Lecture 27

Periodic Potentials: Electrons in Crystals

Silicon crystal

In this lecture you will learn:

- Atomic potentials
- Electrons in periodic potentials
- Energy bands in solids

$V(\vec{r})$

Bandgaps

Vacuum level

0

Energy bands

Potential in a crystal

Core energy levels

0

$\vec{R}$

$\vec{r}$
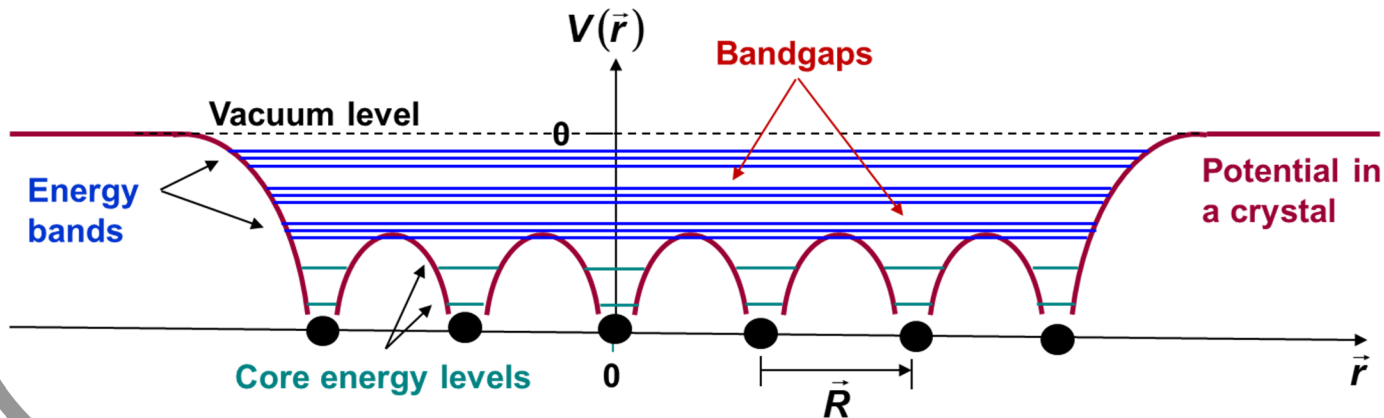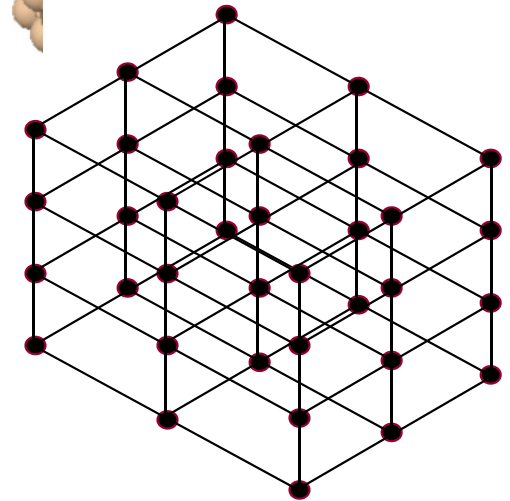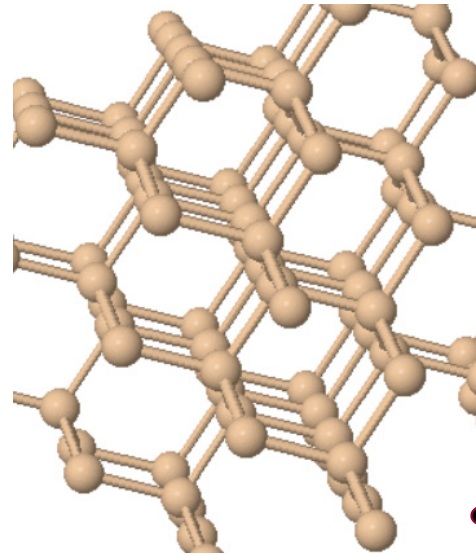
Electron Potential Energy in an Atom

The potential energy of an electron in a single isolated atom looks like:

$$V(\vec{r}) \approx -\frac{Ze^2}{4\pi\varepsilon_o r}$$

Energy levels
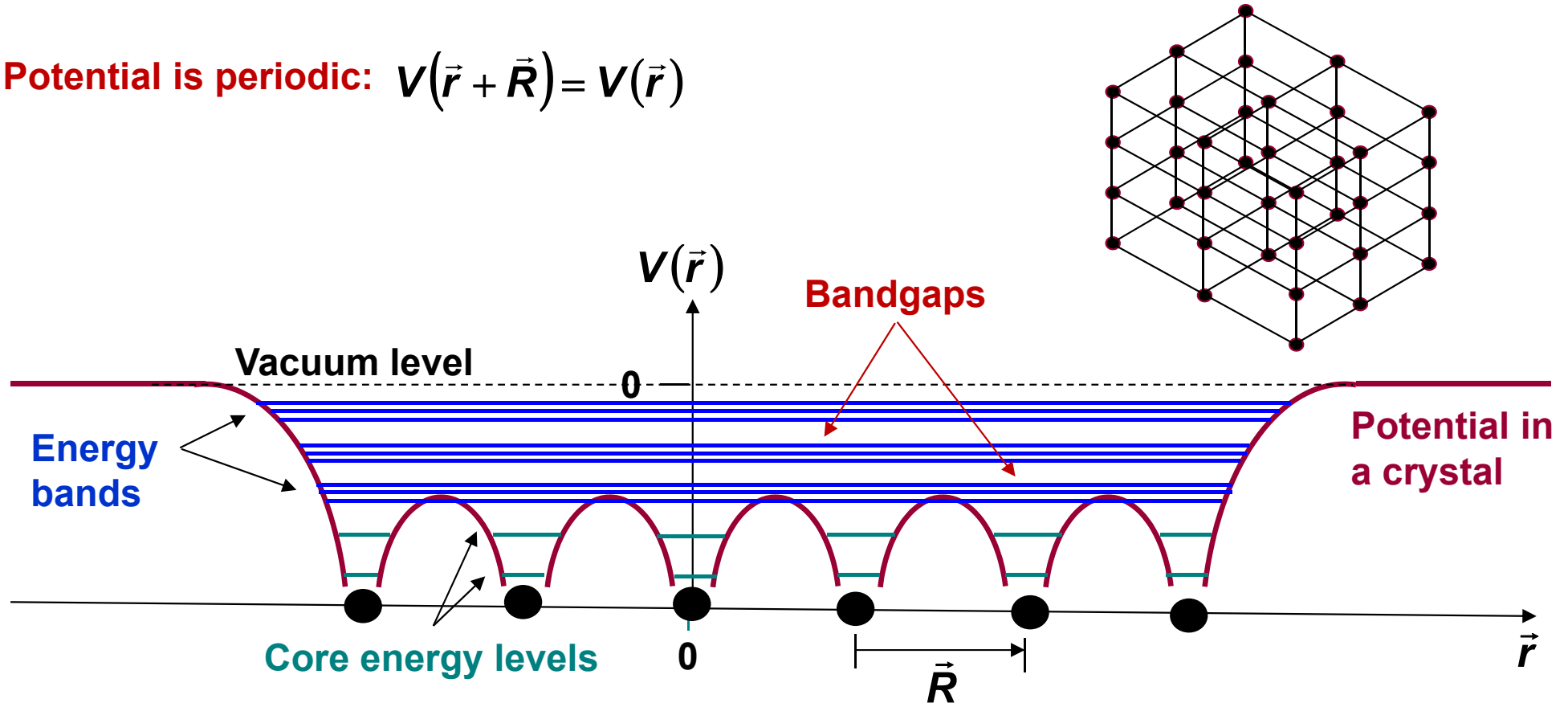
Coulomb potential of an isolated atom
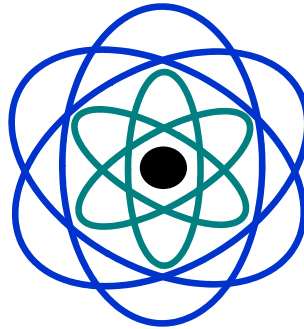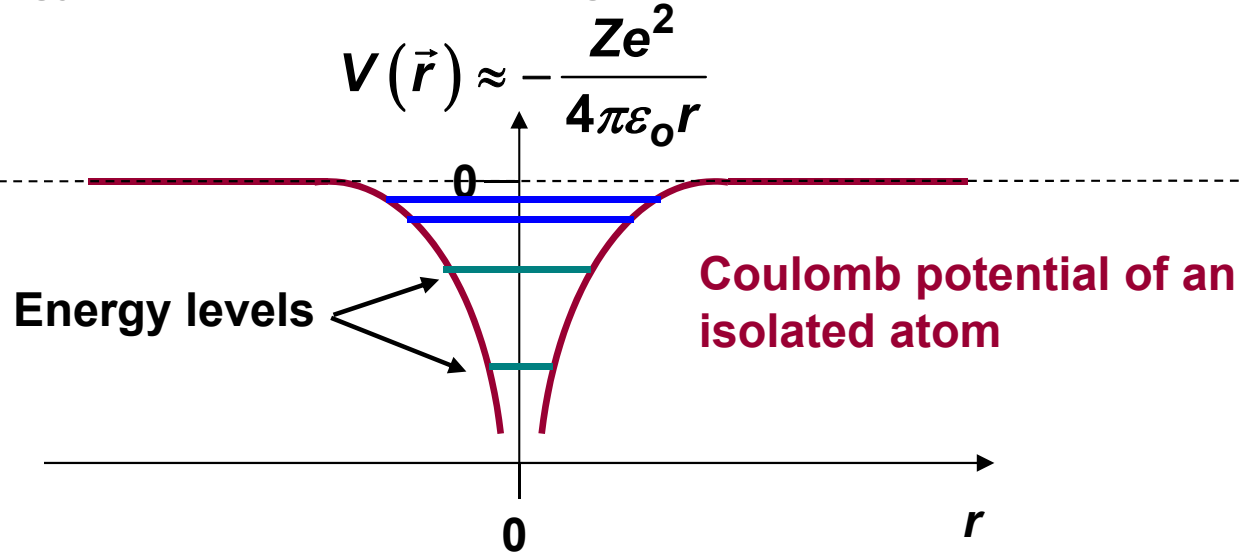
$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\,\psi(\vec{r})$$

If you solve the Schrodinger equation for the potential shown, you will obtain the atomic wavefunctions and the atomic energy levels

