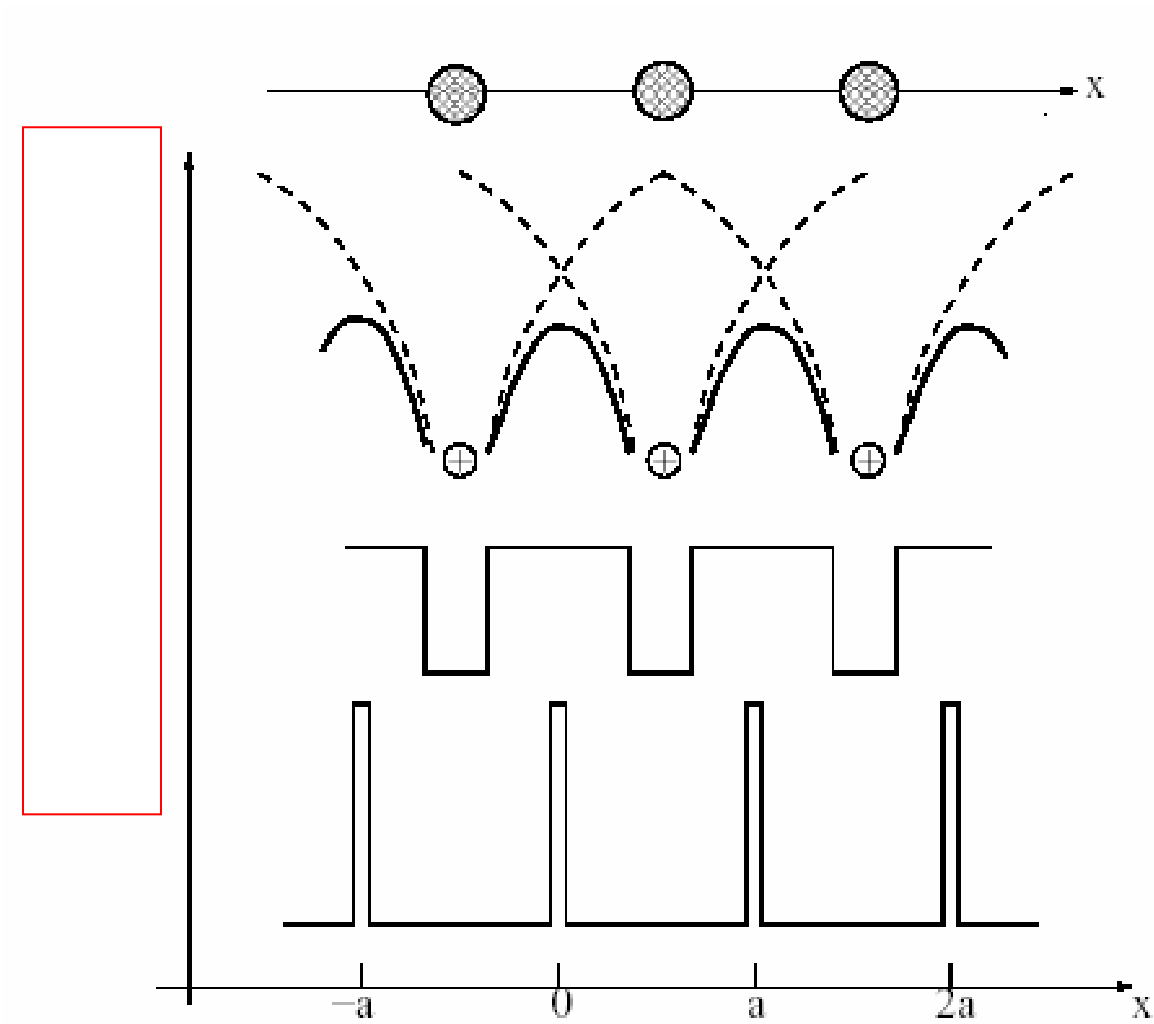
ENERGY BANDS

LECTURE 2

- Periodic potential
- Bloch's Theorem
- Energy bands
- Reduced-zone plot
- Bragg reflection
- Quantum states
- Material classification

Sec. 2.2

Periodic potential



1-D periodic array of primitive cells, each containing 1 monovalent atom.

