Studying Bloch's Theorem

Quick Definitions:

The crystal potential $V(\vec{r})$ describes the ideal crystal: static cores in a perfect periodic arrangement surrounded by electrons[1].

$$V(\vec{r}+\vec{R_n}) = V(\vec{r}) \tag{1}$$

-The crystal appears the same at $\vec{r}$ and $\vec{r}+\vec{R_n}$.

- The **Bravais Lattice** is the collection of all vectors $\{\vec{R}\}$ (called Lattice Vectors).

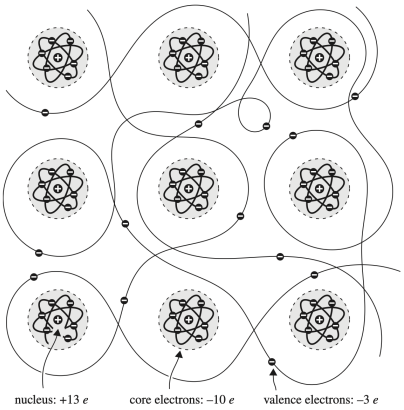


Figure 1: Schematic of a solid with atoms with atomic number z =13 containing cores and valence electrons.

Any periodic lattice $\{\vec{R}\}$ can be written as:

$$\vec{R_n} = n_1\vec{a_1} + n_2\vec{a_2} + n_3\vec{a_3} \tag{2}$$

- The $\vec{a_i}$ vectors are called **primitive lattice vectors**.

- The Bravais lattice have a lattice point density of $1/\Omega_p$ with $\Omega_p = |(\vec{a_1} \times \vec{a_2}).\vec{a_3}|$

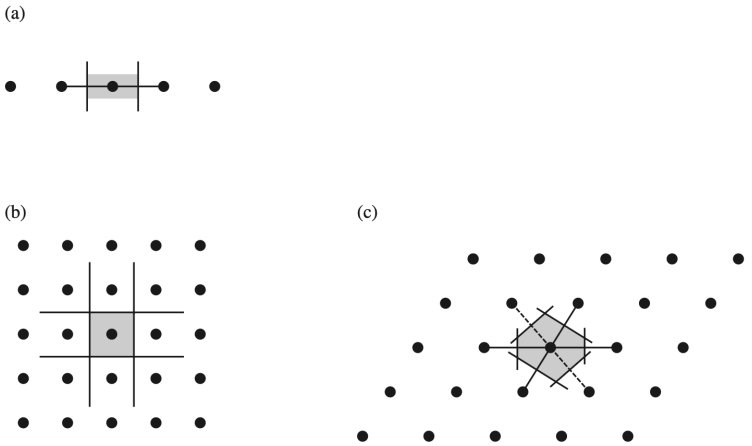
- **Primitive Cell**
  - A region of space that, when translated by all Bravais lattice vectors, fills the entire crystal without overlaps or voids.
  - Contains exactly one lattice point.
  - Volume is constant and equal to Ω_p.
  - A parallelepiped formed by primitive lattice vectors is one possible primitive cell.
- **Unit Cell**
  - A region that fills space by translation via a subset of Bravais lattice vectors.
  - Volume satisfies $\Omega_u = \nu\Omega_p$, where $\nu = 1, 2, 3, \ldots$.

[1]Cohen, Marvin and Louie, Steven G. Fundamentals of condensed matter physics.

  - A primitive cell is a unit cell with the minimum possible volume ($\nu = 1$).

- **Basis**
  - The set of atoms and their coordinates within a unit cell that form the crystal.
  - Represented as a set of vectors $\{\tau_\mu\}$, $\mu = 1, 2, \ldots, N_b$, where N_b is the number of atoms in the basis.
  - A primitive basis is the minimal basis associated with a primitive cell.
  - Two bases differing by a constant displacement vector $\{\tau_\mu + \tau_0\}$ describe the same crystal.
  - Changing any basis vector by a lattice translation $(\tau_\mu + R_n)$ alters the unit cell but not the crystal itself.

- **Wigner–Seitz Cell**
  - A special type of primitive cell.
  - Constructed by:
    * Drawing lines from the origin to all neighboring lattice points.
    * Constructing planes that bisect and are perpendicular to these lines.
    * Forming the smallest polyhedron that encloses the origin.
  - It is the most compact and symmetric of all primitive cells.



(a) One-dimensional Wigner–Seitz cell. (b) and (c) Two-dimensional Wigner–Seitz cells.