Electron Potential Energy in a Crystal of Atoms

Potential is periodic: $V(\vec{r} + \vec{R}) = V(\vec{r})$

$V(\vec{r})$

Bandgaps

Vacuum level

0

Energy bands

Potential in a crystal
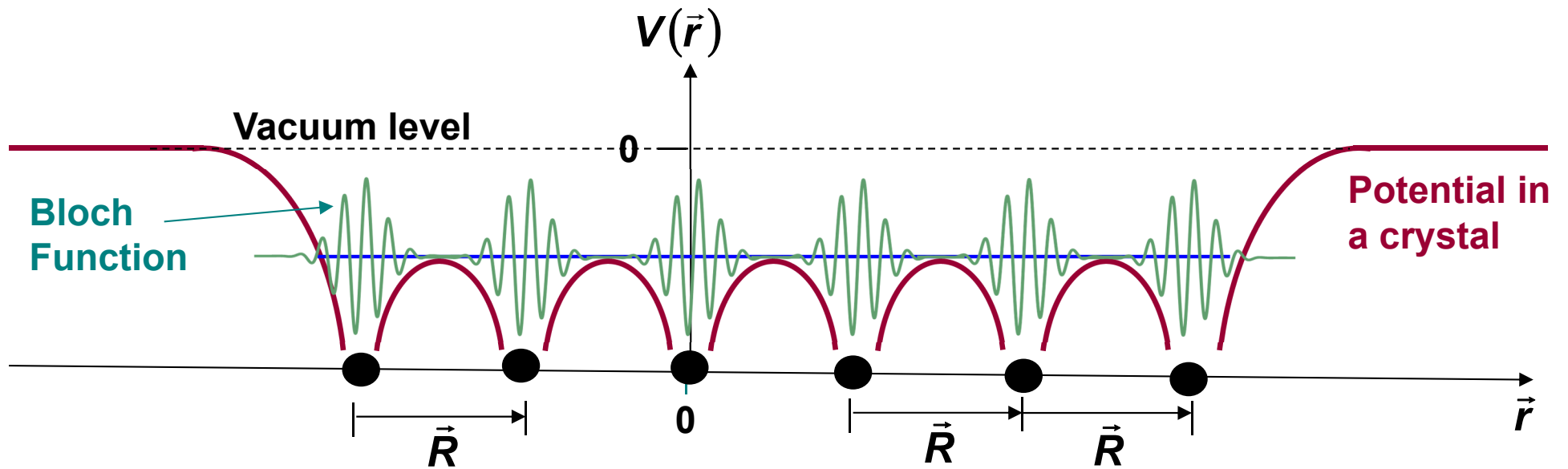
Core energy levels

0

$\vec{R}$

$\vec{r}$

1) The core (innermost) atomic energy eigenfunctions and energy levels remain unchanged

2) The higher energy atomic levels and corresponding wavefunctions get drastically modified:

    - The wavefunctions are not localized at any particular atom
    - The energy levels are organized in bands of energy that are separated by energy gaps or **bandgaps**

Electron Wavefunctions in Periodic Potentials

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})+V(\vec{r})\psi(\vec{r})=E\,\psi(\vec{r})$$

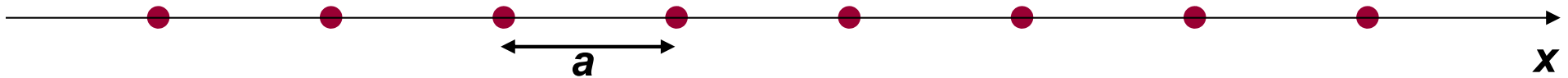$V(\vec{r})$

Vacuum level

0

Bloch
Function

Potential in
a crystal

$\vec{R}$

0

$\vec{R}$

$\vec{R}$

$\vec{r}$

Note that:

$$\left|\psi(\vec{r}+\vec{R})\right|^2=\left|\psi(\vec{r})\right|^2$$

Probability of finding the electron is
also periodic

A 1D Periodic Potential: Fourier Series

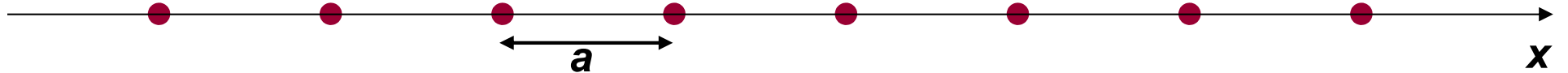**Consider the 1D crystal:**

Potential is periodic:

$$V(x + n\,a) = V(x) \qquad \{n = 0, \pm1, \pm2, ...$$

Consequently, the Fourier series expansion of $V(x)$ will be:

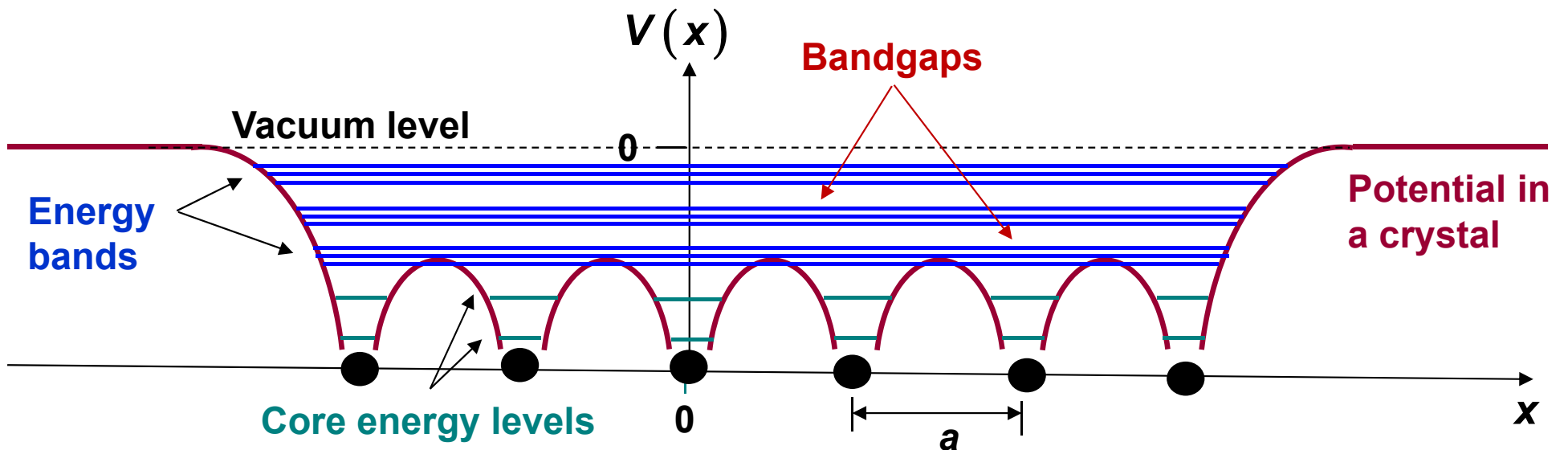$$V(x) = \sum_m V_m\, e^{i\frac{2\pi m}{a}x} \qquad \begin{cases} m = 0, \pm1, \pm2, ... \\ V_{-m} = V_m^* \quad \text{since V(x) is real} \end{cases}$$

Potential has wavevectors that are all integer multiples of $2\pi/a$

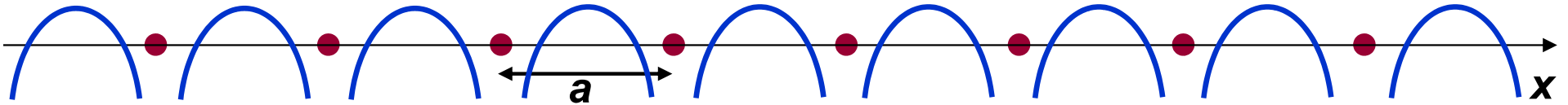# Solving the Schrodinger Equation with a 1D Periodic Potential

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

Free-Electron Approach:

We will suppose that the periodic atomic potential $V(x)$ is small, and that the electrons are essentially free, and we will treat the potential as a perturbation and see how it effects the free electrons.

Solving Schrodinger Equation: Free-Electron Approach

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} + \left(\sum_m V_m\, e^{i\frac{2\pi m}{a}x}\right)\psi(x) = E\,\psi(x)$$

Approximation:

Keep only the fundamental harmonic of the periodic potential:

$$V(x) = V_1 e^{i\frac{2\pi}{a}x} + V_{-1} e^{-i\frac{2\pi}{a}x} = 2V_1 \cos\left(\frac{2\pi}{a}x\right)$$

If $V_1 = V_{-1}$ is real
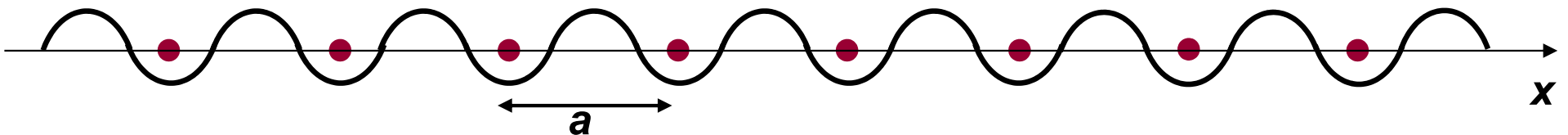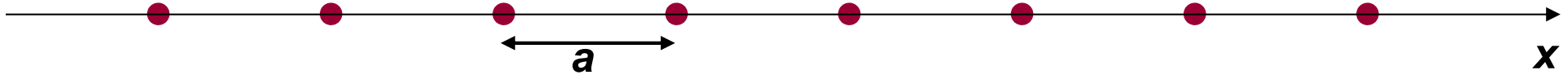
Solving Schrodinger Equation: Free-Electron Approach

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+\left(\sum_m V_m e^{i\frac{2\pi m}{a}x}\right)\psi(x)=E\,\psi(x)$$

Approximation:

Keep only the fundamental harmonic of the periodic potential

$$V(x)=V_1 e^{i\frac{2\pi}{a}x}+V_{-1}e^{-i\frac{2\pi}{a}x}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+\left(V_1 e^{i\frac{2\pi}{a}x}+V_{-1}e^{-i\frac{2\pi}{a}x}\right)\psi(x)=E\,\psi(x)$$

$$\left[\hat{H}_o+\hat{V}\right]|\psi\rangle=E|\psi\rangle$$

The original Hamiltonian is just the standard free-space Hamiltonian:

$$\hat{H}_o=\frac{\hat{p}^2}{2m}$$

Electron in a 1D Periodic Potential: Original Hamiltonian

The original free-space Hamiltonian $\hat{H}_o$ has the standard plane wave eigenstates:

$$\hat{H}_o = \frac{\hat{p}^2}{2m}$$

$$\hat{H}_o|\phi_k\rangle = e(k)|\phi_k\rangle = \frac{\hbar^2 k^2}{2m}|\phi_k\rangle$$

$$\langle x|\phi_k\rangle = \frac{1}{\sqrt{L}}e^{ikx}$$

$$\sum_k |\phi_k\rangle\langle\phi_k| = \hat{1}$$

The eigenstates are normalized in a crystal of length L

Energy $e(k) = \dfrac{\hbar^2 k^2}{2m}$

k
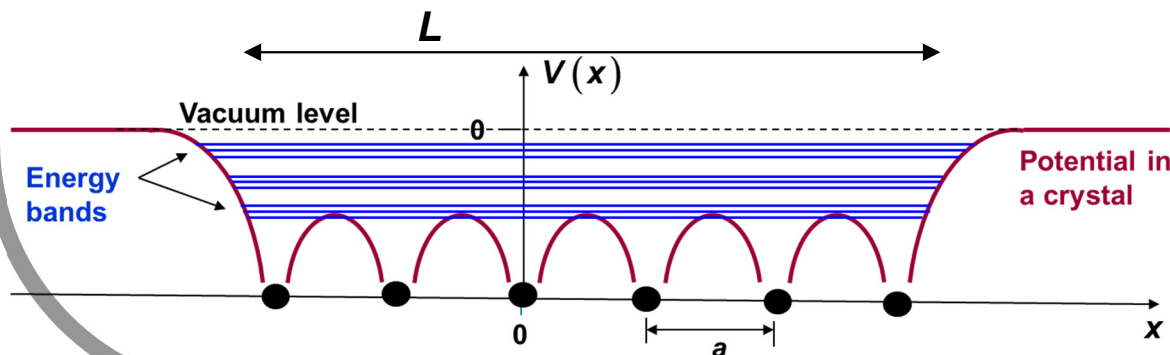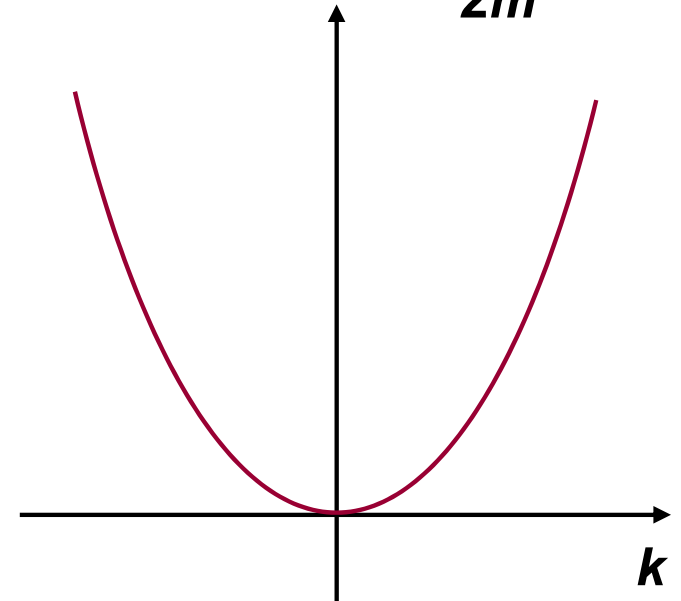
The energy dispersion relation of free electrons is parabolic, as shown in the figure above

L

$V(x)$

Vacuum level

θ

Energy bands

Potential in a crystal

0

a

x

Electron in a 1D Periodic Potential: Free-Electron Approach

Now the Hamiltonian is:

$$\hat{H} = \hat{H}_o + \hat{V}$$

$$\Rightarrow \hat{H} = \hat{1}\hat{H}\hat{1} \qquad\qquad\qquad\qquad \left\{ \quad \sum_k |\phi_k\rangle\langle\phi_k| = \hat{1} \right.$$

$$= \sum_k e(k)|\phi_k\rangle\langle\phi_k| + \sum \langle\phi_{k'}|\hat{V}|\phi_k\rangle |\phi_{k'}\rangle\langle\phi_k|$$
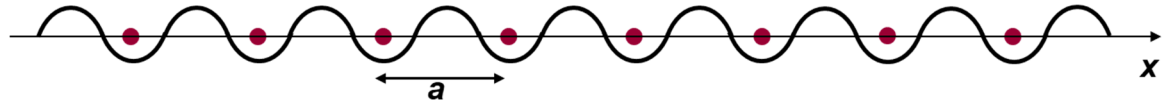
The periodic potential matrix element is non-zero in only special cases:

$$\langle\phi_{k'}|\hat{V}|\phi_k\rangle = \int_{-L/2}^{L/2} dx \sqrt{\frac{1}{L}} e^{-i k' x} V(x) \sqrt{\frac{1}{L}} e^{i k x}$$

$$= \frac{1}{L} \int_{-L/2}^{L/2} dx\, e^{-i k' x} \left[V_1 e^{i \frac{2\pi}{a} x} + V_{-1} e^{-i \frac{2\pi}{a} x} \right] e^{i k x}$$

$$= \begin{cases} V_{-1} & \text{if } k - k' = +\dfrac{2\pi}{a} \\[2mm] V_1 & \text{if } k - k' = -\dfrac{2\pi}{a} \\[2mm] 0 & \text{otherwise} \end{cases}$$

Perturbation Theory: A Review

Consider a Hamiltonian with eigenstates and energies given by:

$$\hat{H}_o |\phi_n\rangle = e_n |\phi_n\rangle$$

In the presence of a perturbing potential, the new eigenstates and energies are given by:

$$\left(\hat{H}_o + \hat{V}\right)|\psi_n\rangle = E_n |\psi_n\rangle$$

If the perturbation is small, then the new eigenstates are slightly perturbed from the original eigenstates and, to first order in the perturbation, can be written as:

$$|\psi_n\rangle \approx |\phi_n\rangle + \sum_{m \neq n} \frac{\langle\phi_m|\hat{V}|\phi_n\rangle}{e_n - e_m}|\phi_m\rangle + \text{higher order terms}$$

Thus, the perturbation "mixes" the eigenstates of the original Hamiltonian to generate the eigensatate of the new Hamiltonian.

Note: The effect of the perturbation is not small, and the perturbation theory breaks down, if for:

$$\langle\phi_m|\hat{V}|\phi_n\rangle \neq 0$$

we have:

$$e_n - e_m \approx 0$$

Electron in a 1D Periodic Potential: Perturbation Theory

So we try perturbation theory and write:

$$\left(\hat{H}_o + \hat{V}\right)|\psi_k\rangle = E(k)|\psi_k\rangle$$

New energy   New eigenstate

And write the new eigenstate to first order in the periodic potential as:

$$|\psi_k\rangle \approx |\phi_k\rangle + \sum_{k'} \frac{\langle\phi_{k'}|\hat{V}|\phi_k\rangle}{e(k) - e(k')}|\phi_{k'}\rangle + \text{higher order terms}$$

And use:

$$\langle\phi_{k'}|\hat{V}|\phi_k\rangle == \begin{cases} V_{-1} & \text{if } k - k' = +\dfrac{2\pi}{a} \\[2ex] V_1 & \text{if } k - k' = -\dfrac{2\pi}{a} \\[2ex] 0 & \text{otherwise} \end{cases}$$

Electron in a 1D Periodic Potential: Perturbation Theory

And write the new eigenfunction as:

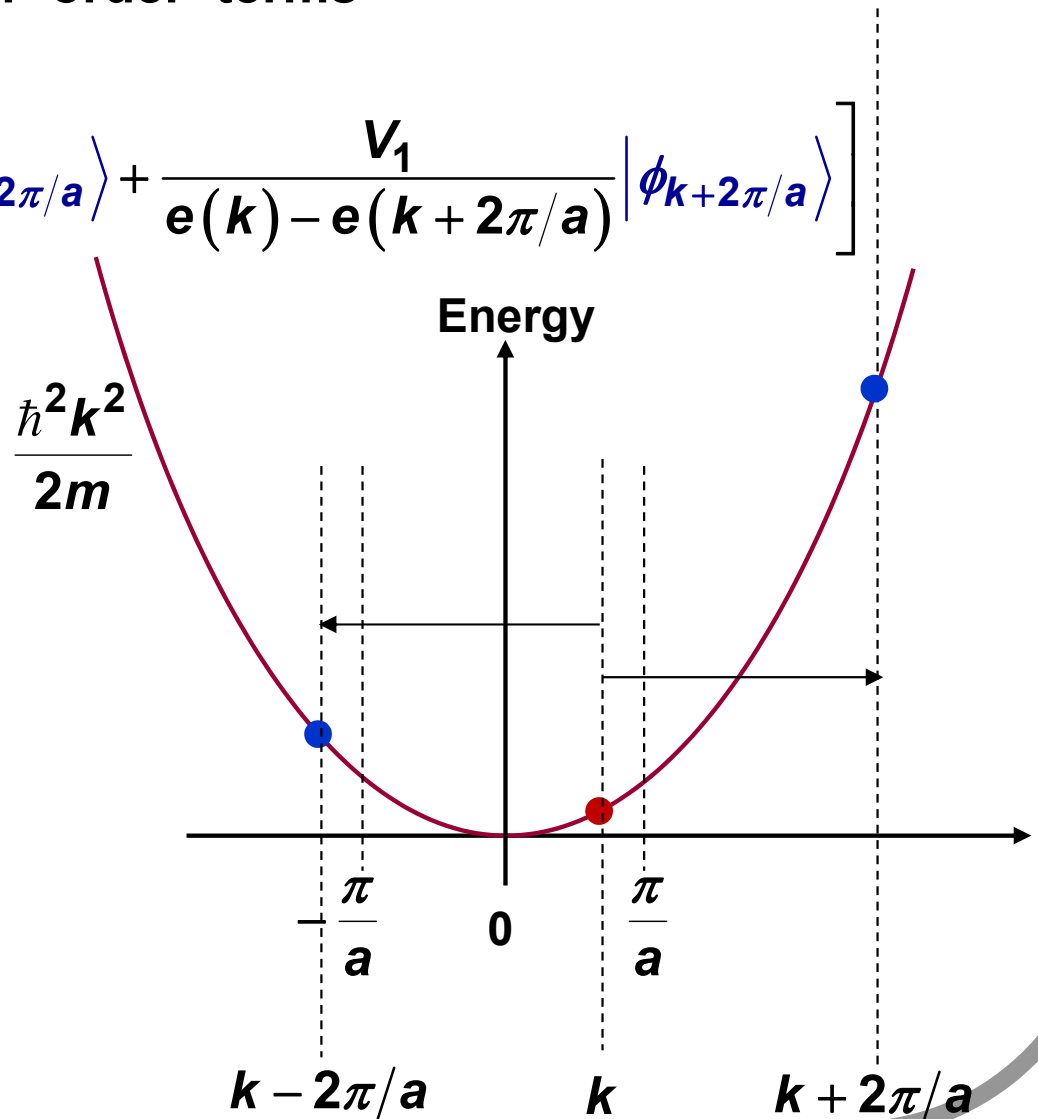$$|\psi_k\rangle \approx |\phi_k\rangle + \sum_{k'} \frac{\langle \phi_{k'}|\hat{V}|\phi_k\rangle}{e(k)-e(k')}|\phi_{k'}\rangle + \text{higher order terms}$$

$$|\psi_k\rangle \approx |\phi_k\rangle + \left[\frac{V_{-1}}{e(k)-e(k-2\pi/a)}|\phi_{k-2\pi/a}\rangle + \frac{V_1}{e(k)-e(k+2\pi/a)}|\phi_{k+2\pi/a}\rangle \right]$$

$$+ \text{higher order terms}$$

Solutions obtained !