1-D Coulombic potential for an array of primitive cells

Square-well representation

Delta-function representation

Any periodic potential will do for our purpose of revealing and

Sec. 2.2

Schrödinger Wave Equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

Can this equation be derived?

What do the symbols represent?

Particularly, what is ψ ?

What is the equation an expression of?

Why do we need to use it for electrons in a solid?

We often write SWE as:

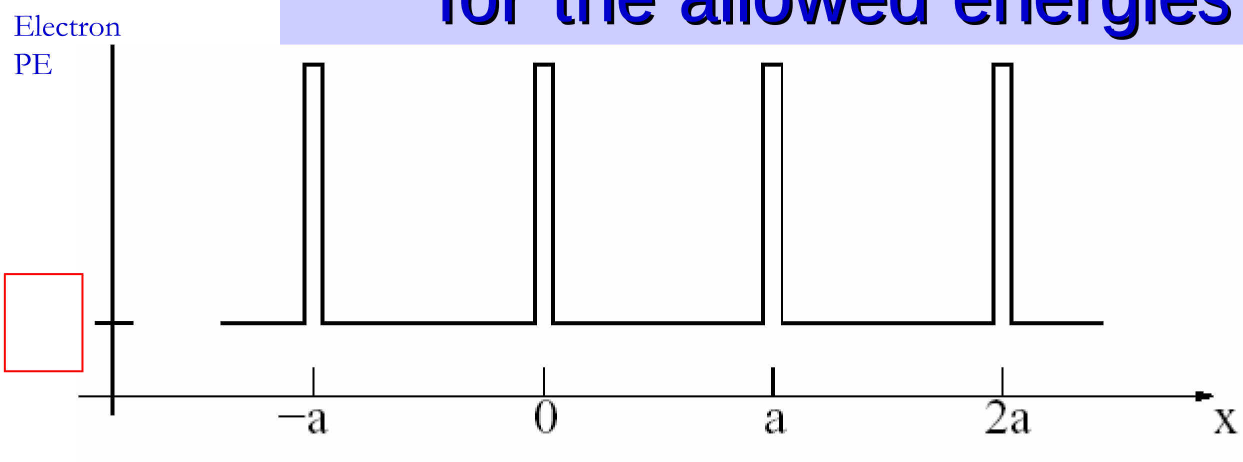
$$\frac{d^2\psi}{dx^2} + g^2\psi(x) = 0\,,$$

where, for U=0, for example,

$$g = \boxed{}\,.$$

Secs. 2.3, 2.4

Setting up the problem to solve for the allowed energies



Solve SWE for the periodic U(x) representing our toy semiconductor

For 0 < x < a

$$g = \frac{\sqrt{2m_0E}}{\hbar}\,.$$

General solution

$$\psi(x) = A\sin(gx) + \qquad, \qquad (0 < x < a)$$

Boundary conditions

1. ψ must be continuous at a boundary;
2. $d\psi/dx$ must be continuous at a boundary, except when the potential energy

