Condensed Matter Physics

PHY 5111

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Non-Interacting Electrons in a Periodic Potential

Condensed Matter Physics – Michael P. Marder

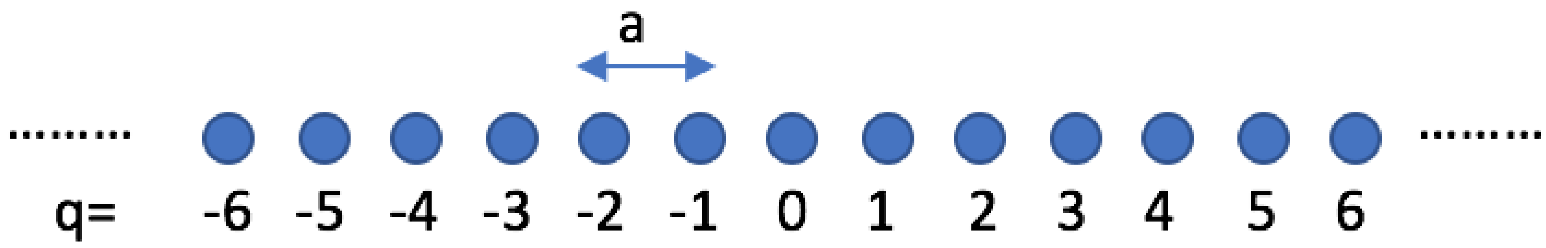
Chapter 7

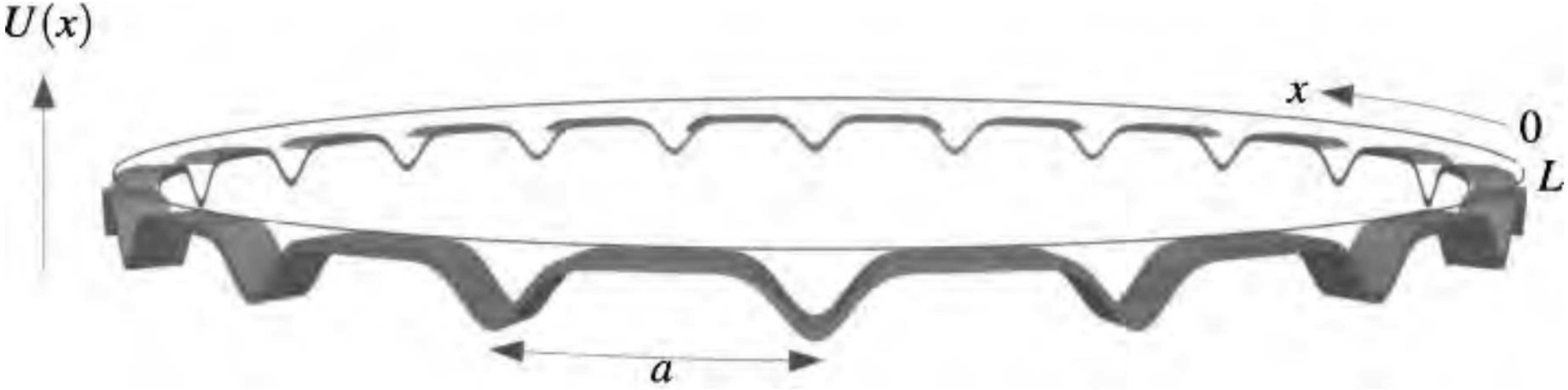
Bloch’s Theorem in One Dimension