- **Reciprocal Lattice**
  - It is a mathematical construction defined as a new lattice:

$$\vec{G_m} = m_1\vec{g_1} + m_2\vec{g_2} + m_3\vec{g_3} \quad (m_1, m_2, m_3 = \text{integer}) \tag{3}$$

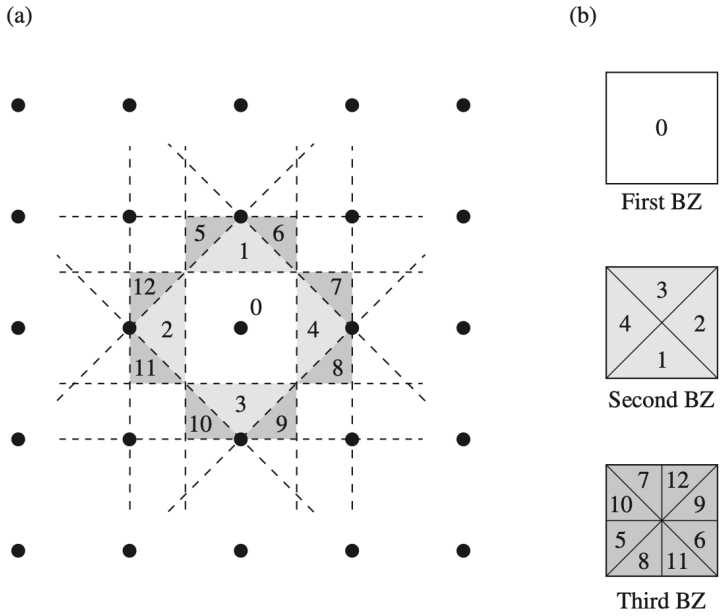
  such that

$$\vec{G_m} \cdot \vec{R_n} = 2\pi\nu \quad (\nu = \text{integer}) \tag{4}$$

- **Brillouin Zone**
  - A primitive cell built as the Wigner-Seitz cell in the Bravais lattice, but in the reciprocal lattice.
  - For three dimensions, the Brillouin zone volume is measured in inverse length.

$$\Omega_{BZ} = \frac{8\pi^3}{\Omega_p} \tag{5}$$

– A second and higher Brillouin zone can be defined by regions in space between the bisecting planes. These regions are mapped back into the first Brillouin zone by mapping reciprocal lattice vectors. The mapping is $\vec{k} = \vec{k} - \vec{G_m}$



Bloch's Theorem

The solutions of the Schrödinger equation of an electron in a periodic lattice can be expressed as a plane wave $e^{i\vec{k}\cdot\vec{r}}$ times a function having the periodic symmetry of the lattice; hence,

$$\Psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}} \tag{6}$$

where

$$u_{\vec{k}}(\vec{r} + \vec{R}n) = u_{\vec{k}}(\vec{r}). \tag{7}$$

Simulation for a 1D Lattice

Let's start with a simple 1D periodic lattice to illustrate Bloch's theorem. We'll assume a periodic potential (e.g., a cosine potential) and construct a Bloch wavefunction. The plot will show an oscillatory wave function modulated by the periodic $u(x)$, with the probability density reflecting the lattice periodicity.

The choice of $k = \pi/(2a)$ in the Mathematica code for the 1D Bloch wavefunction simulation is a specific value selected to illustrate the wavefunction within the **first Brillouin zone**. Below, we break down why this value is chosen and why the first Brillouin zone is defined as $[-\pi/a, \pi/a]$.

For a 1D lattice with lattice constant a, the first Brillouin zone is the interval of $\mathbf{k}$-values where the wavefunction is not redundant due to the lattice's translational symmetry.

- **Lattice vectors**: In a 1D lattice, the lattice points are at positions $R = na$, where $n \in \mathbb{Z}$ and a is the lattice constant.
- **Reciprocal lattice**: The reciprocal lattice vectors are defined such that $e^{i\mathbf{G}\cdot\mathbf{R}} = 1$. For a 1D lattice, the reciprocal lattice vectors are:

$$G = \frac{2\pi}{a}m, \quad m \in \mathbb{Z}.$$

- **First Brillouin zone in 1D**: This is the Wigner-Seitz cell[2] in reciprocal space, which in 1D is the interval centered at $k = 0$ and bounded by the points where the reciprocal lattice vectors cause a Bragg reflection[3] . The boundaries occur at:

$$k = \pm\frac{\pi}{a},$$

because the wavevector k satisfies the Bragg condition for diffraction at these points. Thus, the first Brillouin zone is:

$$k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right].$$

Any k outside this range is equivalent to a k inside it by adding a reciprocal lattice vector $\mathbf{G}$.