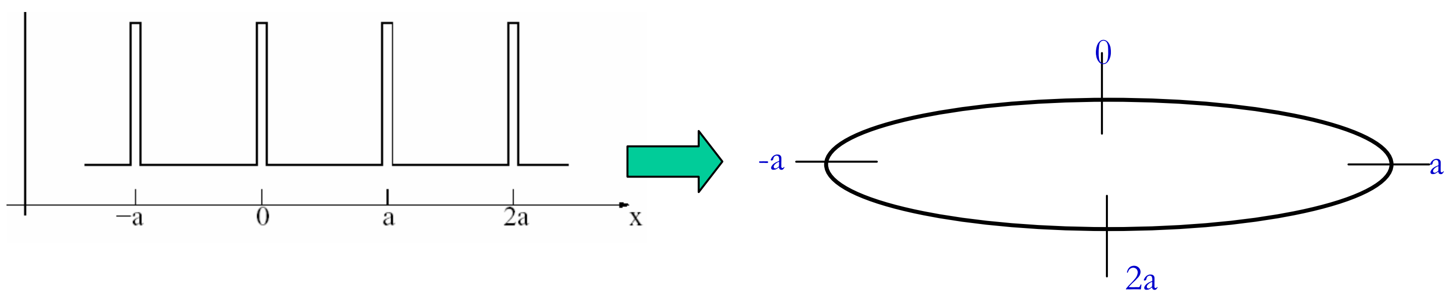
Bloch's Theorem

In a periodic potential, U(x+a)=U(x), the solutions to SWE are: $\psi_k(x) =$

This Bloch wave is a modulated plane wave; u is periodic; k is the

Alternatively, $\psi_k(x+a) =$

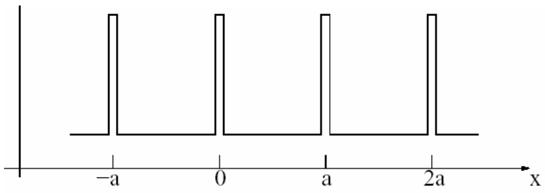
Employ periodic BC's



This allows us to write: $\psi_k(x+Na) = \psi_k(x)$ $\equiv$

$$\therefore \quad k = \frac{2\pi n}{Na}\,, \qquad (n = 0, \pm 1, \pm 2, \pm 3, \cdots)\,,$$ i.e., k is

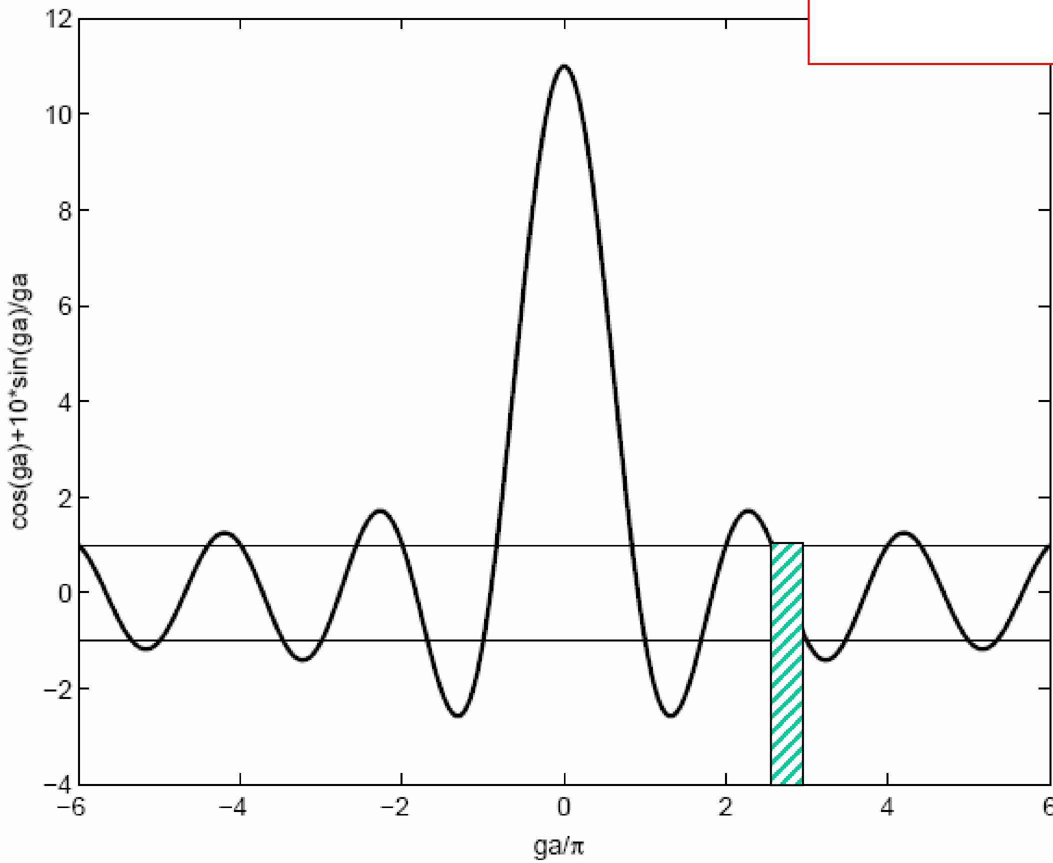
Allowed values of E



Solution for -a<x<0

$$\psi_k(x) = e^{-ika}[A \sin g(x+a) + B \cos g(x+a)]$$

Apply matching conditions to get A and B



Plot this function and note:

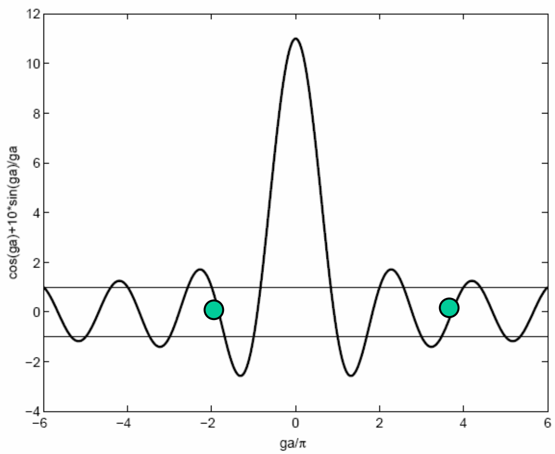
- Only certain values of g are allowed
- Recall: g is f(E)

$$g = \frac{\sqrt{2m_0 E}}{\hbar}$$

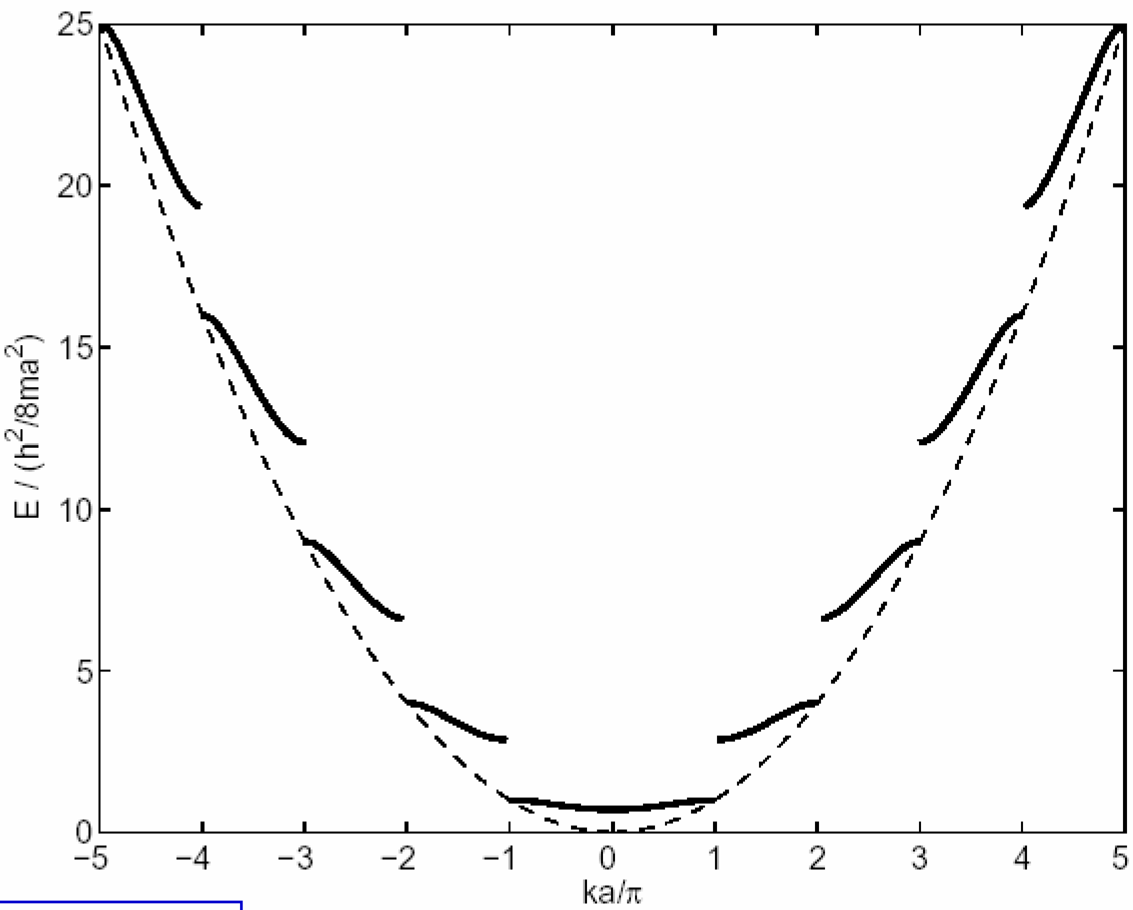
- ∴Only certain ______ of E are allowed.