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

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

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



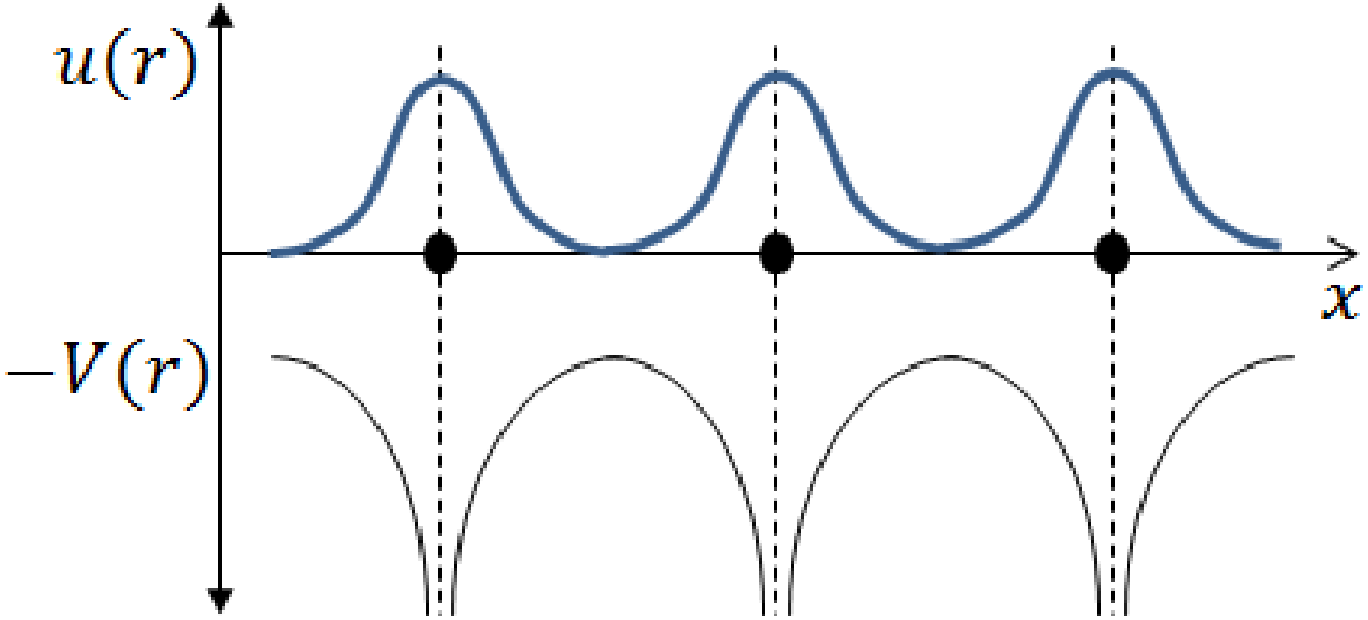


The setting for Bloch's theorem in one dimension is a potential $U(x)$ of period a on a periodic domain of length L

