7

Energy Bands

Ref: textbook, Chapter 7
Q: Why are there insulators and conductors?
Q: What will happen when an electron moves in a crystal?

In the previous chapter, we discussed free electron gases, where we made three approximations

- Ignore the lattice background
- Ignore the interactions between electrons
- Ignore the interactions between phonons and electrons

In this chapter, we will take the lattice background into consideration and see what will happen.

### 7.1. Energy Bands and Band Gap

#### 7.1.1. Phenomenon

Consider a 1D solid. In the absence of a lattice background, the kinetic energy of one electron can take any positive values ($\epsilon = \frac{p^2}{2m} > 0$).

In the presence of a lattice background, the kinetic energy (as a function of the momentum) breaks into pieces. Each piece is known as an energy band. Between two energy bands, there may be a forbidden region, which the energy of an electron can never enter. This forbidden region is called the band gap.

![Fig. 1. The dispersion relation for (a) a free electron gas and (b) electrons moving in a crystal.](image)

Fig. 1. The dispersion relation for (a) a free electron gas and (b) electrons moving in a crystal.
7.1.2. Why are there two possible energy at \( k = \pi / a \)?

Here we consider the gap that appears at the momentum \( k = \pm \pi / a \). At these two momentum points, there are two linear-independent plane waves

\[
\psi_+(x) = \frac{1}{\sqrt{2a}} e^{i\pi x/a}, \quad \psi_-(x) = -\frac{1}{\sqrt{2a}} e^{-i\pi x/a}.
\]

We can form two standing waves using these two plane waves

\[
\begin{align*}
\psi_+(x) &= \frac{1}{\sqrt{2a}} e^{i\pi x/a} + \frac{1}{\sqrt{2a}} e^{-i\pi x/a} = \sqrt{2/a} \cos \left( \frac{\pi}{a} x \right) \\
\psi_-(x) &= \frac{1}{\sqrt{2a}} e^{i\pi x/a} - \frac{1}{\sqrt{2a}} e^{-i\pi x/a} = \sqrt{2/a} \sin \left( \frac{\pi}{a} x \right)
\end{align*}
\]

The probability density is

\[
\rho = |\psi_+(x)|^2 = \frac{1}{a} \cos \left( \frac{\pi}{a} x \right) \quad \text{for } +
\]

\[
|\psi_+(x)|^2 = \frac{1}{a} \sin \left( \frac{\pi}{a} x \right) \quad \text{for } -
\]

In the absence of lattices, these two standing waves have exactly the same energy

\[
\epsilon = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 (\pm \pi/a)^2}{2m} = \frac{\hbar^2 \pi^2}{2m a^2}
\]

So, we have \( \epsilon_+ = \epsilon_- = \hbar^2 \pi^2 / 2m a^2 \)

However, in the presence of the lattice, the \( \psi_+ \) wave has a lower energy than \( \psi_- \), because the electron has a higher probably to appear near an ion for \( \psi_+ \). This is the reason why at momentum \( k = \pi / a \) we have two possible energies (point A and B in figure 1).

- Similar band gaps will arise at \( k = n \pi / a \) for any integer \( n \).
- The momentum region \(-n \frac{\pi}{a} < k < -(n - 1) \frac{\pi}{a}\) and \((n - 1) \frac{\pi}{a} < k < n \frac{\pi}{a}\) is called the \(n\)th Brillouin zones (This is the same Brillouin zones as we learned in the reciprocal lattice).
- In side the of these Brillouin zones, the energy is a smooth function and this smooth function is called the \(n\)th band.
- At each boundary of the Brillouin zones, the energy curve shows a jump and thus an energy gap opens up.

### 7.1.3. Magnitude of the band gap

The size of the gap can be estimated as the following

\[
E_g = \left| \int_0^a U(x) \rho_+(x) \, dx - \int_0^a U(x) \rho_-(x) \, dx \right|
\]  \hspace{1cm} (7.5)

where \(U(x)\) is the potential energy from the ions. Because the lattice is periodic, \(U(x)\) is a periodic function \(U(x + a) = U(x)\) where \(a\) is the lattice constant. In addition, with out loss of generality, we can assume that \(U(x)\) is an even function \(U(x) = -U(x)\).