Sec. 2.5

Allowed bands



• Link the green dots with its band on the plot.



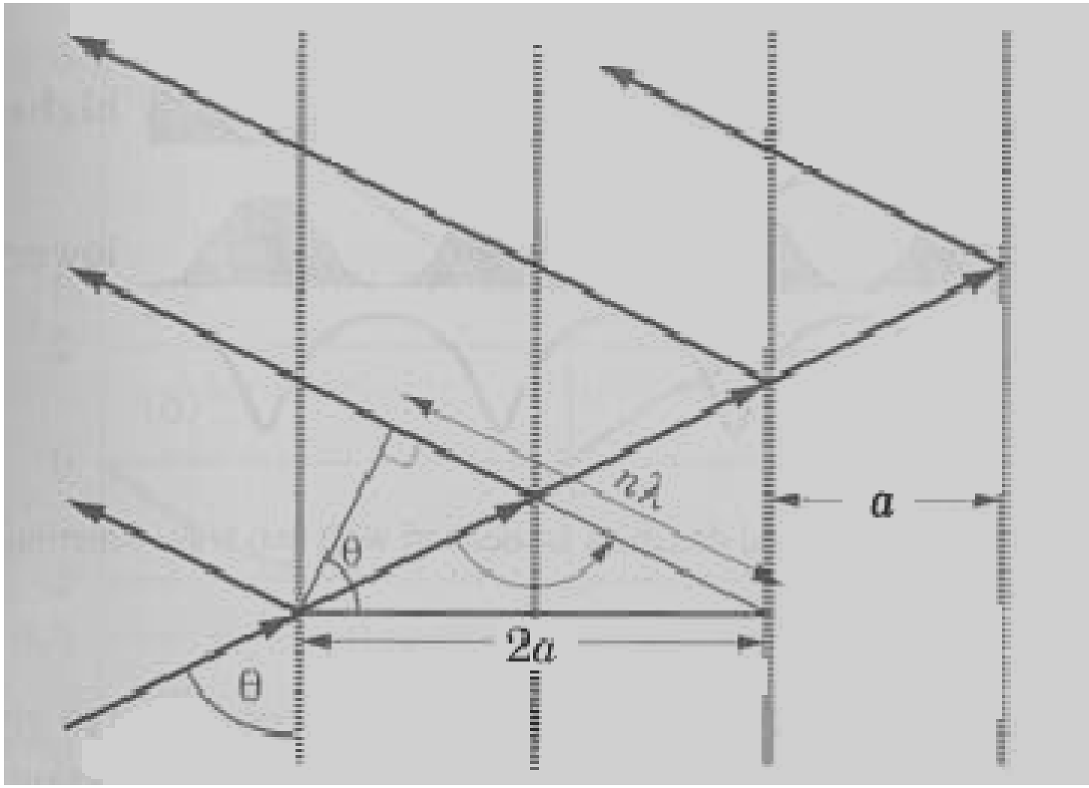
What is the dashed line?

What is k related to for a free electron?

What is k related to in a crystal?