The Hamiltonian is

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

Periodic Potential



SEMANTIC SCHOLAR

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 $U(x) = 0$

$$\psi(x+L)=\psi(x)$$

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

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

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

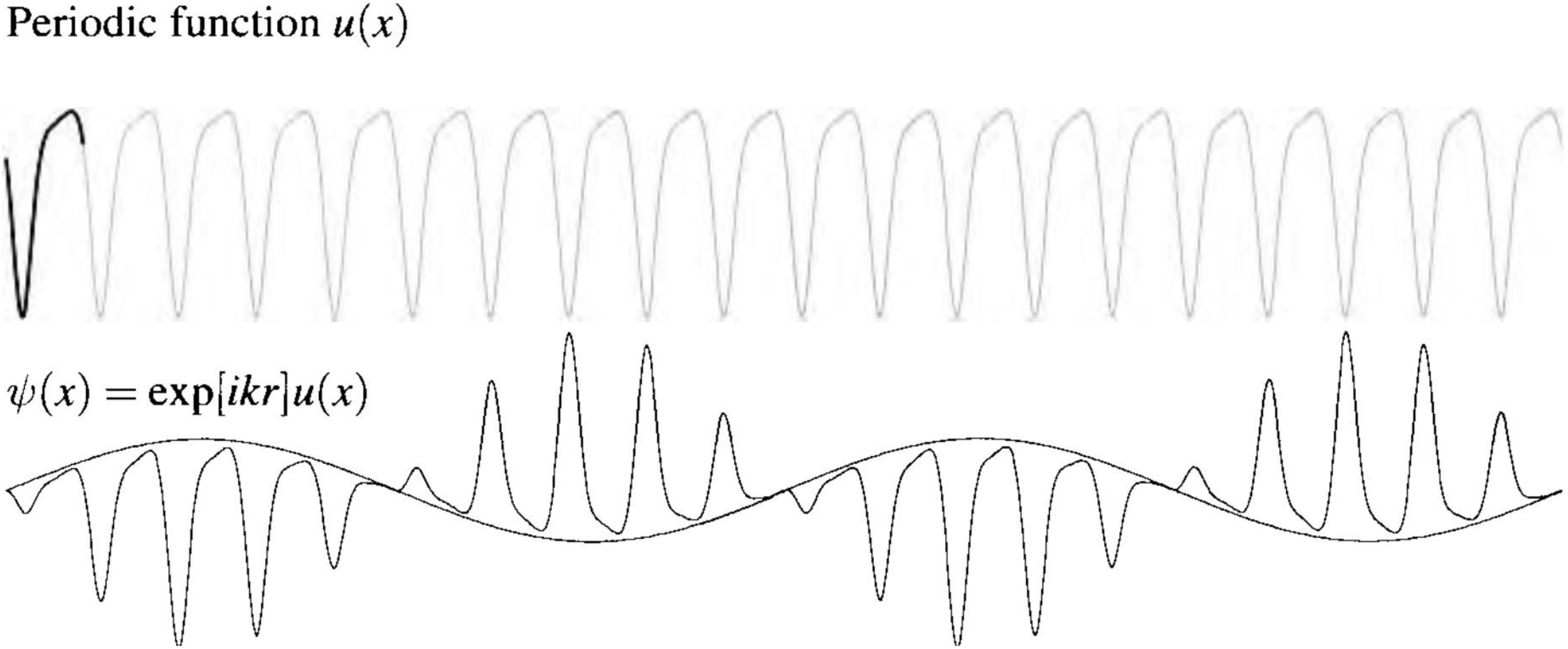
Bloch wave function

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

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



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 $l' \in (-\infty \ldots -1, 0, 1 \ldots \infty)$ 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

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

$$\Rightarrow (\mathcal{E}^0_{k-K'} - \mathcal{E})\psi(k-K') + \sum_K \psi(k-K)\, U_{K-K'} = 0.$$

Send $K \to K - K'$ as the sum index.

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

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

Bloch' Theorem

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

$$\Rightarrow \psi(x) = \frac{e^{ikx} u(x)}{\sqrt{N}} \quad \text{where} \quad u(x) \equiv \frac{1}{\sqrt{a}} \sum_K u_K\, e^{iKx}.$$

$N = L/a$ 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

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

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

$$k = \frac{2\pi m}{L} \text{ where } k \in [-\frac{\pi}{2a}, \frac{\pi}{2a}]$$

Taking k in the interval $[0, 2\pi/a]$ 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

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

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

Bloch's Theorem in Three Dimensions

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

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

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

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

Bloch's Theorem in Three Dimensions

Bloch's Theorem in Three Dimensions

$$(\mathcal{E}^0_{\vec{q}} - \mathcal{E})\psi(\vec{q}) + \sum_{\vec{K}} U_{\vec{K}}\psi(\vec{q} - \vec{K}) = 0$$

