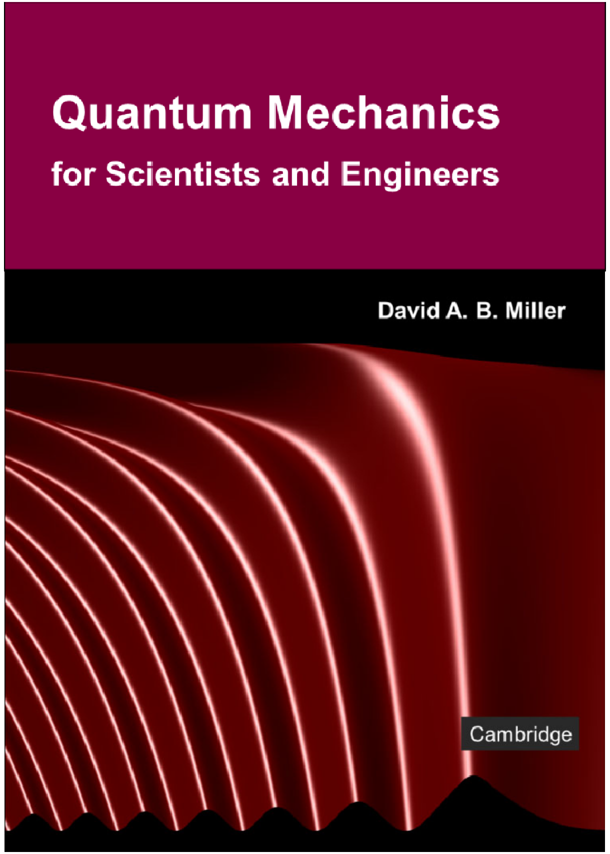
29 Band structures

Slides: Lecture 29a Band structures

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.5 introduction



Band structures

Quantum mechanics for scientists and engineers

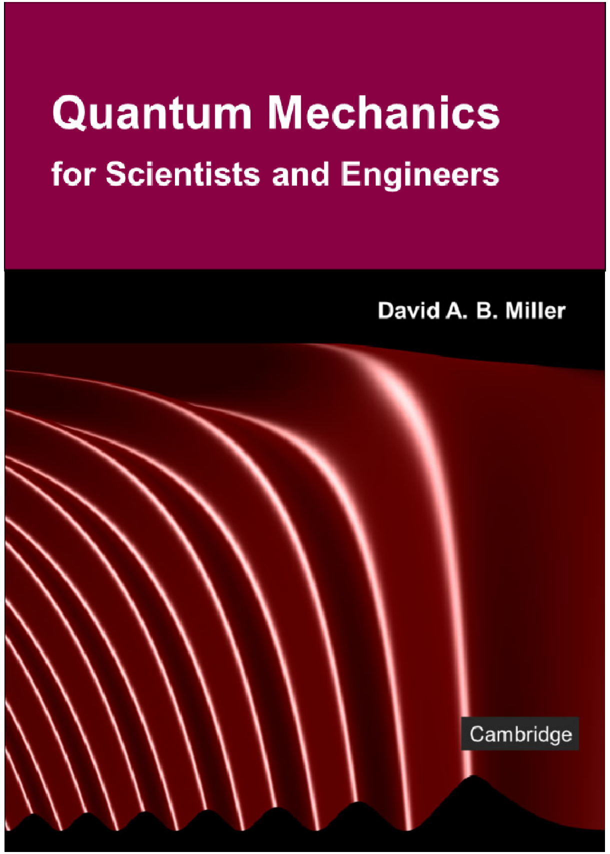
David Miller

29 Band structures

Slides: Lecture 29b Band structure diagrams

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.5



Band structures

Band structure diagrams

Quantum mechanics for scientists and engineers

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Band structure

If we knew the periodic potential $V_P(\mathbf{r})$

we could solve the resulting one-electron Schrödinger equation

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi(\mathbf{r})+V_P(\mathbf{r})\psi(\mathbf{r})=E\psi(\mathbf{r})$$

using the Bloch function form $\psi(\mathbf{r})=u(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$

calculating the energies E of all the possible states

These calculations give a "band structure"