Now lets go home ……………

Wait ………..

Electron in a 1D Periodic Potential: Perturbation Theory

$$\left|\psi_k\right\rangle \approx \left|\phi_k\right\rangle + \left[\frac{V_{-1}}{e(k)-e(k-2\pi/a)}\left|\phi_{k-2\pi/a}\right\rangle + \frac{V_1}{e(k)-e(k+2\pi/a)}\left|\phi_{k+2\pi/a}\right\rangle\right]$$

$$+ \text{ higher order terms}$$

The new wavefunction becomes:

$$\psi_k(x) \approx \left\langle x|\psi_k\right\rangle$$

$$= \frac{1}{\sqrt{L}}e^{ikx} + \left[\frac{V_{-1}}{e(k)-e(k-2\pi/a)}\frac{1}{\sqrt{L}}e^{i\left(k-\frac{2\pi}{a}x\right)} + \frac{V_1}{e(k)-e(k+2\pi/a)}\frac{1}{\sqrt{L}}e^{i\left(k+\frac{2\pi}{a}x\right)}\right]$$
$$+ \text{ higher order terms}$$

$$= \frac{1}{\sqrt{L}}e^{ikx}\left[\frac{V_{-1}}{e(k)-e(k-2\pi/a)}\frac{1}{\sqrt{L}}e^{-i\frac{2\pi}{a}x} + \frac{V_1}{e(k)-e(k+2\pi/a)}\frac{1}{\sqrt{L}}e^{i\frac{2\pi}{a}x}\right]$$
$$+ \text{ higher order terms}$$

$$= \frac{1}{\sqrt{L}}e^{ikx}u_k(x)$$

A periodic function: $u_k(x+a) = u_k(x)$

Electron in a 1D Periodic Potential: Perturbation Theory

$$|\psi_k\rangle \approx |\phi_k\rangle + \left[\frac{V_{-1}}{e(k) - e(k - 2\pi/a)}|\phi_{k - 2\pi/a}\rangle + \frac{V_1}{e(k) - e(k + 2\pi/a)}|\phi_{k + 2\pi/a}\rangle\right]$$

$+$ **higher order terms**

What if k = π/a ?

The denominator blows up !!

Energy

$\dfrac{\hbar^2 k^2}{2m}$

$-\dfrac{\pi}{a}$ 0 $\dfrac{\pi}{a}$

$k - 2\pi/a$ k $k + 2\pi/a$

Electron in a 1D Periodic Potential: Perturbation Theory

$$\left|\psi_k\right\rangle \approx \left|\phi_k\right\rangle + \left[\frac{V_{-1}}{e(k)-e(k-2\pi/a)}\left|\phi_{k-2\pi/a}\right\rangle + \frac{V_1}{e(k)-e(k+2\pi/a)}\left|\phi_{k+2\pi/a}\right\rangle\right]$$

+ higher order terms

What if k = -π/a ?

The denominator blows up !!

$$\frac{\hbar^2 k^2}{2m}$$

Energy

$-\dfrac{\pi}{a}$ **0** $\dfrac{\pi}{a}$

$k-2\pi/a$ k $k+2\pi/a$
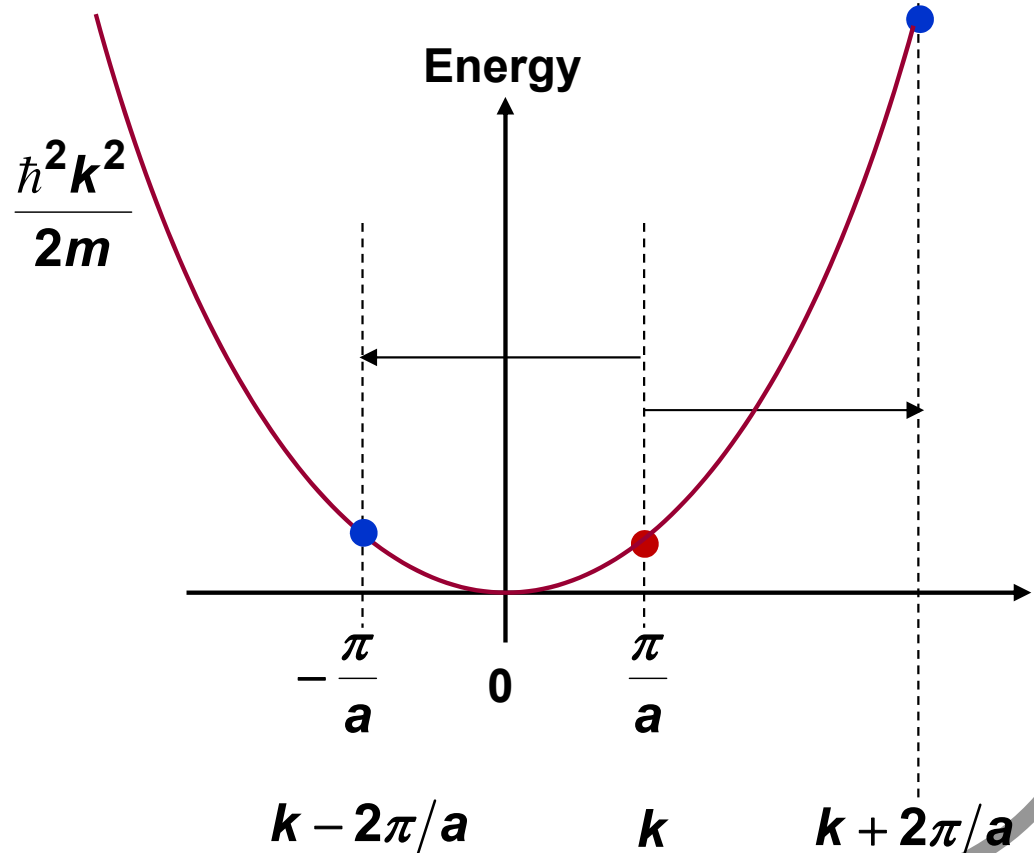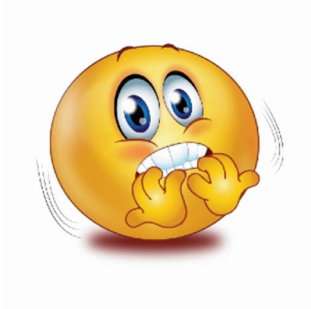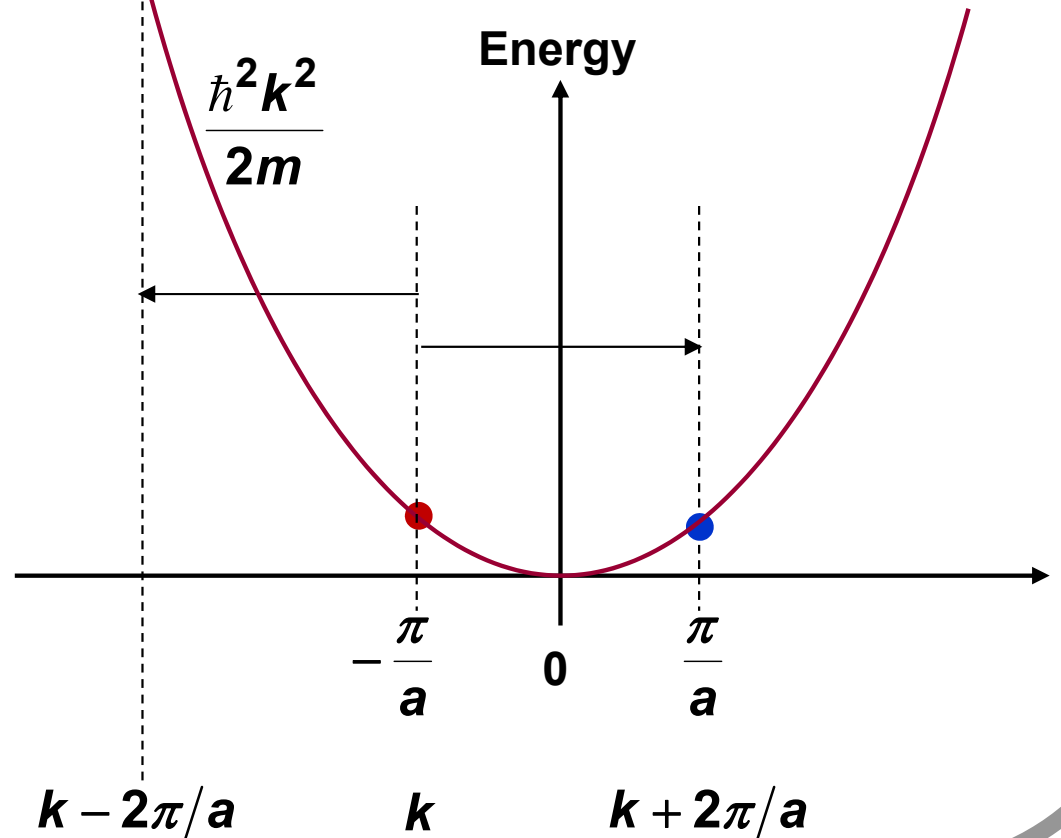
Electron in a 1D Periodic Potential: Bragg Scattering

$\sim e^{ikx}$ a $\sim e^{-ikx}$

x
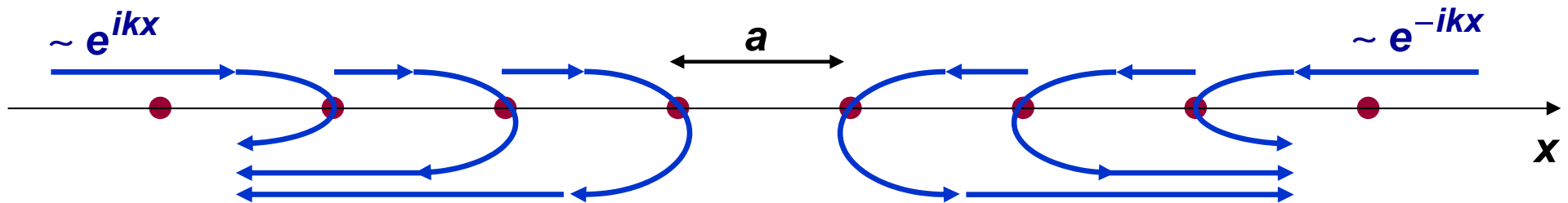
The scattering of the electron wave from each successive atom in the periodic chain would add up constructively in phase in the backward direction if the extra phase accumulated by the wave in the round trip from one atom to the next one is a multiple of 2π:

$$k2a = 2\pi$$

$$\Rightarrow k = \frac{\pi}{a}$$

Bragg condition!
When this is satisfied, a forward moving electron is strongly reflected in the backward direction