The value $k = \pi/(2a)$ is chosen for the following reasons:

- **Inside the First Brillouin Zone**: The wavevector k must lie within $[-\pi/a, \pi/a]$ to represent a unique electronic state. The choice $k = \pi/(2a)$ is well within this range:

$$-\frac{\pi}{a} \leq \frac{\pi}{2a} \leq \frac{\pi}{a}.$$

It's a convenient value that's neither at the center ($k = 0$) nor at the edge ($k = \pm\pi/a$) of the Brillouin zone, making it illustrative for visualizing the Bloch wavefunction.

- **Physical Significance**: At $k = \pi/(2a)$, the plane wave part of the Bloch wavefunction, e^{ikx}, has a wavelength that is related to the lattice periodicity but not at the extreme cases:
  - At $k = 0$, the wavefunction is purely periodic with no overall phase progression.
  - At $k = \pi/a$, the wavefunction is at the Brillouin zone boundary, where band gaps often appear due to Bragg scattering.
  - $k = \pi/(2a)$ is an intermediate case, showing a wavefunction with both a propagating plane wave character and the periodic modulation from $u_k(x)$.

- **Visualization**: This value produces a wavefunction with a clear oscillatory behavior in the plane wave component ($e^{i(\pi/(2a))x}$) that interacts with the periodic function $u(x)$, making the plots (real part, imaginary part, and probability density) visually informative. The wavelength of the plane wave is:

$$\lambda = \frac{2\pi}{k} = \frac{2\pi}{\pi/(2a)} = 4a,$$

which spans four lattice constants, providing a nice scale for plotting over a few unit cells.

- **Arbitrary but Representative**: The exact value isn't critical for a qualitative demonstration. Any k within $[-\pi/a, \pi/a]$ could be used, but $\pi/(2a)$ is a simple, non-zero value that avoids the special cases at the zone center or boundary, making it a good choice for pedagogical purposes.

The boundaries of the first Brillouin zone arise from the periodicity of the lattice in real space, which imposes constraints on the wavevector in reciprocal space:

- The wavefunction satisfies:

$$\psi_k(x + a) = e^{ika}\psi_k(x).$$

[2]Following the same steps previously explained

[3]The condition for constructive interference is $\vec{k} \cdot \vec{G} = \frac{1}{2}|\vec{G}|^2$. So, for maximum interference, let's say in 1D, $\vec{k} = \frac{\pi}{a}\hat{i}$. $\lambda = \frac{2\pi}{k} = 2a$, and if $\lambda = 2a$ the Bragg's law will have the maximum value: $n\lambda = 2a\sin\theta$.

This phase factor e^{ika} defines the wavevector k. However, adding a reciprocal lattice vector $\mathbf{G} = 2\pi m/a$ to k leaves the physics unchanged:

$$e^{i(k+\mathbf{G})x} = e^{ikx}e^{i(2\pi m/a)x} = e^{ikx}e^{i2\pi m(x/a)}.$$

Since x/a is an integer at lattice points, $e^{i2\pi m(x/a)} = 1$, so k and $k+\mathbf{G}$ describe equivalent states.

- $k = 0$: The wavefunction becomes purely periodic, $\psi(x) = u(x)$, resembling a standing wave.
- $k = \pi/a$: The wavefunction is at the Brillouin zone edge, often showing standing wave behavior due to interference (e.g., $\psi(x) \propto \cos(\pi x/a)u(x)$).
- $k = \pi/(4a)$: A different intermediate value, with a longer wavelength ($\lambda = 8a$).

The choice $k = \pi/(2a)$ is a practical one for visualization, balancing the plane wave's oscillation frequency with the periodic modulation.

For higher-dimensional lattices (e.g., 2D square or hexagonal), the first Brillouin zone is a region in $\mathbf{k}$-space determined by the reciprocal lattice vectors. For example:

- **2D Square Lattice**: Reciprocal lattice vectors are $\mathbf{b}_1 = (2\pi/a, 0)$, $\mathbf{b}_2 = (0, 2\pi/a)$, and the first Brillouin zone is a square $[-\pi/a, \pi/a]^2$. The code used $k_x = k_y = \pi/(2a)$ for similar reasons: it's within the zone and produces clear visualizations.
- **Hexagonal Lattice**: The Brillouin zone is hexagonal, and the choice of $\mathbf{k}$ depends on the reciprocal lattice vectors, but the principle remains the same.