There are various band structure calculation methods

Many methods "guess" $V_P(\mathbf{r})$, adjusting it to fit data

Band structure diagrams

To construct a band structure

presuming we know $V_P(\mathbf{r})$

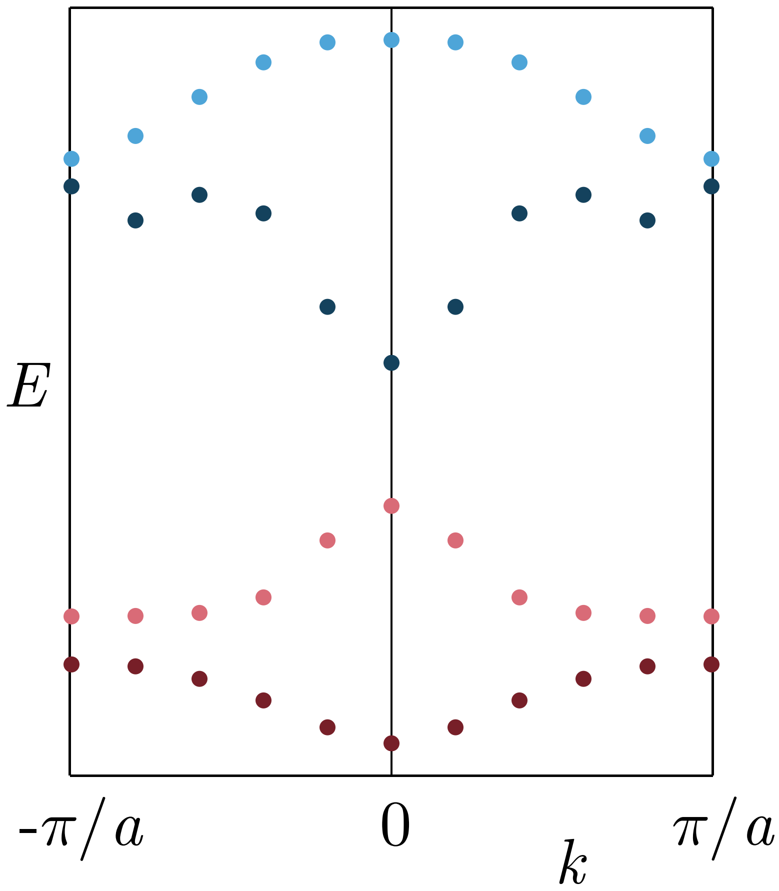
we choose one of the allowed values of k