For such an even periodic function, we can write it as a a Fourier series.

\[
U(x) = \frac{U_0}{2} + \sum_{n} U_n \cos \left( \frac{2\pi n}{a}x \right)
\]  \hspace{1cm} (7.6)

and

\[
U_n = \frac{2}{a} \int_0^a U(x) \cos \left( \frac{2\pi n}{a}x \right) \, dx
\]  \hspace{1cm} (7.7)

The energy gap at \(k = \pm \pi / a\) is

\[
E_k = \left| \int_0^a U(x)[\rho_+(x) - \rho_-(x)] \, dx \right| = \left| \frac{2}{a} \int_0^a U(x) \left[ \cos \left( \frac{\pi}{a}x \right) - \sin \left( \frac{\pi}{a}x \right) \right] \, dx \right| = \left| \frac{2}{a} \int_0^a U(x) \cos \left( \frac{2\pi}{a}x \right) \, dx \right| = |U_1| \hspace{1cm} (7.8)
\]

The energy gap at \(k = \pm n \pi / a\) is

\[
E_k = \left| \int_0^a U(x)[\rho_+(x) - \rho_-(x)] \, dx \right| = \left| \frac{2}{a} \int_0^a U(x) \cos \left( \frac{\pi}{a}x \right) - \sin \left( \frac{\pi}{a}n \right) \, dx \right| = \left| \frac{2}{a} \int_0^a U(x) \cos \left( \frac{2\pi}{a}n x \right) \, dx \right| = |U_n| \hspace{1cm} (7.9)
\]

### 7.2. Bloch waves

#### 7.2.1. The effect of the lattice potential: the Hamiltonian and the Schrodinger equation

The Hamiltonian

\[
H = \frac{\hbar^2}{2m} + U(x) = -\frac{\hbar^2}{2m} \partial_x^2 + U(x)
\]  \hspace{1cm} (7.10)

The Schrodinger equation

\[
\frac{\hbar^2}{2m} \partial_x^2 \psi(x) + U(x) \psi(x) = \epsilon \psi(x)
\]  \hspace{1cm} (7.11)

This equation is in general hard (or impossible) to solve analytically. However, F. Bloch managed to prove a very important theorem, which states that the solution to this equation must take the following form:

\[
\psi_k(x) = u_k(x) e^{i k \cdot x}
\]  \hspace{1cm} (7.12)

Here, \(u(x)\) is a periodic function \(u_k(x + a) = u_k(x)\), which has the same period as the lattice.

- This conclusion is true in any dimensions. For example, in 3D, we have \(\psi(r) = u_k(r) \exp \left( i \cdot \frac{r}{k} \right) \) where \(u_k(r)\) is a 3D periodic function \(u_k(r + T) = u_k(r)\) where \(T\) is any lattice vector.

This type of waves are known as the Bloch wave. They have some nice properties

- The plane waves are a special type of Bloch waves with the function \(u(x) = \text{constant}\).
The Bloch wave is NOT an eigenstate of the momentum operator. In other words, it doesn’t have a well-defined momentum (unless \( u(x) = \text{constant} \)). However, the parameter \( k \) in the Bloch wave behaves very similarly to the momentum. We call \( h k \) the lattice momentum.

Lattice momentum is not the momentum, but it is conserved in a lattice.

### 7.2.2. The proof of the Bloch theorem

Define the translation operator

\[
T_a \psi(r) = \psi(r + a)
\]

(7.13)

where \( a \) is the lattice constant. This operator shift our quantum system in real space by the lattice constant \( a \).

Under translation by \( a \), a quantum operator \( O \) changes as \( O \rightarrow T_a O T_a^{-1} \). Therefore, for the Hamiltonian

\[
T_a H(x) T_a^{-1} = H(x + a)
\]

(7.14)

Because

\[
H(x) = -\frac{\hbar^2}{2m} \partial_x^2 + U(x)
\]

(7.15)

and

\[
H(x + a) = -\frac{\hbar^2}{2m} \partial_{x+a}^2 + U(x + a) = -\frac{\hbar^2}{2m} \partial_x^2 + U(x)
\]

(7.16)

we know immediately that \( H(x) = H(x + a) \). And thus

\[
T_a H(x) T_a^{-1} = H(x + a) = H(x)
\]

(7.17)

In other words,

\[
T_a H(x) = H(x) T_a
\]

(7.18)

so

\[
[T_a, H] = 0
\]

(7.19)

If two operators commute, we know that we can find common eigenstates of these two operators. For \( T_a \) and \( H \), this means that we can find a set of (complete orthonormal) basis \( \psi_k(x) \), such that

\[
H \psi_k(x) = \epsilon \psi_k(x) \quad \text{and} \quad T_a \psi_k(x) = e^{i k a} \psi_k(x)
\]

(7.20)

Here, we used the fact that \( H \) is an Hermitian operator, so that its eigenvalues \( \epsilon \) must be real. For \( T_a \), because it is a unitary operator, its eigenvalue must be a complex with absolute value 1.

Define

\[
\psi_k(x) = e^{-i k x} \psi_k(x)
\]

(7.21)

It is easy to prove that \( u_k(x) \) is a periodic function \( u_k(x) = u_k(x + a) \).

\[
u_k(x + a) = e^{-i k (x+a)} \psi_k(x + a) = e^{-i k x} T_a \psi_k(x) = e^{-i k x} e^{i k a} \psi_k(x) = e^{-i k x} \psi_k(x) = u_k(x)
\]

(7.22)

Therefore,

\[
\psi_k(x) = u_k(x) e^{i k x}
\]

(7.23)

where \( u_k(x) \) is a periodic function.

