_3 = |\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)|
\]

In all dimensions the following relationship holds between the “volumes” of the direct and reciprocal lattice primitive cells:

\[
\Pi_d = \frac{(2\pi)^d}{\Omega_d}
\]
The common building blocks for most high temperature (high T_c) superconductors are copper oxide layers, as depicted in Figure 1.6(a). Assume the distance between copper atoms (filled circles) is \( a \). For simplicity let us also assume that in the third dimension these \( \text{CuO}_2 \) layers are simply stacked with spacing \( c \), and there are no other atoms in the crystal. In first approximation the layers have a fourfold symmetry; the crystal is tetragonal.

(a) Sketch the Bravais lattice and indicate a possible set of primitive vectors for this crystal. What is the unit cell, and what is the basis?

(b) In LaCuO_4 one discovers, at closer inspection, that the \( \text{CuO}_2 \) lattice is actually not flat, but that the oxygen atoms are moved a small amount out of the plane ("up" or "down") in an alternating fashion (in Figure 1.6(b), \( \oplus \) means up and \( \ominus \) means down). What is the primitive cell and lattice spacing for this crystal? What is the reciprocal lattice? Describe (qualitatively) what happens in the X-ray diffraction pattern as the distortion is decreased gradually to zero.

(a) One of many choices for the Bravais lattice is shown in Figure 11.2 along with its unit cell, basis, and primitive vectors.

(b) A choice for the Bravais lattice in this case, as well as for the new primitive unit cell, is shown in Figure 11.3. Note the new lattice spacing is \( \sqrt{2}a \).

Figure 11.4 Reciprocal lattices for distorted (new) and pristine (old) \( \text{CuO}_2 \) lattices.

The reciprocal lattices for both Bravais lattices are shown in Figure 11.4: the open circles correspond to weak X-ray diffraction peaks and the filled circles are strong peaks. As the distortion decreases, the structure factor of the weaker Bragg peaks of the distorted crystal goes to zero. Hence the X-ray pattern returns to the original reciprocal lattice pattern.
Reciprocal Lattice as the Fourier Transform of the Direct Lattice

Consider a 1D Bravais lattice of delta functions (“Dirac comb”):

\[ \delta(x - na) = \begin{cases} \infty & x = na \\ 0 & x \neq na \end{cases} \]

\[ \int \delta(x - na) \, dx = 1 \]

\[ \int \text{d}x \sum_{n=-\infty}^{\infty} \delta(x - na) \, e^{ikx} = \frac{2\pi}{a} \sum_{m=-\infty}^{\infty} \delta \left( k - m \frac{2\pi}{a} \right) \]

The FT of a train of delta functions is also a train of delta functions in the \( k \)-space.

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

Homework problem
Reciprocal Lattice as the Fourier Transform of the Direct Lattice (cont’d)

\[ f(\mathbf{k}) = \frac{(2\pi)^2}{a_1 a_2} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta \left( k_x - n \frac{2\pi}{a_1} \right) \delta \left( k_y - m \frac{2\pi}{a_2} \right) \]

\[ f(\mathbf{k}) = \frac{(2\pi)^3}{a_1 a_2 a_3} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \left( k_x - n \frac{2\pi}{a_1} \right) \delta \left( k_y - m \frac{2\pi}{a_2} \right) \delta \left( k_z - n \frac{2\pi}{a_3} \right) \]
Crystal structure = Bravais Lattice + Basis

- The Wigner-Seitz primitive cell (reflects the symmetry of the lattice).

Reciprocal Lattice

- Scattering by lattices: **Bragg** \( 2d \sin \theta = n\lambda \) and **Laue** \( \vec{k} \cdot \vec{G} = \left( \frac{\vec{G}}{2} \right)^2 \).
- The first Brillouin zone is the Wigner-Seitz cell of the reciprocal lattice. It contains all physically different \( k \) for the waves with the periodicity of direct lattice.
- The reciprocal lattice is a Fourier transform of the direct lattice.

\[ \vec{k} - \vec{k}' = \vec{G} \]

Today: Simon Ch. 12,13. Next lecture: Simon Ch. 2.