For simplicity we restrict to one dimension for the moment

Solving the equation

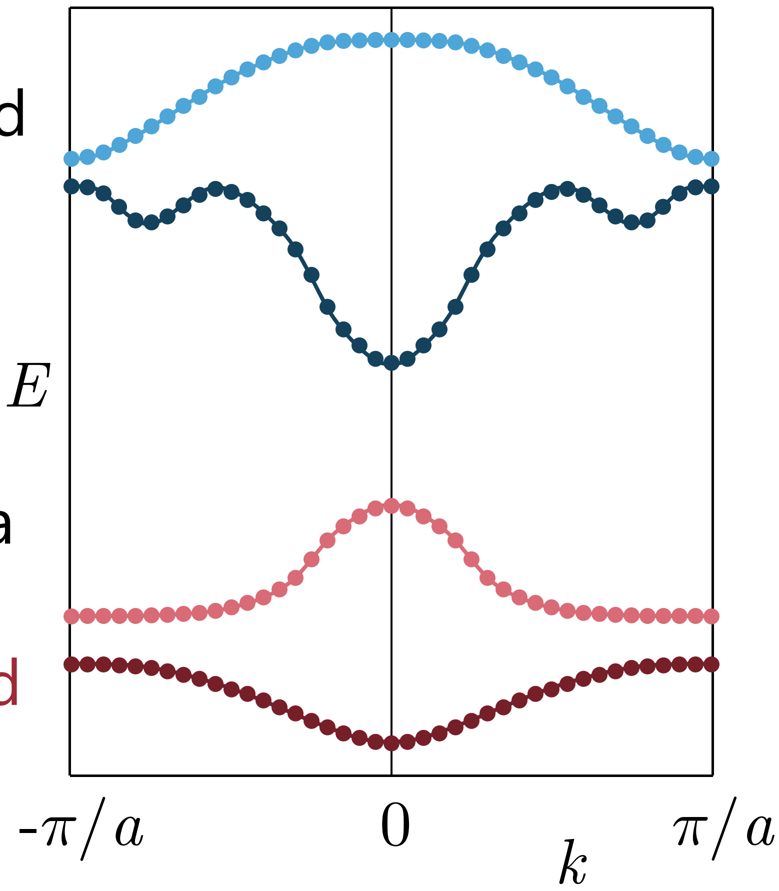
gives energy eigensolutions

We continue with the other allowed values of k



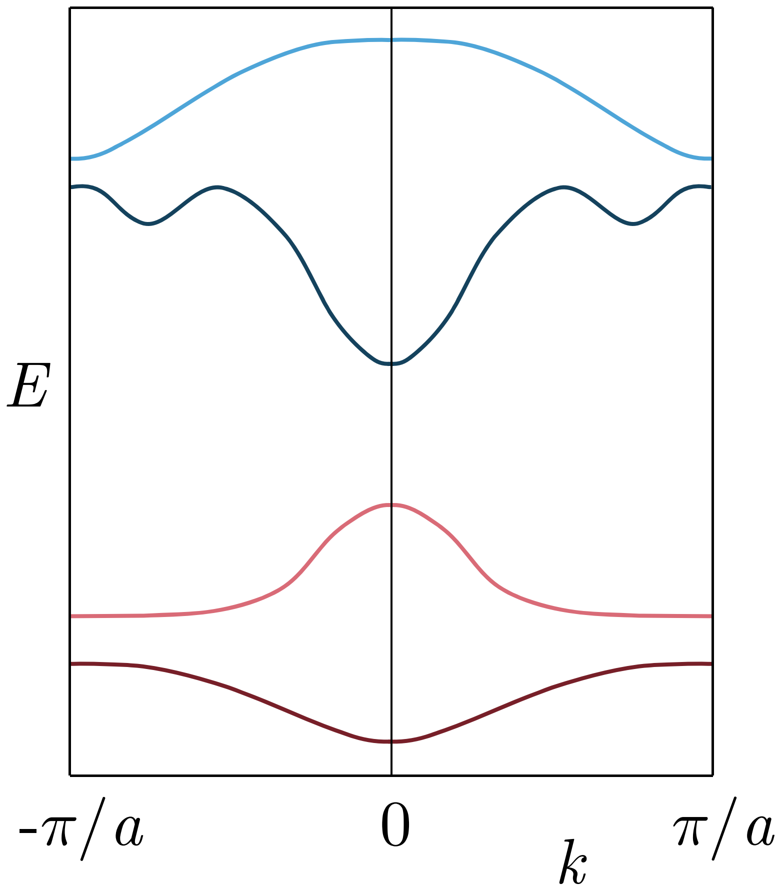
Band structure diagrams

- A larger crystal gives more allowed values of k
- For a large crystal
  - the sets of "dots" effectively become like lines
- We refer to the group of dots on a line as a "band"
  - The number of k-states in a band
    - is the number of unit cells in the crystal
- In practice, we just show the lines



Band structure diagrams

- There are multiple bands in a band structure
  - in fact an infinite number
    - but usually only a few are important for the properties of a material
- In each band, we only have to plot k-values from $-\pi/a$ to π/a
  - This range is known as
    - the (first) Brillouin zone