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

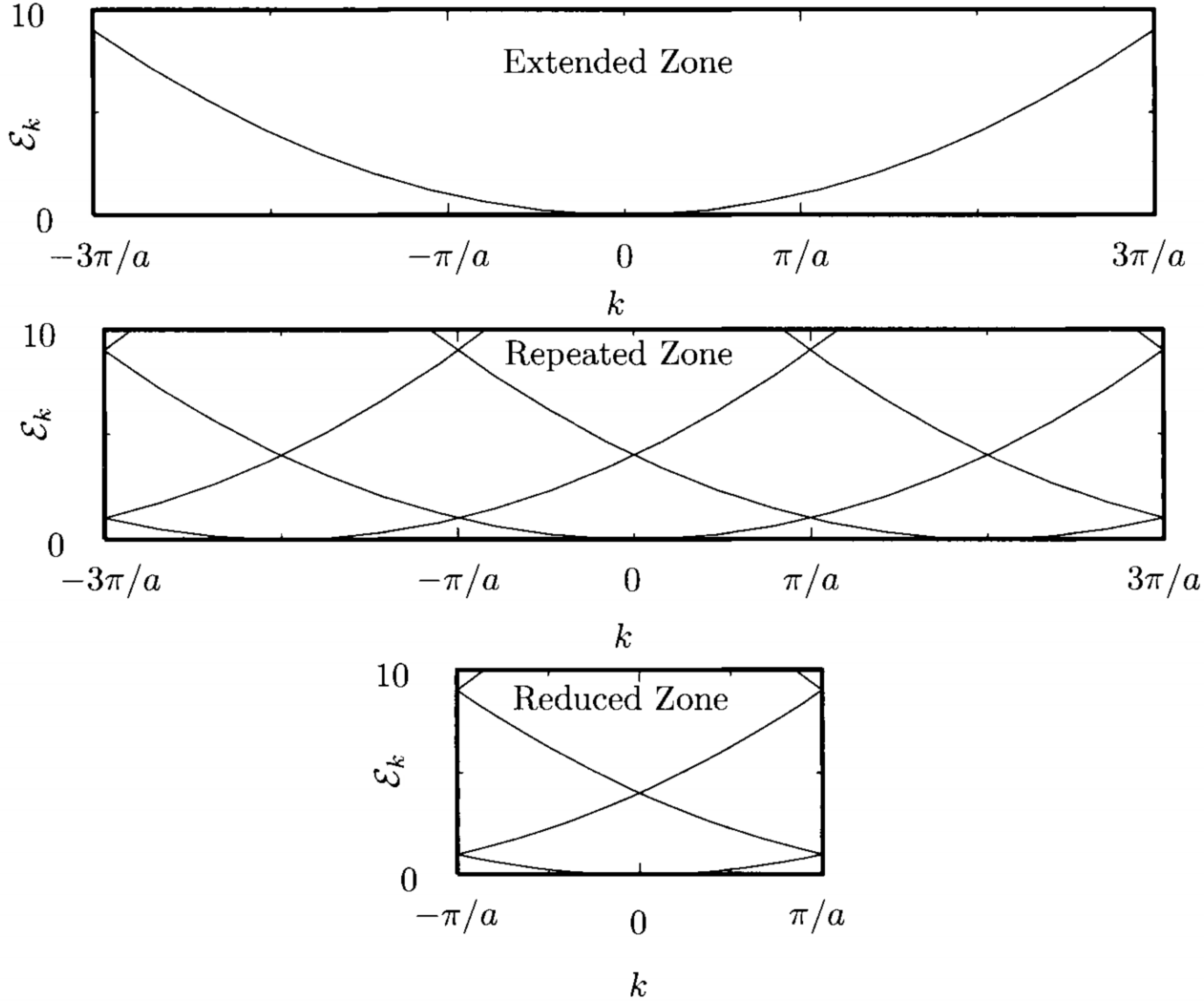
$$\psi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})}{\sqrt{N}}$$

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

Implication of Bloch's Theorem

- Effective Hamiltonian
- Counting $\vec{k}$
- Brillouin Zone
- Density of States
- Energy Bands

Implication of Bloch's Theorem



Energy diagram for free electron

Kronig-Penney Model

Kronig and Penney (1931) found an exactly soluble model that illustrates the nature of energy bands. Suppose that in each unit cell of a one-dimensional lattice with lattice points $R = na$ and reciprocal lattice vectors K, there is a potential of the form

$$U_0 a \delta(x), \quad a \text{ is the lattice spacing.}$$

where U_0 has dimensions of energy. Then U_K as defined in Eq. (7.26) is simply

$$U_K = U_0,$$

$$0 = (\mathcal{E}_q^0 - \mathcal{E})\psi(q) + \sum_K U_0 \psi(q-K).$$

Kronig-Penney Model

$$\psi(q) + \frac{U_0}{\mathcal{E}_q^0 - \mathcal{E}} Q_q = 0.$$

$$\psi(k-K) + \frac{U_0}{\mathcal{E}_{k-K}^0 - \mathcal{E}} Q_{k-K} = 0$$

$$\Rightarrow \sum_K \left[\psi(k-K) + \frac{U_0}{\mathcal{E}_{k-K}^0 - \mathcal{E}} Q_k\right] = 0$$

$$\Rightarrow Q_k + \sum_K \frac{U_0}{\mathcal{E}_{k-K}^0 - \mathcal{E}} Q_k = 0.$$