Similarly, a backward moving electron is strongly Bragg scattered in the forward direction when

$$k = -\frac{\pi}{a}$$

Electron in a 1D Periodic Potential: Perturbation Theory
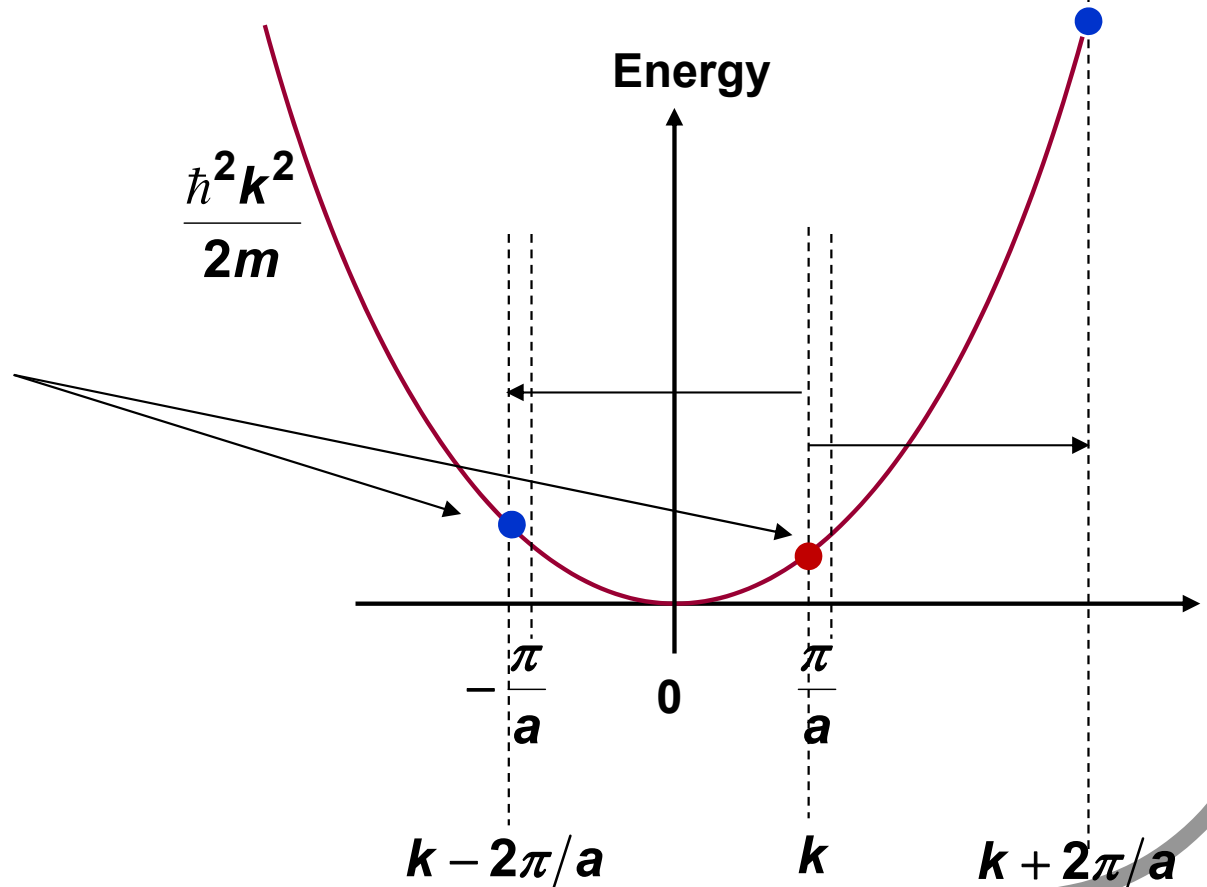
Suppose k is near π/a :

$$\left|\psi_k\right\rangle \approx \left|\phi_k\right\rangle + \left[\frac{V_{-1}}{e(k)-e(k-2\pi/a)}\left|\phi_{k-2\pi/a}\right\rangle + \frac{V_1}{e(k)-e(k+2\pi/a)}\left|\phi_{k+2\pi/a}\right\rangle\right]$$

$$+ \text{ higher order terms}$$

Then $\left|\phi_k\right\rangle$ is strongly coupled To $\left|\phi_{k-2\pi/a}\right\rangle$ and $\left|\phi_{k-2\pi/a}\right\rangle$ is strongly coupled to $\left|\phi_k\right\rangle$

Way forward: abandon standard perturbation theory and use finite basis expansion !

Energy

$$\frac{\hbar^2 k^2}{2m}$$

$$-\frac{\pi}{a} \qquad 0 \qquad \frac{\pi}{a}$$

$$k-2\pi/a \qquad k \qquad k+2\pi/a$$

Electron in a 1D Periodic Potential: Finite Basis Expansion

Now the Hamiltonian is:
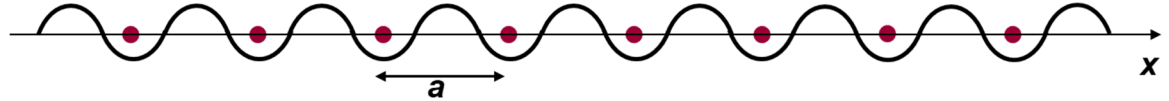
$$\hat{H} = \hat{H}_o + \hat{V}$$

$$\Rightarrow \hat{H} = \hat{1}\hat{H}\hat{1}$$
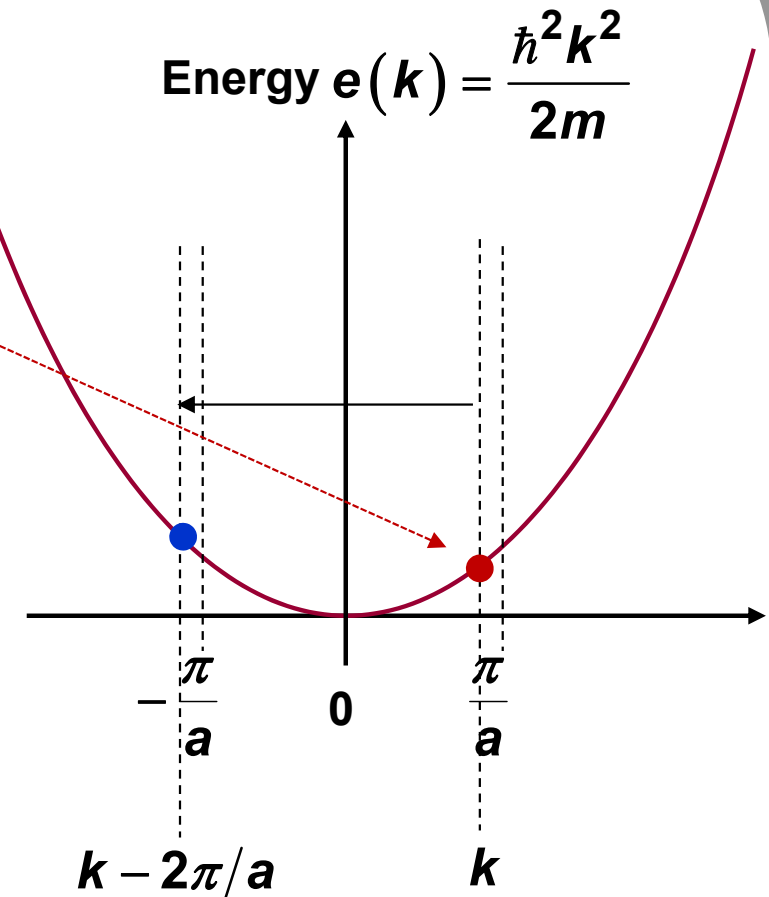
$$= \sum_k e(k)|\phi_k\rangle\langle\phi_k| + \sum \langle\phi_{k'}|\hat{V}|\phi_k\rangle |\phi_{k'}\rangle\langle\phi_k|$$

The periodic potential matrix element is non-zero in only special cases:

$$\langle\phi_{k'}|\hat{V}|\phi_k\rangle == \begin{cases} V_{-1} \ \delta_{k-k'=\frac{2\pi}{a}} \\[2em] V_1 \ \delta_{k-k'=-\frac{2\pi}{a}} \end{cases}$$

Electron in a 1D Periodic Potential: Finite Basis Expansion

Suppose k is near π/a :

Keep the most important strongly coupled basis functions:

$$\left|\psi_k\right\rangle \approx a\left|\phi_k\right\rangle + b\left|\phi_{k-2\pi/a}\right\rangle$$

Plug this into the Schrodinger equation:

$$\left(\hat{H}_o + \hat{V}\right)\left|\psi_k\right\rangle = E(k)\left|\psi_k\right\rangle$$

$$\hat{H}_o + \hat{V} = \sum_k e(k)\left|\phi_k\right\rangle\left\langle\phi_k\right| + \sum \left\langle\phi_{k'}\right|\hat{V}\left|\phi_k\right\rangle\left|\phi_{k'}\right\rangle\left\langle\phi_k\right|$$

To get the matrix equation:

$$\begin{bmatrix} e(k) & V_1 \\ V_{-1} & e(k-2\pi/a) \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = E(k)\begin{bmatrix} a \\ b \end{bmatrix}$$

The new energies are:

$$E(k) = \frac{e(k) + e(k-2\pi/a)}{2} \pm \sqrt{\left(\frac{e(k) - e(k-2\pi/a)}{2}\right)^2 + |V_1|^2}$$

Energy $e(k) = \dfrac{\hbar^2 k^2}{2m}$

$-\dfrac{\pi}{a}$ $\quad 0 \quad$ $\dfrac{\pi}{a}$

$k - 2\pi/a$ $\qquad\qquad$ k

Electron in a 1D Periodic Potential: Finite Basis Expansion

Energy $e(k) = \dfrac{\hbar^2 k^2}{2m}$

Suppose k is near $-\pi/a$:

Keep the most important strongly coupled basis functions:

$$\left|\psi_k\right\rangle \approx c\left|\phi_k\right\rangle + d\left|\phi_{k+2\pi/a}\right\rangle$$

Plug this into the Schrodinger equation:

$$\left(\hat{H}_o + \hat{V}\right)\left|\psi_k\right\rangle = E(k)\left|\psi_k\right\rangle$$

$$\hat{H}_o + \hat{V} = \sum_k e(k)\left|\phi_k\right\rangle\left\langle\phi_k\right| + \sum \left\langle\phi_{k'}\right|\hat{V}\left|\phi_k\right\rangle\left|\phi_{k'}\right\rangle\left\langle\phi_k\right|$$