Extended Brillouin zone scheme

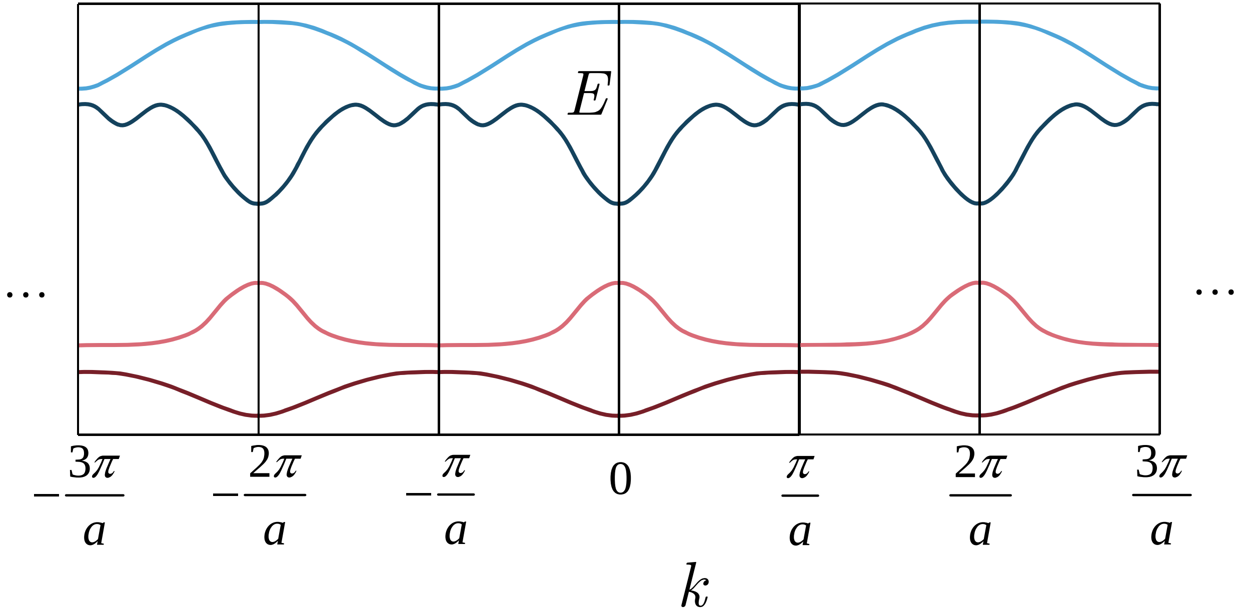
If we continue to larger k

the band structure just repeats

in multiple Brillouin zones

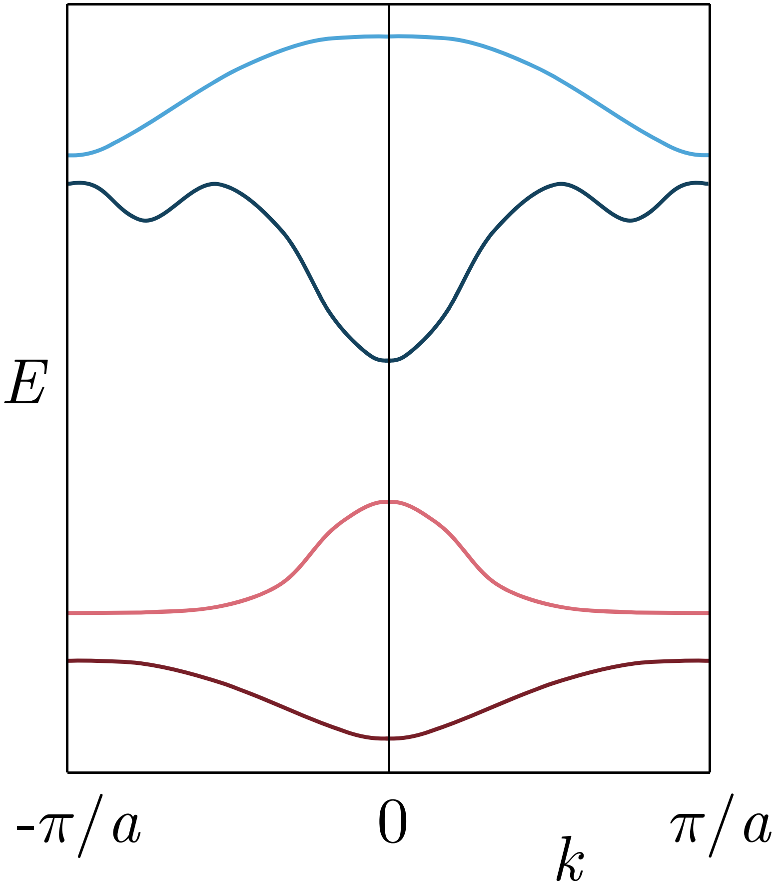
an "extended zone scheme"

so we only need to plot one Brillouin zone



Band structure diagrams

- Each band loosely corresponds to a different atomic state in the constituent atoms
  - or at least orthogonal combinations of atomic states
- The bands are formed from the atomic states
  - as the atoms are "pushed together" to make the crystal



