

Non-Interacting Electrons in a Periodic Potential

Condensed Matter Physics – Michael P. Marder

Chapter 7

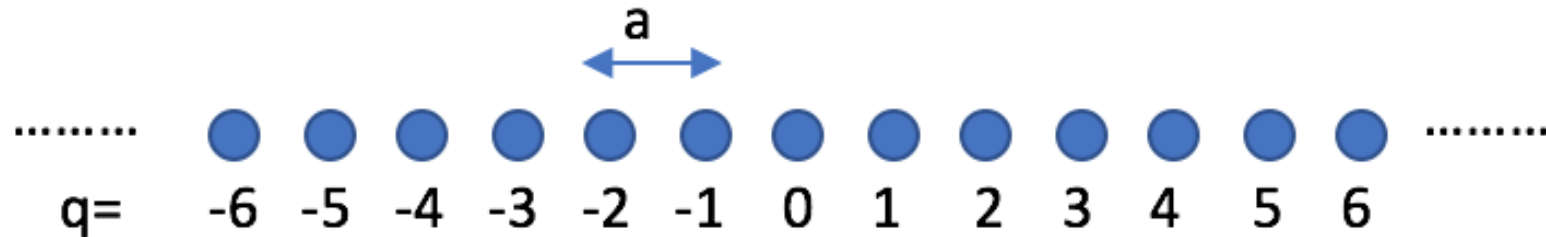


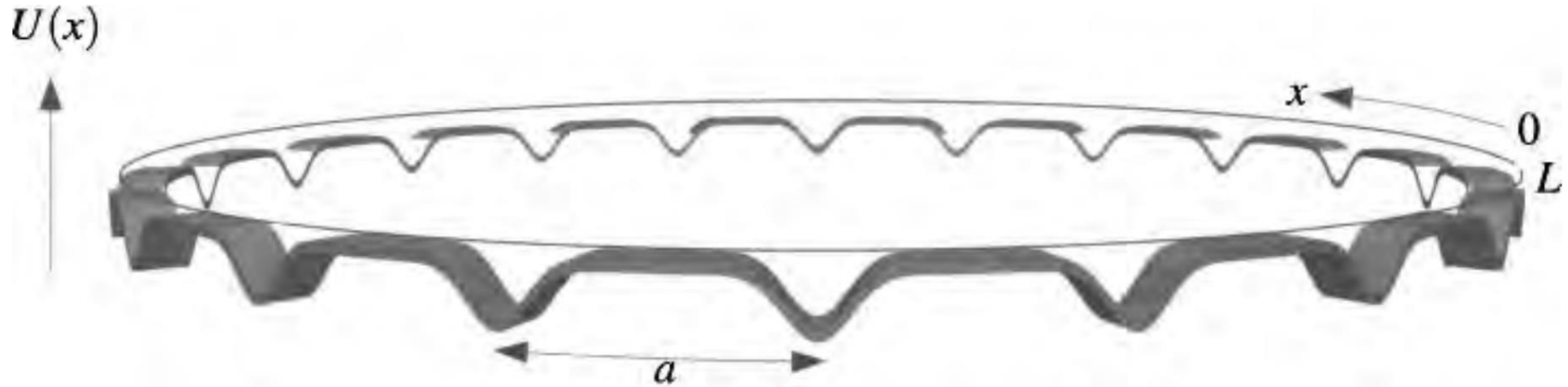
Bloch's Theorem in One Dimension

Bloch proposed that the electron move in a periodic potential $U(\vec{r})$, making the problem nearly tractable, which obeys

$$U(\vec{r} + \vec{R}) = U(\vec{r})$$

For all \vec{R} in a Bravais lattice.