To get the matrix equation:

$$\begin{bmatrix} e(k) & V_{-1} \\ V_1 & e(k+2\pi/a) \end{bmatrix}\begin{bmatrix} c \\ d \end{bmatrix} = E(k)\begin{bmatrix} c \\ d \end{bmatrix}$$

k

$k + 2\pi/a$

$-\dfrac{\pi}{a}$ 0 $\dfrac{\pi}{a}$

The new energies are:

$$E(k) = \frac{e(k) + e(k+2\pi/a)}{2} \pm \sqrt{\left(\frac{e(k) - e(k+2\pi/a)}{2}\right)^2 + |V_1|^2}$$
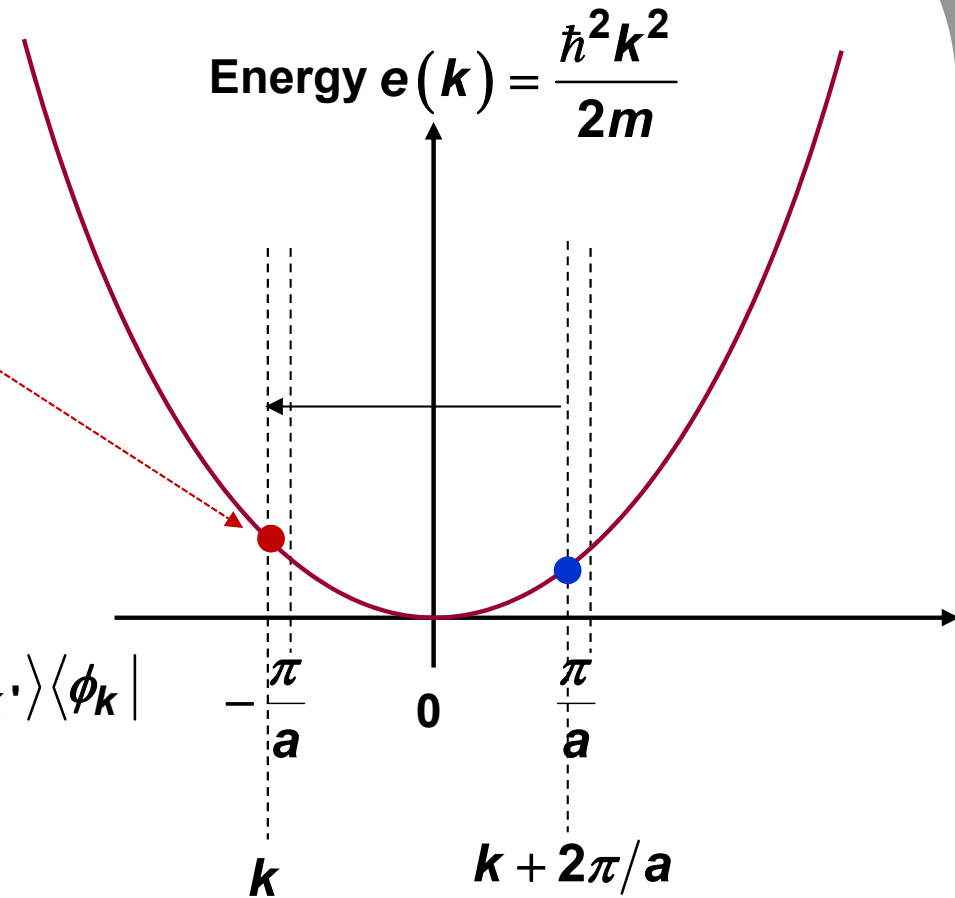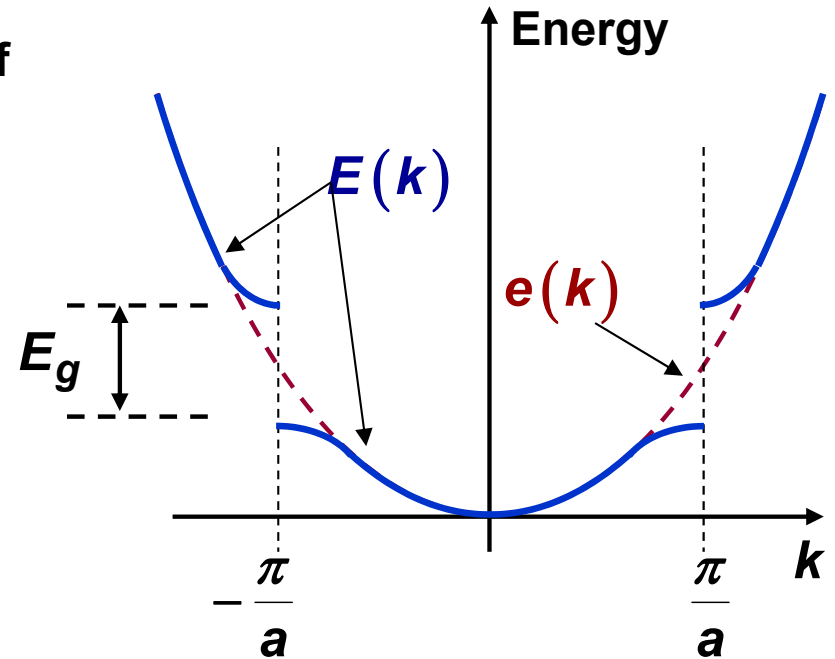
Electron in a 1D Periodic Potential: Finite Basis Expansion

The obtained solutions $E(k)$ are plotted on top of the free-electron energy dispersion $e(k)$ so that you can see the difference.

An energy gap opens up!!

$$E_g = 2\left|V_1\right|$$

$$E(k) = \frac{e(k)+e(k-2\pi/a)}{2} \pm \sqrt{\left(\frac{e(k)-e(k-2\pi/a)}{2}\right)^2 + \left|V_1\right|^2} \quad \begin{cases} \text{for } k \text{ near } +\pi/a \\ + \\ \quad \text{sign for } k \begin{smallmatrix} > \\ < \end{smallmatrix} \pi/a \\ - \end{cases}$$

$$E(k) = \frac{e(k)+e(k+2\pi/a)}{2} \pm \sqrt{\left(\frac{e(k)-e(k+2\pi/a)}{2}\right)^2 + \left|V_1\right|^2} \quad \begin{cases} \text{for } k \text{ near } -\pi/a \\ + \\ \quad \text{sign for } k \begin{smallmatrix} < \\ > \end{smallmatrix} -\pi/a \\ - \end{cases}$$

Electron in a 1D Periodic Potential: Origin of the Bandgaps

We have: $E_\pm(k = \pi/a) = e(k = \pi/a) \pm |V_1|$

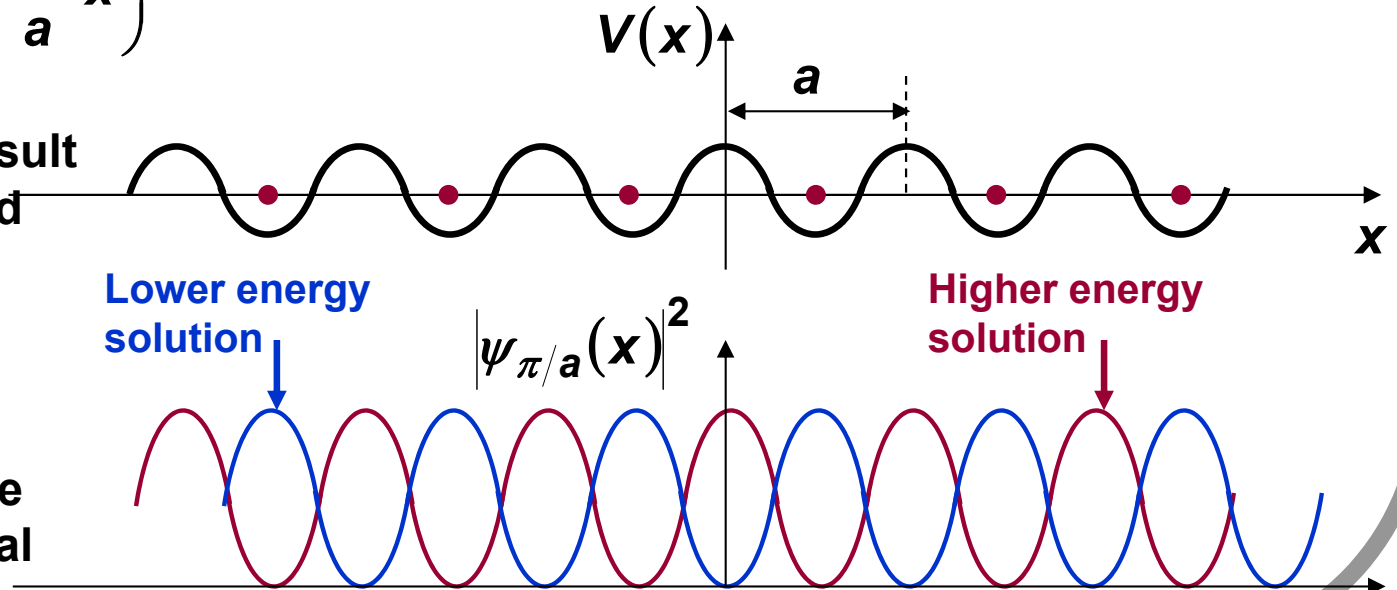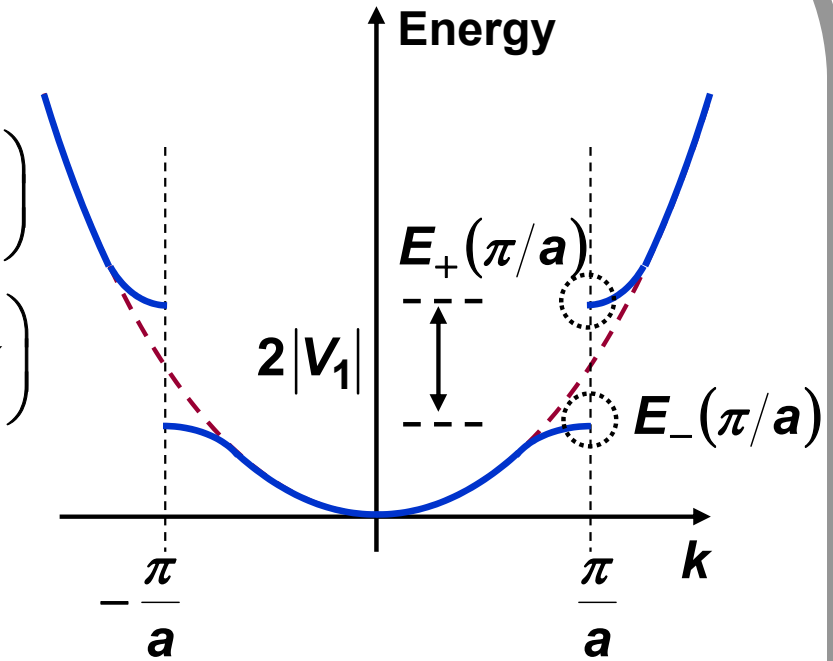$$|\psi_k\rangle \approx a|\phi_k\rangle + b|\phi_{k-2\pi/a}\rangle$$

$$\psi_{k=\pi/a}(x) \approx \sqrt{\frac{1}{2L}}\left(e^{i\frac{\pi}{a}x} \pm e^{-i\frac{\pi}{a}x}\right) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(\frac{\pi}{a}x\right) \\ i\sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{a}x\right) \end{cases}$$