$$Q_q = \sum_K \psi(q-K)$$

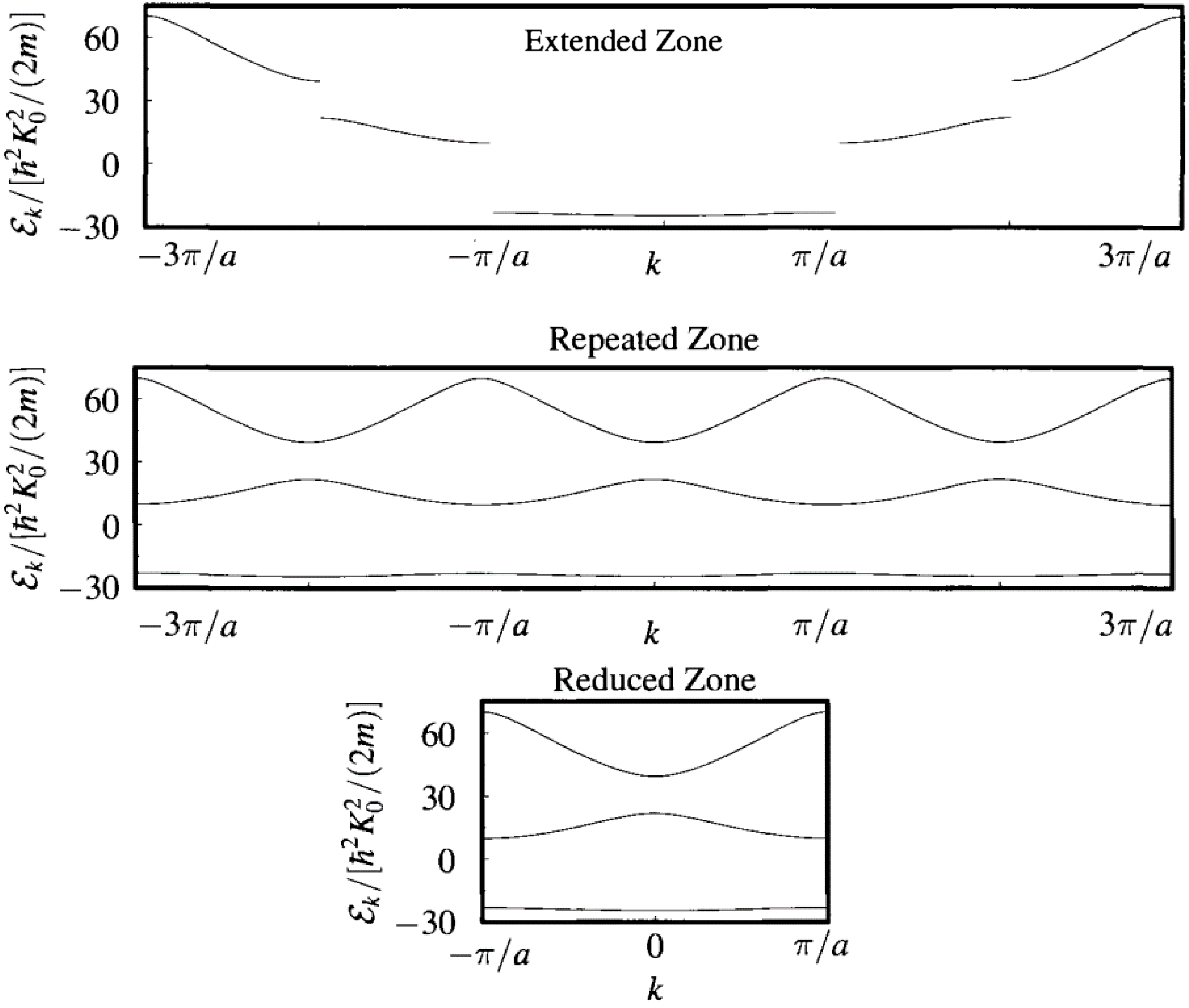
$$Q_q = Q_{q-K}$$

Kronig-Penney Model

$$Q_k + \sum_K \frac{U_0}{\mathcal{E}^0_{k-K} - \mathcal{E}} Q_k = 0.$$

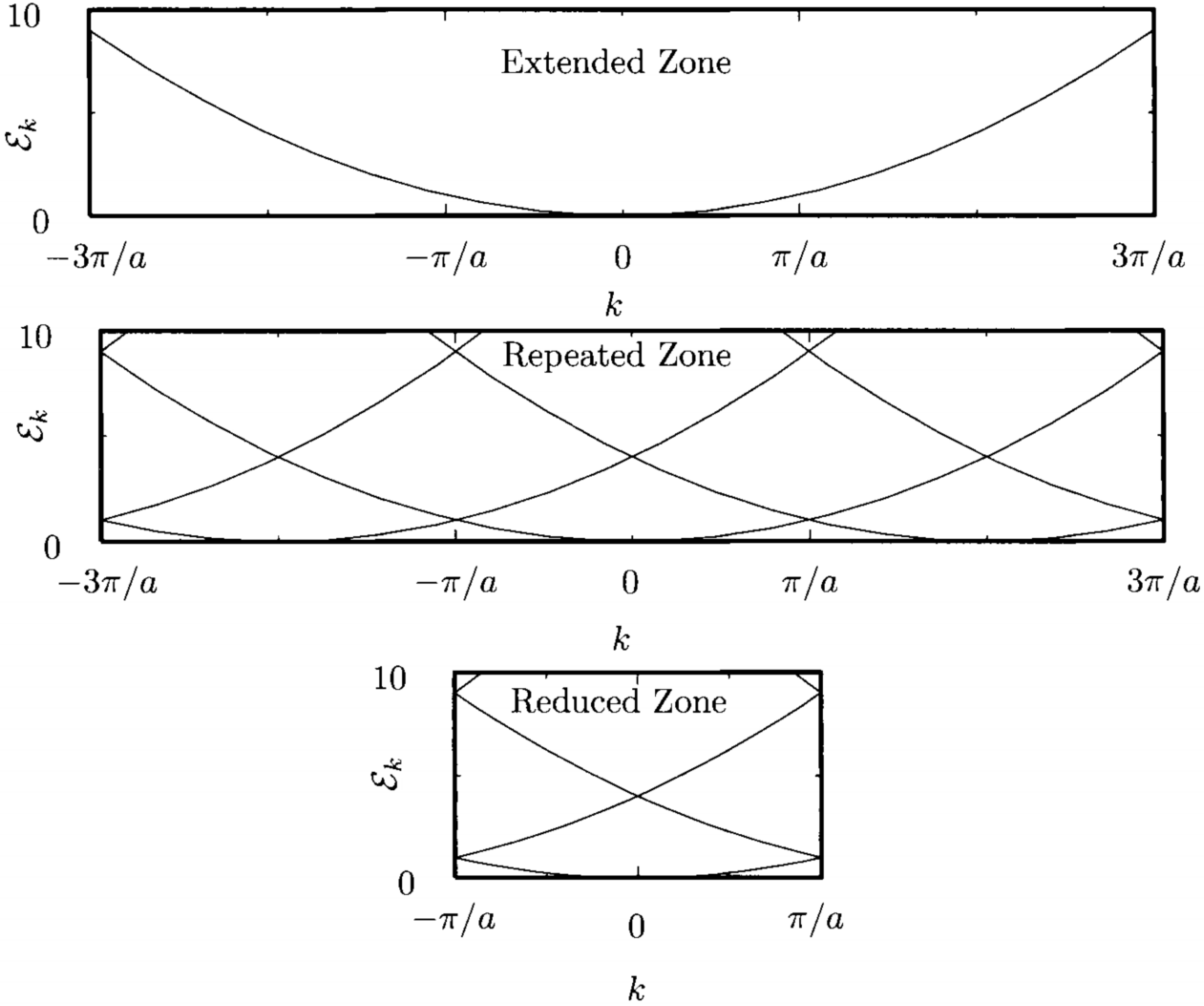
Assuming that Q_k does not vanish,

$$-\frac{1}{U_0} = \sum_K \frac{1}{\mathcal{E}^0_{k-K} - \mathcal{E}}$$



Energy bands with

$$U_0 = -10\hbar^2 K_0^2/(2m)$$



Energy band for free electron

Brillouin zone for the
(a) simple cubic,
(b) face-centred cubic,
(c) body-centred cubic, and
(d) hexagonal lattice.

The most important points and lines of symmetry are shown, together with their nomenclature.