Sec. 2.6

Band gaps: physical origin



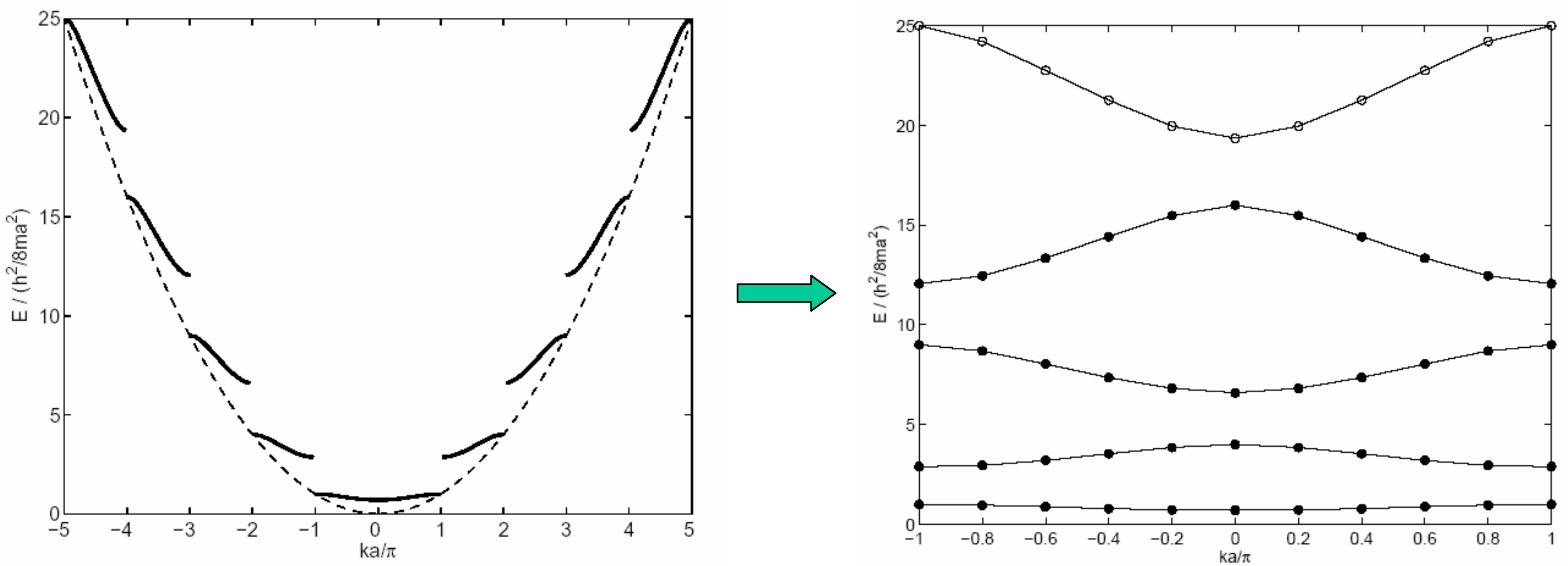
Electron wavefront of wavelength λ incident at angle θ on the planes of a crystal separated by spacing *a* (From Davies, *loc. cit.*, p.49)

Bragg reflection occurs when 2a sin θ =

i.e., in our 1-D example when k= instead of propagating waves, we get waves.

Sec. 2.5

Extended- and Reduced-zone plots



- Consider the 4th and 5th bands

$$k = \frac{4\pi}{a} + k'$$

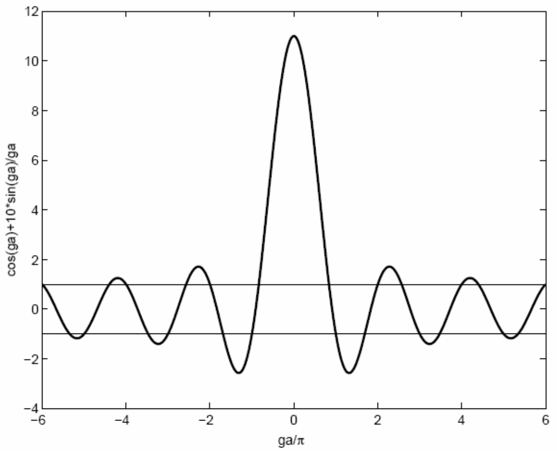
where k' is a Bloch wavevector in the first zone