Kramers degeneracy

The band structure is drawn to be symmetric about $k = 0$

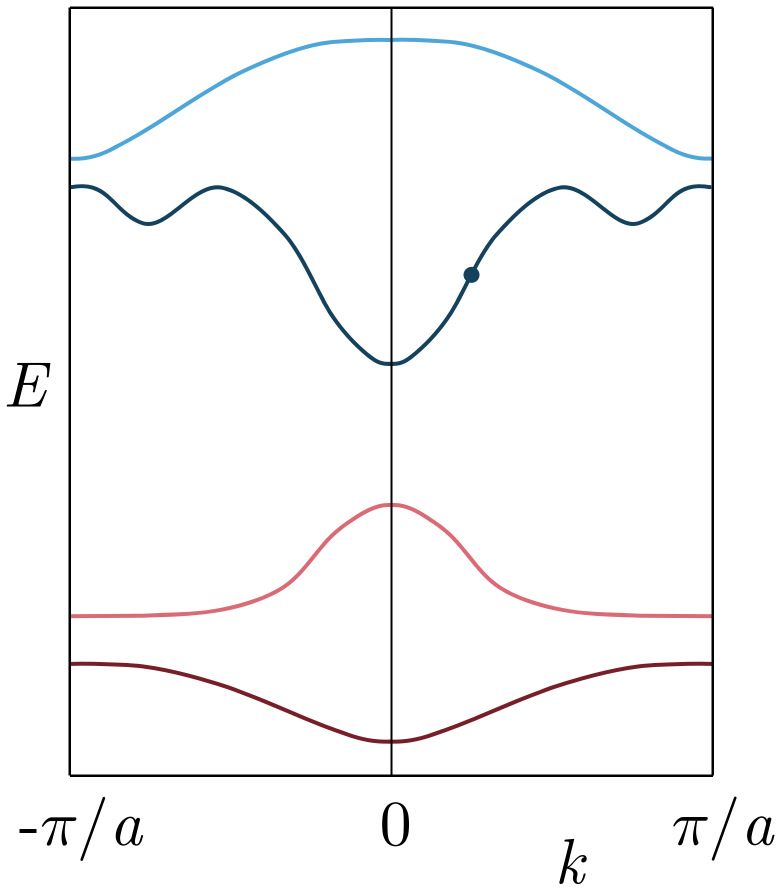
This common symmetry is easily proved

Suppose that the Bloch function

$$\psi(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$$

satisfies the Schrödinger equation for a specific $\mathbf{k}$

Note the unit cell function $u_{\mathbf{k}}(\mathbf{r})$ may be different for different $\mathbf{k}$



Kramers degeneracy

Hence we have

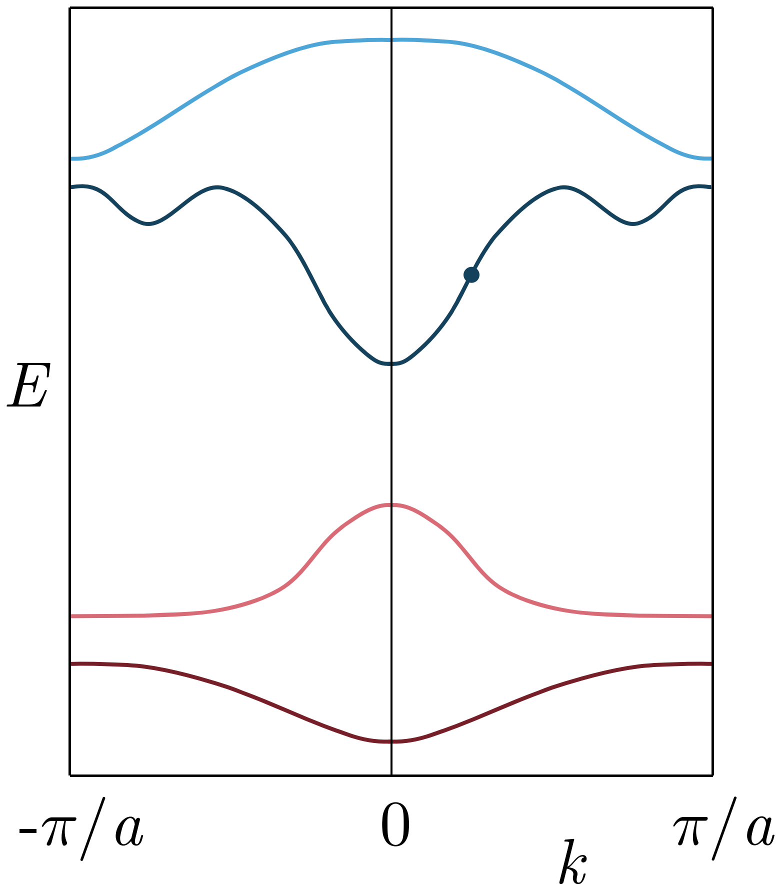
$$H\psi(\mathbf{k},\mathbf{r}) = E_{\mathbf{k}}\psi(\mathbf{k},\mathbf{r})$$