Note that (for V_1 real):

$$V(x) = V_1 e^{i\frac{2\pi}{a}x} + V_{-1} e^{-i\frac{2\pi}{a}x}$$

$$= 2V_1\cos\left(\frac{2\pi}{a}x\right)$$

• The solutions are standing waves (as a result of forward and backward Bragg scattering)

• The higher energy solution has larger probability density in the region of higher potential

Energy

$E_+(\pi/a)$

$2|V_1|$

$E_-(\pi/a)$

$-\frac{\pi}{a}$ $\frac{\pi}{a}$ k

$V(x)$

a

Lower energy solution

Higher energy solution

$|\psi_{\pi/a}(x)|^2$

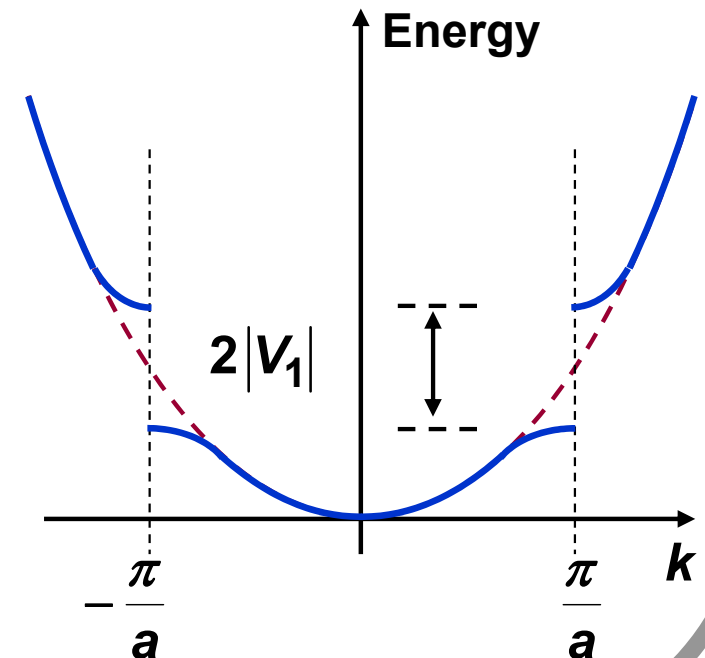# Electron in a 1D Periodic Potential: Summary

Summary of Findings:

• **For a perturbative periodic potential with the following Fourier Series representation,**

$$V(x) = V_1 e^{i\frac{2\pi}{a}x} + V_{-1} e^{-i\frac{2\pi}{a}x}$$

the plane wave eigenfunctions of the free electron with wavevector k get coupled with the wavevectors $(k + 2\pi/a)$ and $(k - 2\pi/a)$ as a result of the fact that the potential had wavevectors $2\pi/a$ and $-2\pi/a$ in its Fourier series
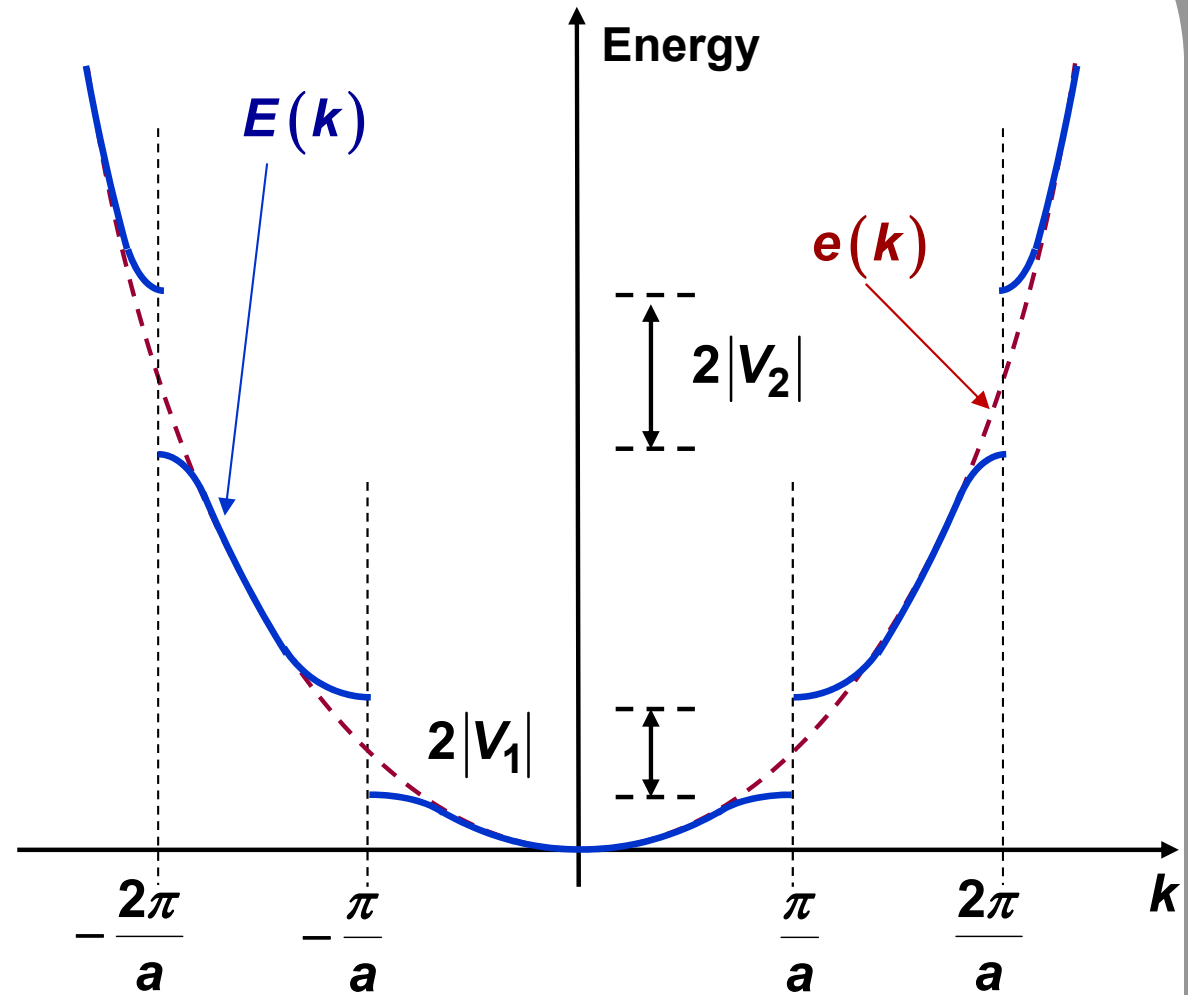
• **If the electron wavevector k is such that $e(k)$ and $e(k-2\pi/a)$ have the same energy, or if $e(k)$ and $e(k+2\pi/a)$ have the same energy, then a bandgap of magnitude $2|V_1|$ will open up in the free electron dispersion for the wavevector value k**
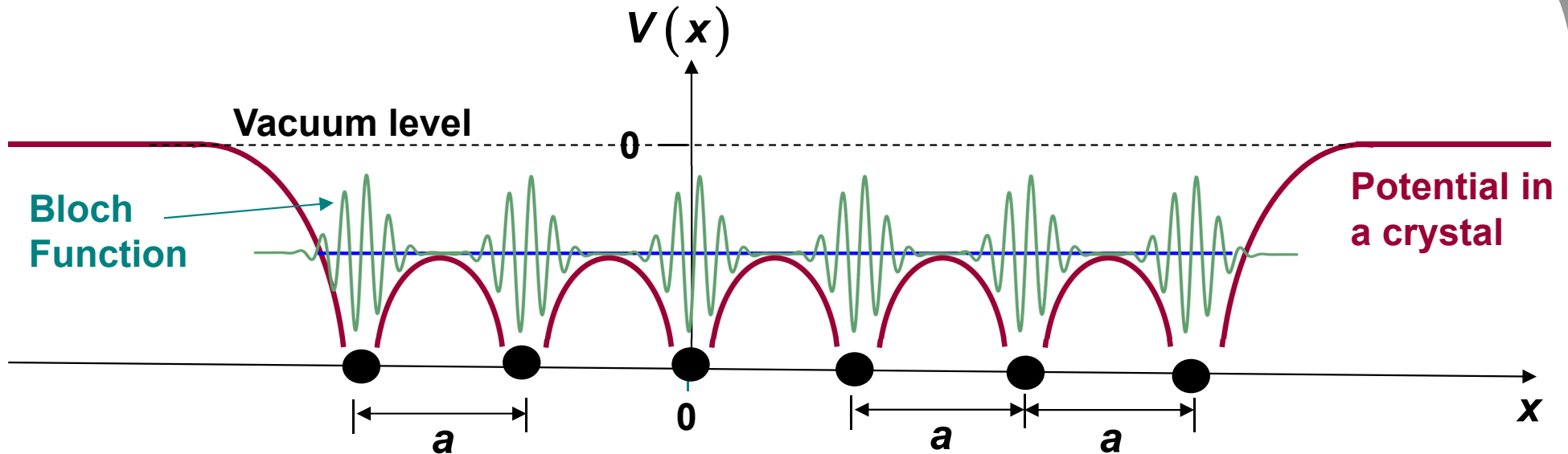
Electron in a 1D Periodic Potential: More General Case

Now suppose the periodic potential looks like:

$$V(x) = V_1 e^{i\frac{2\pi}{a}x} + V_{-1} e^{-i\frac{2\pi}{a}x}$$

$$+ V_2 e^{i\frac{4\pi}{a}x} + V_{-2} e^{-i\frac{4\pi}{a}x}$$

$E(k)$

$e(k)$

Energy

$2|V_2|$

$2|V_1|$

$-\dfrac{2\pi}{a}$ $-\dfrac{\pi}{a}$ $\dfrac{\pi}{a}$ $\dfrac{2\pi}{a}$ k

Electron in a 1D Periodic Potential: Bloch's Theorem

$V(x)$

Vacuum level

0

Bloch Function

Potential in a crystal

a

0

a a

x

Note that:

$$\left|\psi\left(x+na\right)\right|^{2}=\left|\psi\left(x\right)\right|^{2} \qquad \{n=0,\pm1,\pm2,......$$