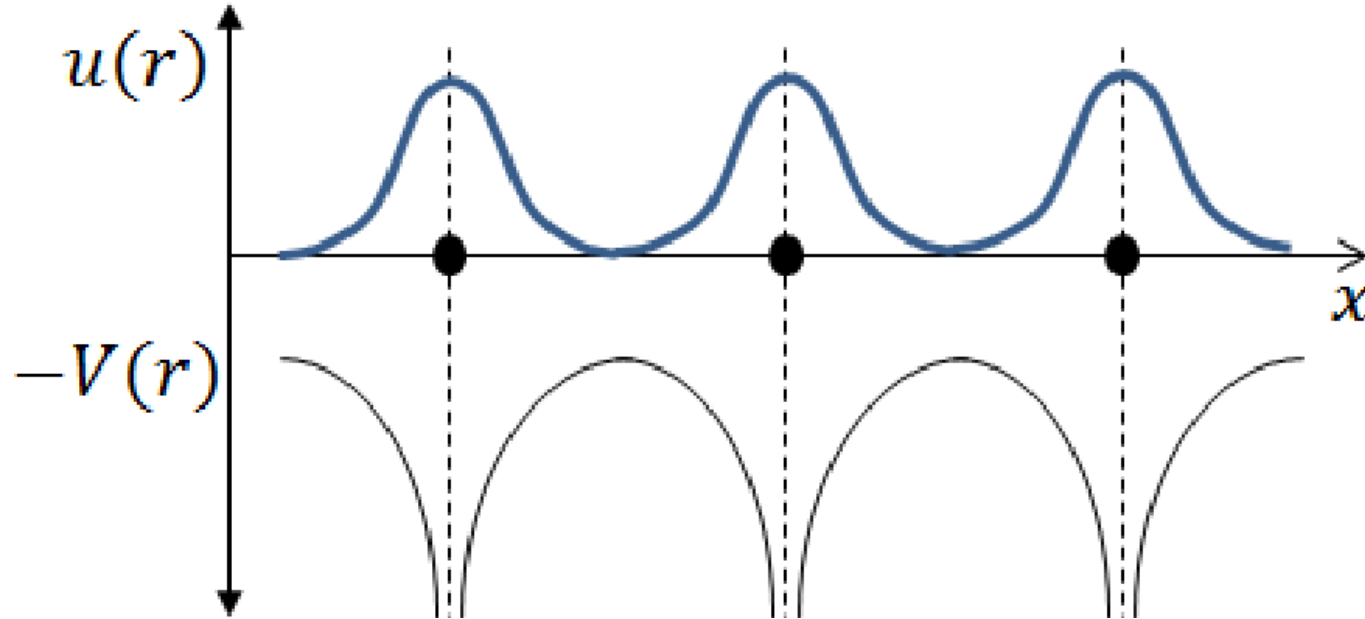


The setting for Bloch's theorem in one dimension is a potential $U(x)$ of period a on a periodic domain of length L

The Hamiltonian is

$$\hat{\mathcal{H}} = \frac{\hat{P}^2}{2m} + U(\hat{R}).$$

Periodic Potential



The periodic potential of a crystal results in a delocalized electron. The Bloch theorem requires the electronic wavefunction have the same periodicity as the lattice and therefore has a slowly varying envelope $u(r)$.

Schrödinger equation in one dimension

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + U(x) \psi(x) = \mathcal{E} \psi(x)$$

The one-dimensional space where ψ is defined is of length L i.e. ψ to be periodic. Suppose that the potential $U(x)$ was just $U(x) = 0$

$$\psi(x + L) = \psi(x) \qquad \psi_k(x) = \frac{e^{ikx}}{\sqrt{L}}$$



Schrödinger equation in one dimension

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + U(x) \psi(x) = \mathcal{E} \psi(x)$$

When the potential $U(x)$ is not zero, the solutions retain the same basic structure, but change to

$$\psi_k(x) = \frac{e^{ikx} u(x)}{\sqrt{N}}$$



Bloch wave function

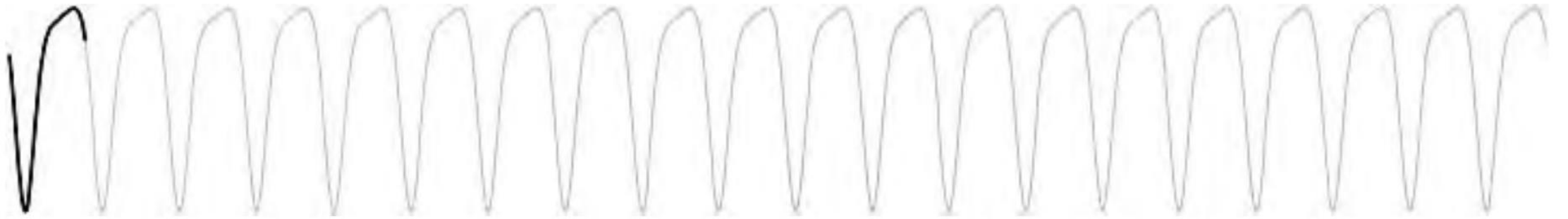
$$\psi_k(x) = \frac{e^{ikx} u(x)}{\sqrt{N}}$$