### 7.3. Properties of Bloch waves and crystal momentum

Eigen wave functions for a single particle moving in a periodic potential: Bloch waves

\[
\psi_{nk}(x) = u_{nk}(x) e^{i k x}
\]

(7.24)

Here \( k \) is known as the crystal momentum. The corresponding eigenenergy is \( \epsilon_{n,k} \), which satisfies
\[ H \psi_{n,k}(x) = \epsilon_{n,k} \psi_{n,k}(x) \]  \hspace{1cm} (7.25)

### 7.3.1. value of \( k \)?

- The crystal momenta are only well-defined modulo \( G \), where \( G \) is a reciprocal vector.
- Therefore, we can limit the crystal momentum to the first Brillouin zone without loss of information (e.g. for a 1D system, \(-\pi/a \leq k < \pi/a\)).

**Proof**: Suppose we have a Bloch wave with crystal momentum \( k \)

\[ \psi_{n,k}(x) = u_{n,k}(x) e^{i k x} \]  \hspace{1cm} (7.26)

Define \( k' = k + G \)

\[ \psi_{n,k} (x) = u_{n,k}(x) e^{i k x} = u_{n,k'-G}(x) e^{i (k'-G) x} = u_{n,k'-G}(x) e^{-i G x} e^{i k' x} \]  \hspace{1cm} (7.27)

Define \( u_{n,k}(x) = u_{n,k'-G}(x) e^{-i G x} \)

\[ \psi_{n,k} (x) = u_{n,k'-G}(x) e^{i k' x} = u_{n,k}(x) e^{i k x} \]  \hspace{1cm} (7.28)

It is easy to check that \( u_{n,k}(x) = u_{n,k}(x+T) \) where \( T \) is any lattice vector.

\[ u_{n,k}(x+T) = u_{n,k'-G}(x+T) e^{-i G (x+T)} = u_{n,k'-G}(x) e^{-i G x} = u_{n,k}(x) \]  \hspace{1cm} (7.29)

Therefore, \( \psi_{n,k}(x) = u_{n,k}(x) e^{i k x} \) \( \) is also a Bloch wave function with crystal momentum \( k' \)

\[ \psi_{n,k'}(x) = u_{n,k}(x) e^{i k' x} = \psi_{n,k}(x) \]  \hspace{1cm} (7.30)

**Conclusion**: as long as \( k \) and \( k' \) differs by a reciprocal lattice vector \( G \), we can write a Bloch wavefunction with crystal momentum \( k \) as a Bloch wavefunction with crystal momentum \( k' \).

In other words, crystal momentum is only well defined modulo \( G \)

![Fig. 3. Dispersion relation \( \epsilon_n(k) \) shown in extended zone, reduced zone and periodic zone. (Figure 4 in text book page 225).](image-url)
### 7.3.2. Reduced Brillouin zone

Since the crystal momentum is only well defined modulo $G$, we can limit the momentum to the first Brillouin zone (e.g. for a 1D system, $-\pi/a \leq k < \pi/a$) without loss of information. We can plot the eigen-energy $\epsilon_{n,k}$ as a function of $k$ in the first Brillouin zone. This way of plotting $\epsilon_{n,k}$ is known as the reduced Brillouin zone (See figure b above)

The band index $n$ is (from bottom to top) $n = 1, 2, 3, ...$

### 7.3.3. Periodic Brillouin zone

There is another way of plotting $\epsilon_{n,k}$. We can start from the reduced Brillouin zone and then we plot $\epsilon_{n,k}$ as a periodic function of $k$, repeating the same curve in the second, third, ... Brillouin zone (See figure c above)

### 7.3.4. Folding, Reduced Brillouin zone and extended Brillouin zone for free particles without lattices

We know that plane waves is a special case of Bloch waves (where the periodic potential is $V = 0$). Therefore, we can present the dispersion of a free particle $\epsilon = \hbar^2 k^2 / 2m$ in the same way (in the reduced BZ and periodic BZ).

The can be achieve using the following procedures:

start from the dispersion $\epsilon(k) = \hbar^2 k^2 / 2m$,
then move the curve in the regions $(2n-1)\pi/a < k < 2n\pi/a$ to $-\pi/a < k < 0$ and move the curve in the regions $2n\pi/a < k < (2n+1)\pi/a$ to $0 < k < \pi/a$.

So we get the figure below.

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This construction is known as Brillouin zone folding. Similarly, the reverse procedure is known as “unfolding”. We can unfold the reduced Brillouin zone to get the “extended Brillouin zone”, going back to the case $-\infty < k < +\infty$ and get one single curve with $k^2/2m$ for a free particle.