

Bloch's Theorem

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \psi = \epsilon \psi$$

Bloch Wavefunctions tell us about the mathematical form of an electron wavefunction in the presence of a periodic potential energy. (In 1-D version "Floquet's theorem")

In the independent-electron approximation, we employ the time-independent Schrödinger equation (SE) for a single electron in a periodic potential: $U(\mathbf{r} + \mathbf{R}) = U(\mathbf{r})$
where $\mathbf{R} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$

Bloch showed that the solutions to the SE are **the product of a plane wave and a function with the periodicity of the lattice**:

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \quad \text{where} \quad u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$$



"Bloch functions"

What does this mean???!?

This represents a phase factor by which a Bloch function is multiplied when we make a crystal lattice translation $\mathbf{r} \rightarrow \mathbf{r} + \mathbf{R}$

To prove Bloch's theorem in 1D, first notice that Bloch's theorem implies:

$$\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) e^{i\mathbf{k} \cdot (\mathbf{r} + \mathbf{R})} = u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} e^{i\mathbf{k} \cdot \mathbf{R}} = \psi_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{R}}$$

Since $\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \psi_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{R}}$ implies Bloch's theorem, if we can prove it then we will have proven Bloch's theorem.



Bloch's Theorem in 1-D

Consider Q identical lattice points around a circular ring, each separated by a distance a . Our task is to prove: $\psi(x+a) = \psi(x) e^{ika}$

Periodic boundary conditions imply: $\psi(x+Qa) = \psi(x)$

The symmetry of the ring implies that there is a solution to the equation: $\psi(x+a) = C \psi(x)$

If we apply this translation Q times we will return to the initial atom position: "phase factor"

$$\psi(x+Qa) = C^Q \psi(x) = \psi(x)$$

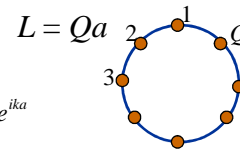
This requires $C^Q = 1$ And has the most general solution: $C^Q = e^{2\pi p i} \quad p = 0, \pm 1, \pm 2, \dots$

Or $C = e^{2\pi p i / Q} = e^{ika}$, where we define the **Bloch wavevector** as $k = \frac{2\pi p}{Qa}$

Now that we know C we can rewrite $\psi(x+a) = C \psi(x) = e^{ika} \psi(x)$ Q.E.D.

Generalize this to 3-D: $\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \psi_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{R}}$ ✓

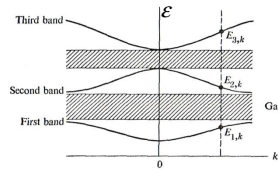
Bloch's theorem allows us to calculate (in principle) the energy bands of electrons in a crystal if we know the potential energy function experienced by the electron...



The Bloch function $\psi_{\mathbf{k}}(\mathbf{r})$ and energy bands

- Has the form of a travelling wave, $\exp(i\mathbf{k}\cdot\mathbf{r})$ *i.e.*, The electron travels through the crystal like a free particle, but since $u_{\mathbf{k}}(\mathbf{r})$ is periodic, the electron is not entirely free.
- Because the electron behaves as a wave of wave-number (-vector) k , it has deBroglie wavelength $\lambda = 2\pi/k$ and hence a **“crystal momentum”** $\mathbf{p} = \hbar\mathbf{k}$.
- The Bloch function is a crystal orbital *i.e.*, it is delocalised throughout the solid – the “crystalline electron” is shared by all the atoms.
- To calculate the energy bands, take the SE, substitute for $\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$, to yield the wave equation for $u_{\mathbf{k}}(\mathbf{r})$:
$$\left[-\frac{\hbar^2}{2m}(\nabla + i\mathbf{k})^2 + U(\mathbf{r}) \right] u_{\mathbf{k}}(\mathbf{r}) = \epsilon_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r})$$
- This is an eigenvalue equation and hence the energy is a multivalued function of \mathbf{k}

For each value of k there are a large number of solutions, giving a set of discrete energies, $\epsilon_{1,k}, \epsilon_{2,k}$



The energies $\epsilon_{1,k}, \epsilon_{2,k}$, etc depend on k and vary continuously. Each level leads to an energy band.



Dynamics of Bloch Electrons in an E Field

We mentioned earlier, and will discuss more later that **metals have partially-filled bands**, while **semiconductors and insulators have completely filled bands**. What is the qualitative difference between filled and partially-filled bands?

For a single electron: $\mathbf{j} = -e\mathbf{v}$

For a collection of electrons: $\mathbf{J} = -e \sum_{\mathbf{k}} \mathbf{v}(\mathbf{k})$

For each electron: $\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k})$
 $v_x = \frac{1}{\hbar} \frac{d\mathcal{E}}{dk}$ in 1D

But the symmetry of an energy bands requires: $\mathcal{E}(-\mathbf{k}) = \mathcal{E}(\mathbf{k})$

Thus we conclude: $\mathbf{v}(-\mathbf{k}) = -\mathbf{v}(\mathbf{k})$

So for a filled band, which has an equal number of electrons with k positive and negative,

$$\mathbf{J} = -e \sum_{1stBZ} \mathbf{v}(\mathbf{k}) = 0$$

Filled energy bands carry no current! We will see that this is true even when an electric field is applied.

Note: the electrons in filled bands are not stationary...there are just the same number moving in each direction, so the net current is zero.