ψ is normalized over the whole system, u is normalized over a single unit cell

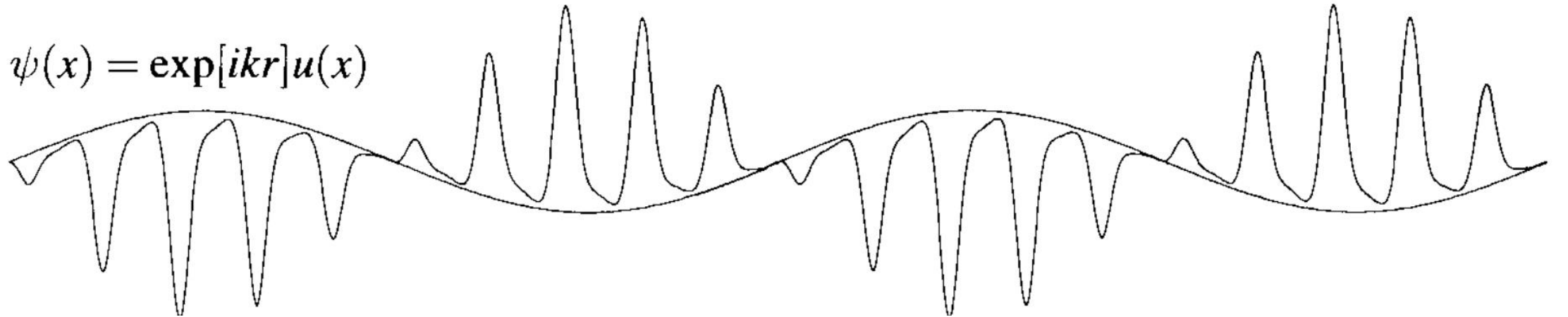
Where $u(x)$ is a function that like $U(x)$ is periodic with period a , and where $N = L/a$ is the number of cells in the full periodic system. That is, the solutions are plane waves $\exp[ikx]$ modulated by a periodic function $u(x)$.

Bloch wave function

Periodic function $u(x)$



$\psi(x) = \exp[ikr]u(x)$



Bloch wave functions are periodic functions $u(r)$ modulated by a plane wave of longer period. The lower portion of the figure displays the real part of $\psi(x)$

Bloch wave function

Fourier's theorem says that every periodic function can be written as a sum of all the complex exponential functions $\exp[ikx]$ that share the same period. Because ψ is periodic with period L , $\psi(x)$ can be written as a sum of Fourier components $\exp[iq'x]$ where q' is of the form $q' = 2\pi l'/L$ and $l' \in (-\infty \dots -1, 0, 1 \dots \infty)$ is any integer:

$$\psi(x) = \frac{1}{\sqrt{L}} \sum_{q'} \psi(q') e^{iq'x}$$

Bloch wave function

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + U(x) \psi(x) = \mathcal{E} \psi(x)$$

U is periodic with period $a = L/N$, and it can be written as a sum of Fourier components $\exp[iKx]$ where the reciprocal lattice vector K is of the form $K = 2\pi l/a$, and l is an integer:

$$U(x) = \sum_K U_K e^{iKx}.$$

$$\sum_{q'} \frac{\hbar^2 q'^2}{2m} e^{iq'x} \psi(q') + \sum_{q'K} e^{i(q'+K)x} \psi(q') U_K = \mathcal{E} \sum_{q'} e^{iq'x} \psi(q')$$



Bloch wave function

This equation must hold separately for each Fourier component $\exp[iqx]$, a condition imposed formally by choosing $q = 2\pi l/L$, multiplying Eq. (7.9) by $\exp[-iqx]/L$ and integrating from 0 to L . It is easy to verify that

$$\frac{1}{L} \int_0^L dx e^{i(q'-q)x} = \delta_{q,q'}; \quad \frac{1}{L} \int_0^L dx e^{i(q'+K-q)x} = \delta_{q',q-K}.$$

Therefore

$$\frac{\hbar^2 q^2}{2m} \psi(q) + \sum_{q'K} \delta_{q',q-K} \psi(q') U_K = \mathcal{E} \psi(q).$$

$$\Rightarrow (\mathcal{E}_q^0 - \mathcal{E}) \psi(q) + \sum_K \psi(q-K) U_K = 0.$$



Bloch wave function

Suppose one has a solution. There must be at least one $k = 2\pi m/L$ for which $\psi(k)$ is not equal to zero. The equation for $\psi(k)$ involves $\psi(k - K)$ for all K of the form $2\pi l/a$. Pick any of these wave function components, say $\psi(k - K')$, and ask what Eq. (7.12) implies. It says

$$(\mathcal{E}_{k-K'}^0 - \mathcal{E})\psi(k - K') + \sum_K \psi(k - K' - K) U_K = 0$$

$$\Rightarrow (\mathcal{E}_{k-K'}^0 - \mathcal{E})\psi(k - K') + \sum_K \psi(k - K) U_{K-K'} = 0. \quad \text{Send } K \rightarrow K - K' \text{ as the sum index.}$$

$$(\mathcal{E}_q^0 - \mathcal{E})\psi(q) + \sum_K \psi(q - K) U_K = 0.$$

$$\psi(q) = \sum_K \delta_{q,k+K} u_K.$$



Bloch's Theorem

$$\psi(x) = \frac{1}{\sqrt{L}} \sum_{q'=K} \delta_{q',k+K} u_K e^{iq'x} = \frac{1}{\sqrt{L}} \sum_K u_K e^{i(k+K)x}$$

$$\Rightarrow \psi(x) = \frac{e^{ikx} u(x)}{\sqrt{N}} \quad \text{where} \quad u(x) \equiv \frac{1}{\sqrt{a}} \sum_K u_K e^{iKx}. \quad N = L/a \text{ is the number of unit cells.}$$

$$(\mathcal{E}_q^0 - \mathcal{E})\psi(q) + \sum_K \psi(q - K) U_K = 0.$$

$$\psi_k(x) = \frac{e^{ikx} u_k(x)}{\sqrt{N}} \Rightarrow \psi_k(x + a) = \psi_k(x) e^{ika}.$$

The Fourier component k is called the wave *number* and $\hbar k$ is called the *crystal momentum*.