where $E_{\mathbf{k}}$ is the eigenenergy associated with this specific $\mathbf{k}$

in this specific band

and

$$H = -\left(\hbar^2/2m_e\right)\nabla^2 + V_P(\mathbf{r})$$



Kramers degeneracy

Taking the complex conjugate of both sides of

$$H\psi(\mathbf{k},\mathbf{r}) = E_{\mathbf{k}}\psi(\mathbf{k},\mathbf{r})$$

noting that $H = H^*$

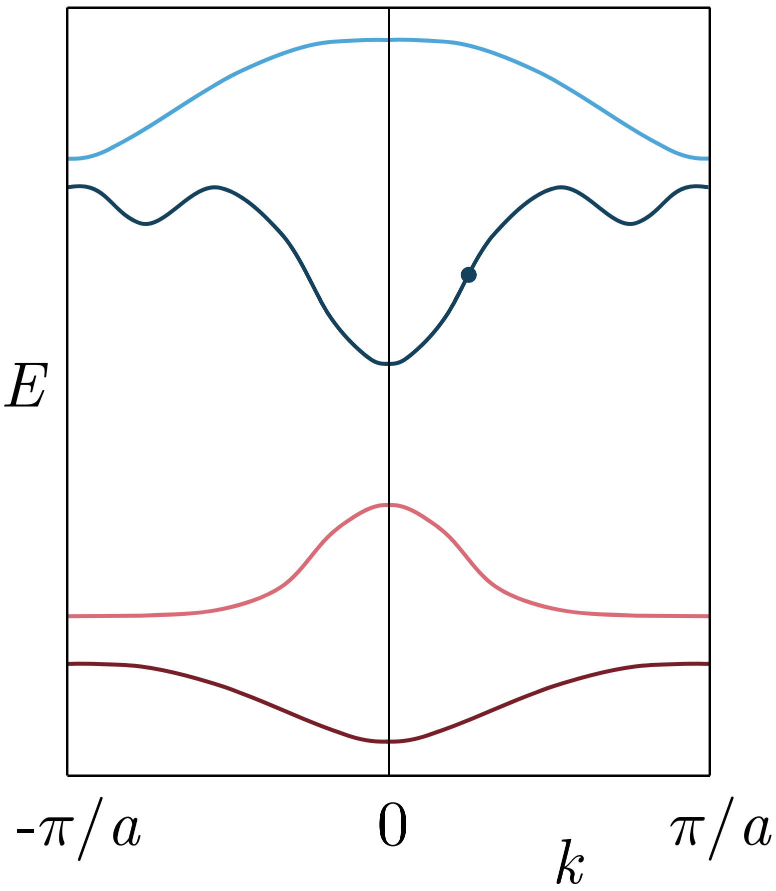
and that $E_{\mathbf{k}}$ is necessarily real

$$H\psi^*(\mathbf{k},\mathbf{r}) = E_{\mathbf{k}}\psi^*(\mathbf{k},\mathbf{r})$$

But $\psi^*(\mathbf{k},\mathbf{r}) = u_{\mathbf{k}}^*(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})$