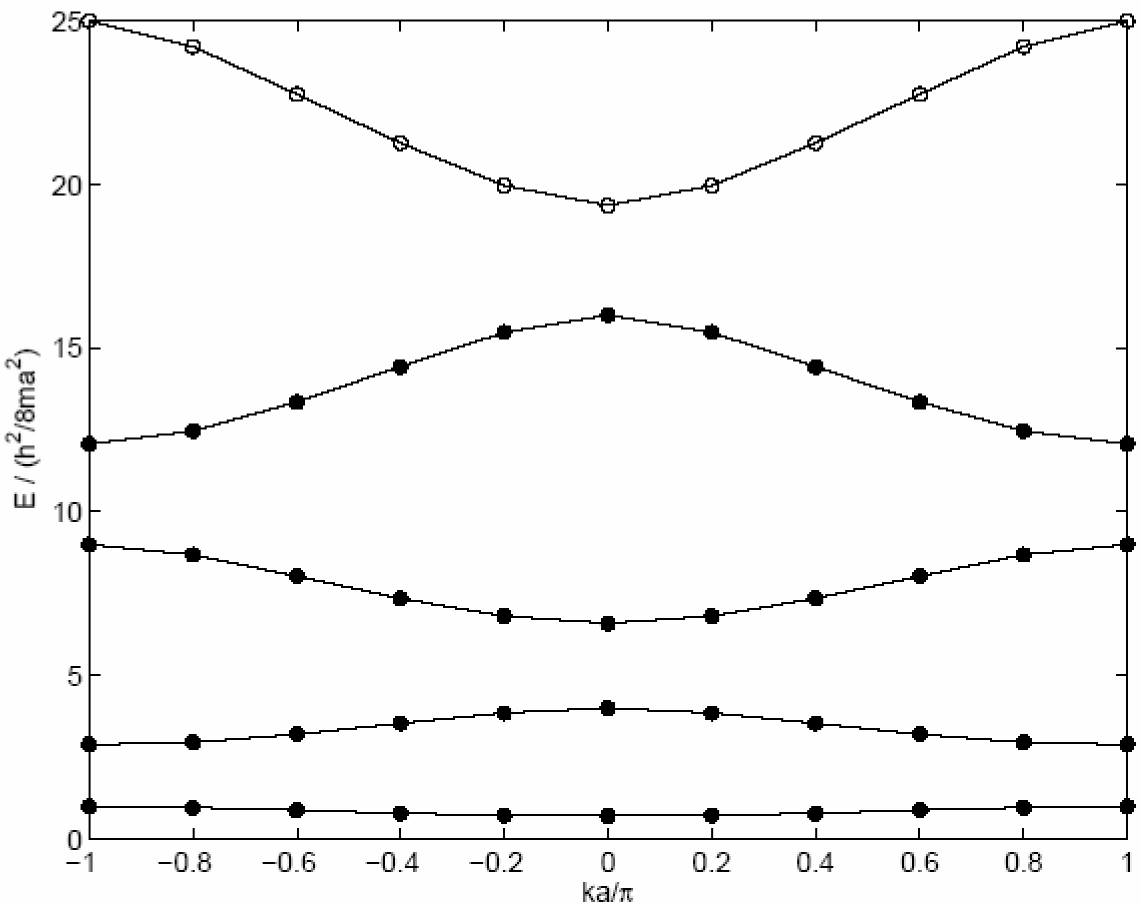
$$\begin{aligned} \psi_k(x) &= u_k(x) e^{i4\pi x/a} e^{ik'x} \\ &\equiv u'_k(x) e^{ik'x} \\ &= \psi_{k'}(x)\,. \end{aligned}$$

∴ shifts of n2π/a leave

Sec. 2.7

Allowed states





For N=

$$k = \frac{2\pi n}{Na}, \quad (n = 0, \pm 1, \pm 2, \ldots \pm N/2)$$

Spacing between

is 0.2 π/a (in this example)

Each state is a state.

How many electrons can there be in each crystal momentum state?

How many electrons in a full band?

Sec. 2.7

Semiconductor, metal, or insulator?

Our N=10 example is for one-electron primitive cells and gives N distinct states per BAND.

Allowing for spin there are 2N states per band

Silicon has 2 atoms per primitive cell, with 4 valence electrons in each atom,

i.e., 8 electrons per primitive cell and 8N valence electrons in total.

Therefore, the first 4 bands are completely filled (at 0K).

What happens at T > 0K ?

Where is the BANDGAP?

One possibility for a metal is that the material has 3N valence electrons.

Why does this make a metal?

What makes an insulator?