Table 7.1. The structure of Bloch's Hamiltonian in reciprocal space

$$\begin{pmatrix}
 \begin{pmatrix}
 \mathcal{E}_{K_0}^0 + U_{K_0} & U_{K_{-1}} & \dots & U_{K_{1-M}} \\
 U_{K_1} & \mathcal{E}_{K_1}^0 + U_{K_0} & \dots & U_{K_{2-M}} \\
 U_{K_2} & U_{K_1} & \dots & U_{K_{3-M}} \\
 \vdots & \vdots & \ddots & \vdots \\
 & & & \mathcal{E}_{K_{M-1}}^0 + U_{K_0}
 \end{pmatrix} & 0 \dots \\
 0 & \begin{pmatrix}
 \mathcal{E}_{k_1}^0 + U_{K_0} & U_{K_{-1}} & \dots \\
 U_{K_1} & \mathcal{E}_{k_1+K_1}^0 + U_{K_0} & \dots \\
 \vdots & \vdots & \ddots \\
 \vdots & \vdots & \vdots & \ddots
 \end{pmatrix} & \dots \\
 \vdots & & &
 \end{pmatrix}
 \begin{pmatrix}
 \psi(K_0) \\
 \psi(K_1) \\
 \psi(K_2) \\
 \vdots \\
 \vdots \\
 \vdots \\
 \psi(K_{M-1}) \\
 \psi(k_1 + K_0) \\
 \psi(k_1 + K_1) \\
 \vdots \\
 \vdots \\
 \vdots \\
 \vdots
 \end{pmatrix}$$

This matrix contains blocks that link together wave function components $\psi(k_m + K_l)$ for a given m , where $k_m = 2\pi m/L$ and $K_l = 2\pi l/a$. There are no matrix elements connecting $\psi(q)$'s when the q 's do not differ by reciprocal lattice vectors. The dimension of each block is M , the number of reciprocal lattice vectors retained in the calculation, while the total number of blocks is equal to the total number of unit cells, $N = L/a$.

Choosing k specifies a *set* of Fourier components $q = k + K$ from which the wave function ψ_k will be constructed. Choosing $k + K'$ picks out *exactly the same set*. From this point of view, two wave numbers k are physically distinct only if they do not differ by any reciprocal lattice vector K . This means that indices k should be chosen from

$$k = \frac{2\pi m}{L} \text{ where } k \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right] \text{ Taking } k \text{ in the interval } [0, 2\pi/a] \text{ would do just as well.}$$

This collection of $k = 2\pi m/L$, $m \in [-N/2, N/2 - 1]$ is called the *first Brillouin zone*, and will be defined in greater generality in Section 7.2.4.

Thus a complete set of solutions to Eq. (7.12) is

$$\psi_{nk}(x) = \frac{e^{ikx} u_{nk}(x)}{\sqrt{N}} \quad \text{with band energy } \mathcal{E}_{nk}.$$

where k lies in the first Brillouin zone, and the band index runs from 0 to ∞ .



Bloch's Theorem in Three Dimensions

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + U(\hat{R}).$$

$$U(\vec{r} + \vec{R}) = U(\vec{r})$$

$$\psi(\vec{r}) = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\vec{q}} \psi(\vec{q}) e^{i\vec{q} \cdot \vec{r}}.$$

$$U(\vec{r}) = \sum_{\vec{K}} e^{i\vec{K} \cdot \vec{r}} U_{\vec{K}}.$$

$$\mathcal{V} = L^3$$

$$\psi(x + L, y, z) = \psi(x, y, z)$$



Bloch's Theorem in Three Dimensions

$$(\varepsilon_{\vec{q}}^0 - \varepsilon)\psi(\vec{q}) + \sum_{\vec{K}} U_{\vec{K}}\psi(\vec{q} - \vec{K}) = 0$$

$$\psi(\vec{q}) = \sum_{\vec{K}} \delta_{\vec{q}, \vec{k} + \vec{K}} u_{\vec{K}}.$$

$$\psi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r})}{\sqrt{N}}$$

$$u_{\vec{k}}(\vec{r} + \vec{R}) = u_{\vec{k}}(\vec{r})$$