Probability of finding the electron is periodic

This implies that:

$$\psi\left(x+na\right)=e^{i\theta(na)}\psi\left(x\right)$$

Electron in a 1D Periodic Potential: Bloch's Theorem

$V(x)$

Vacuum level

0

Bloch Function

Potential in a crystal

0

a a a

x
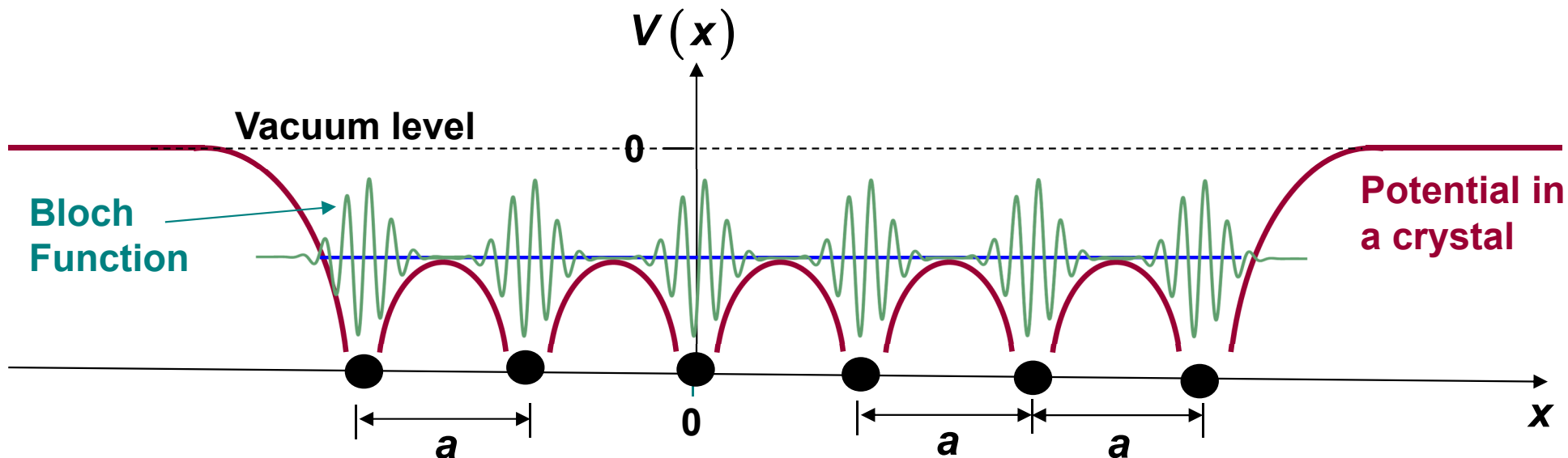
$$\psi(x + na) = e^{i\theta(na)}\psi(x)$$

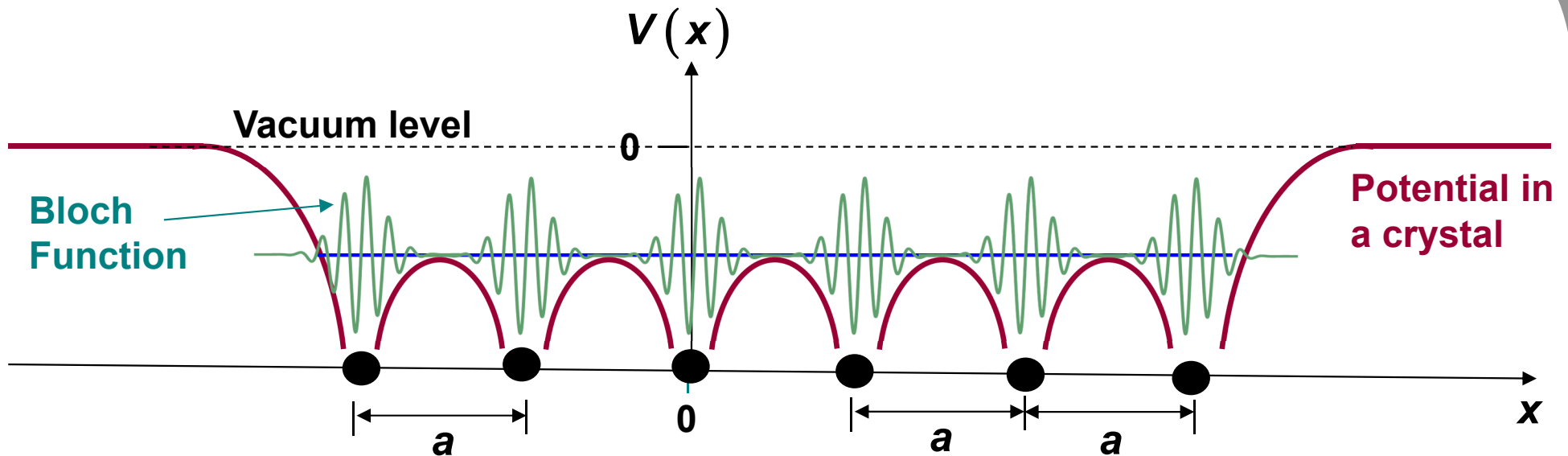$$\Rightarrow \psi(x + a) = e^{i\theta(a)}\psi(x) \qquad \Rightarrow \psi(x + a) = e^{i\theta(a)}\psi(x)$$

$$\Rightarrow \psi(x + 2a) = e^{i\theta(2a)}\psi(x) \qquad \Rightarrow \psi(x + a + a) = e^{i\theta(a)}\psi(x + a) = e^{i\theta(a)}e^{i\theta(a)}\psi(x)$$

$$\theta(2a) = 2\theta(a)$$

$$\Rightarrow \theta(a) \propto a \qquad \longrightarrow \quad \text{The phase is a linear function of } a$$

Electron in a 1D Periodic Potential: Bloch's Theorem

$V(x)$

Vacuum level

0

Bloch Function

Potential in a crystal

a

0

a a

x

$$\psi(x+a) = e^{i\theta(a)}\psi(x)$$

$$\Rightarrow \theta(a) \propto a$$

Let: $\theta(a) = ka$ ⟶ **k is the constant of proportionality**

Then: $\psi(x+a) = e^{ika}\psi(x)$ ⟶ **Bloch's theorem**

$$\Rightarrow \psi_k(x) = \frac{e^{ikx}}{\sqrt{L}} u_k(x)$$ ⟶ $u_k(x+a) = u_k(x)$

Bloch function

A periodic function

Electron in a 1D Periodic Potential: Bloch's Theorem

$$\psi_k(x) = \frac{e^{ikx}}{\sqrt{L}} u_k(x) \longrightarrow u_k(x+a) = u_k(x)$$

Bloch function

A periodic function

Any periodic function can be expanded in a Fourier series:

$$u_k(x) = \sum_m u_m e^{i\frac{2\pi}{a}m x}$$

Fourier Series

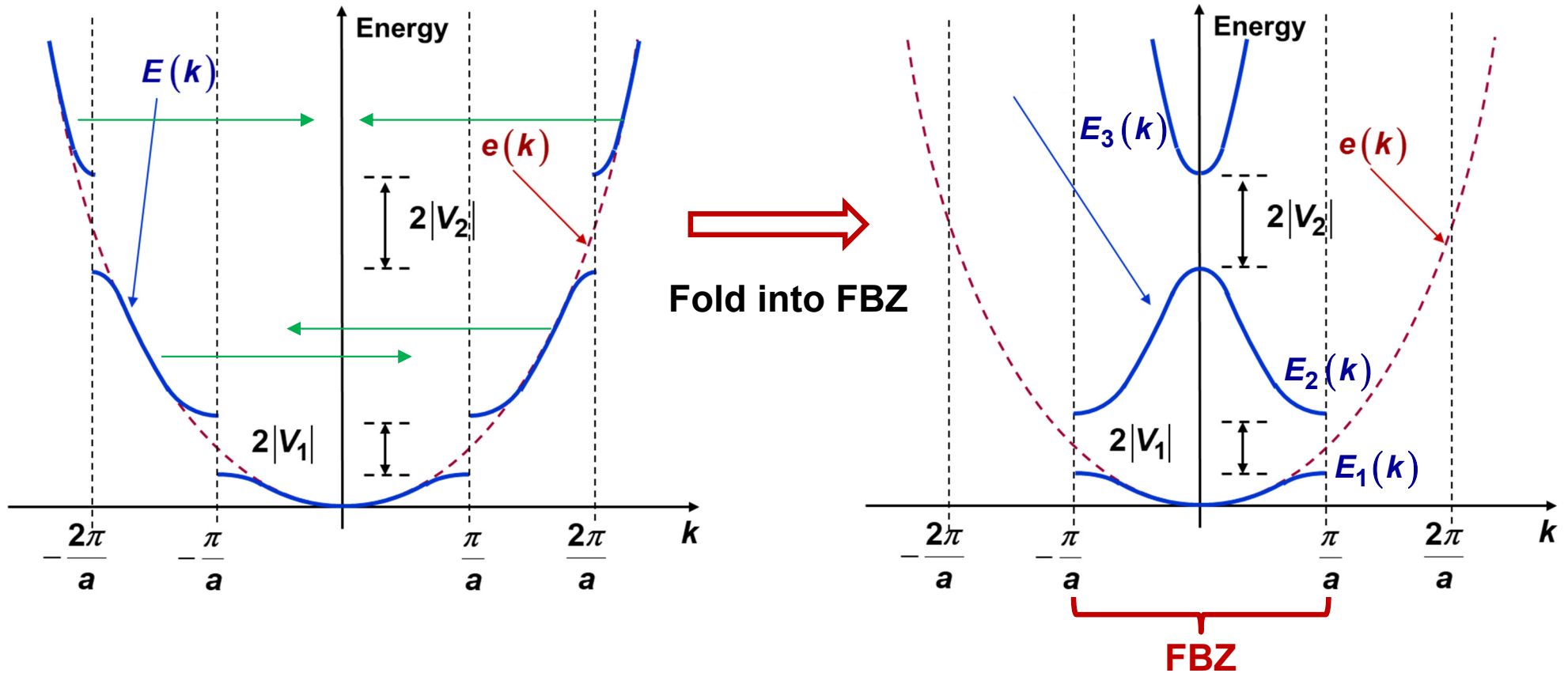$$\psi_k(x) = \frac{1}{\sqrt{L}} \sum_m u_m e^{i\left[k+\frac{2\pi}{a}m\right]x} \implies$$

Since summation over *m* includes all integers, *k* can be restricted to satisfy:

$$-\pi/a < k \le \pi/a$$

The above convention is used almost always!

Electron in a 1D Periodic Potential: Folded Bands and FBZ

Since **k** has been restricted to the range $-\pi/a < k \leq \pi/a$, the energy dispersion outside this range is folded into this range via translations by vectors that are multiples of $2\pi/a$

The dispersion thus obtained is split into energy bands

The interval $-\pi/a < k \leq \pi/a$ is called the **First Brillouin Zone (FBZ)**