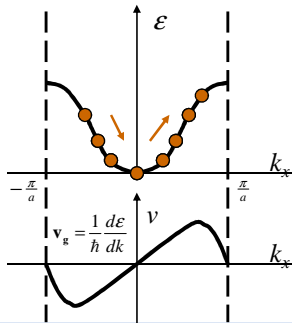
Dynamics of Bloch Electrons in an E Field

The same argument that we made for filled bands also applies to a partially filled band in the absence of an electric field. However, when an external electric field is applied to a periodic solid, the electrons all experience a force F that causes a change in their \mathbf{k} values:

$$\mathbf{F} = \hbar \frac{d\mathbf{k}}{dt}$$

Notice how a change in the external electric field causes a change in the \mathbf{k} vectors of all electrons:

$$\mathbf{F} = \hbar \frac{d\mathbf{k}}{dt} = -e\mathbf{E} \longrightarrow \frac{d\mathbf{k}}{dt} = \frac{-e\mathbf{E}}{\hbar}$$



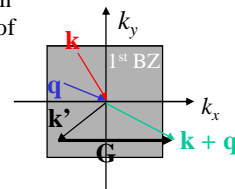
If the electrons are in a partially filled band, this will break the symmetry of electron states in the 1st BZ and produce a net current. But if they are in a filled band, even though all electrons change k vectors, the symmetry remains, so $J = 0$.



Dynamics of Bloch Electrons in an E Field

Note: $\hbar\mathbf{k}$ is not the electron's real momentum, because \mathbf{F} is only the external force: it does not include the force of the lattice on the moving electron. It is labeled the crystal momentum.

“ \mathbf{k} ” enters in the conservation laws that govern collision processes in crystals (like real momentum) *e.g.*, an electron \mathbf{k} absorbs a phonon of wavevector \mathbf{q} , the selection rule is $\mathbf{k} + \mathbf{q} = \mathbf{k}' + \mathbf{G}$ *i.e.* electron is scattered from state \mathbf{k} to \mathbf{k}'



Can you see how an AC current may result from the application of a DC field?
“Bloch Oscillations”

Hint: When an electron reaches the 1st BZ edge (at $k = \pi/a$) it immediately reappears at the opposite edge ($k = -\pi/a$) and continues to increase its k value.

Look what happens to its velocity.

Bloch oscillations are not routinely observed because the electrons in a periodic system undergo collisions with impurities and defects in the lattice much too frequently. In practice this occurs on the time scale of the collision time τ ($\approx 10^{-14}$ s) (*i.e.* electron “lifetime”).

Let's analyze the effect of an external electric field in this more realistic case...

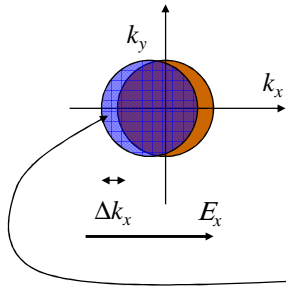


Dynamics of Bloch Electrons in an E Field

$$\frac{d\mathbf{k}}{dt} = \frac{-e\mathbf{E}}{\hbar} \equiv \frac{\Delta\mathbf{k}}{\tau} \longrightarrow \Delta k_x \equiv \frac{-eE_x}{\hbar} \tau$$

average displacement

The steady-state situation can be represented (for a nearly free electron metal) by a very small shift in the Fermi sphere:



This leads to a net current, since there is no longer perfect cancellation of terms corresponding to $\pm k$ values, as when $E=0$.

$$J_x = -e \sum_{1st\text{BZ}} v_x(k)$$

We can also write this as:

$$J_x = - \underbrace{(g(\mathcal{E}_F)\Delta\mathcal{E})}_{\text{density of "uncompensated" electrons}} \cdot e \cdot v_{Fx} \quad \Delta\mathcal{E} = \text{energy shift of Fermi sphere}$$

We can simplify this expression through the chain rule:

$$J_x = - (g(\mathcal{E}_F)\Delta\mathcal{E}) \cdot e \cdot v_{Fx} = -e v_{Fx} g(\mathcal{E}_F) \left(\frac{d\mathcal{E}}{dk_x} \right)_{\mathcal{E}_F} \Delta k_x$$



Electrical conductivity – a more general description

Now using the approximation of a free-electron band $\mathcal{E}(k)$:

$$J_x = -e v_{Fx} g(\mathcal{E}_F) (\hbar v_{Fx}) \Delta k_x = -e v_{Fx}^2 g(\mathcal{E}_F) \hbar \left(\frac{-eE_x}{\hbar} \tau_F \right)$$

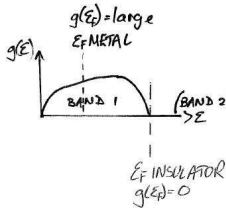
$$v_x = \frac{d\omega}{dk} = \frac{1}{\hbar} \frac{d\mathcal{E}}{dk} \quad \Delta k_x \equiv \frac{-eE_x}{\hbar} \tau_F$$

$$J_x = e^2 v_{Fx}^2 \tau_F g(\mathcal{E}_F) E_x$$

For a spherical Fermi surface, we can write $v_F^2 = v_{Fx}^2 + v_{Fy}^2 + v_{Fz}^2 = 3v_{Fx}^2 \longrightarrow v_{Fx}^2 = \frac{1}{3} v_F^2$

Which then yields:

$$J_x = \frac{1}{3} e^2 v_F^2 \tau_F g(\mathcal{E}_F) E_x = \sigma E_x \longrightarrow \boxed{\sigma = \frac{1}{3} e^2 v_F^2 \tau_F g(\mathcal{E}_F)}$$



This result reduces to the free-electron gas expression when the FEG values of $g(\mathcal{E}_F)$ and \mathcal{E}_F are substituted [CHECK THIS!].

But note that our new equation for σ is much more general and highlights the importance of the $g(\mathcal{E}_F)$ (rather than n) and τ_F in determining the conductivity of a metal.