which is also a wavefunction in Bloch form

but for -$\mathbf{k}$



Kramers degeneracy

Hence we are saying that

for every solution with

wavevector $\mathbf{k}$ and energy $E_{\mathbf{k}}$

there is one with wavevector

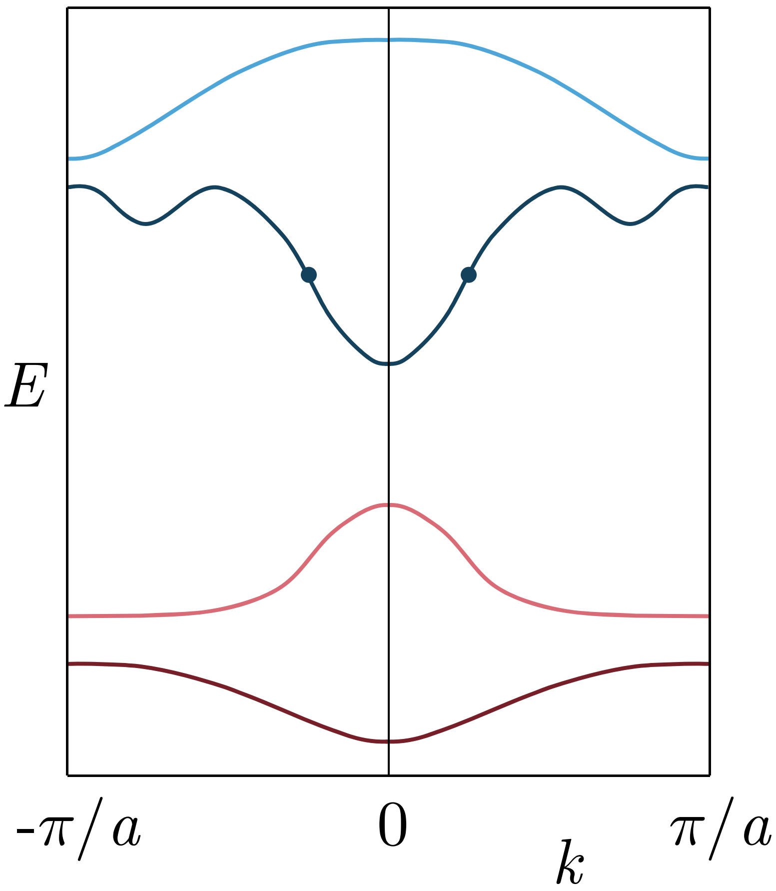
$-\mathbf{k}$ with the same energy

Hence the band structure is symmetric about $k = 0$

We can choose to write

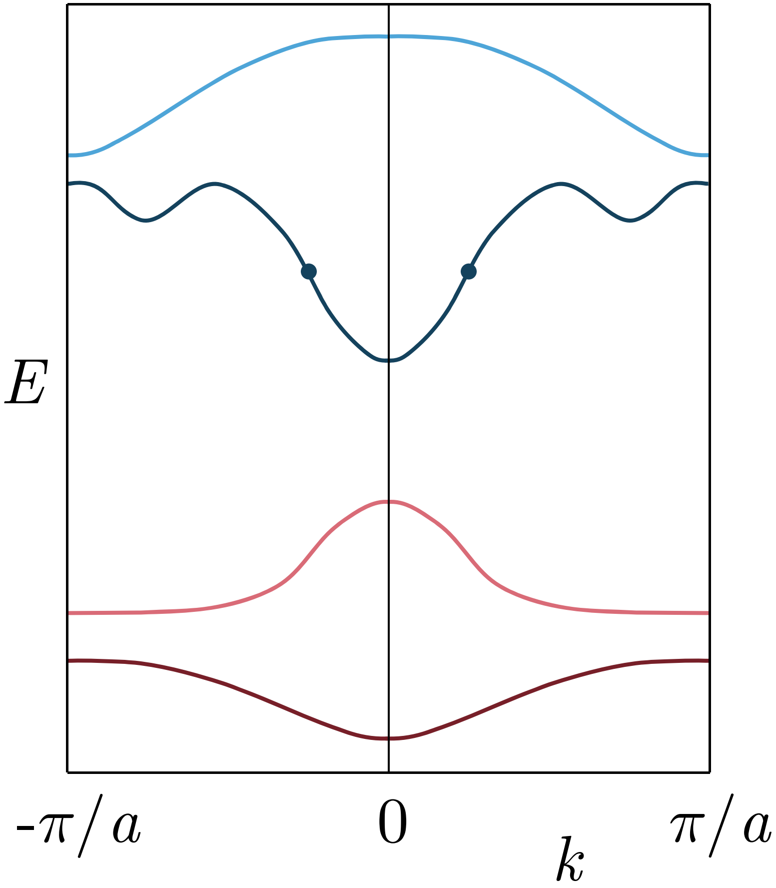
$$\psi^*(\mathbf{k},\mathbf{r}) = u_{\mathbf{k}}^*(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})$$

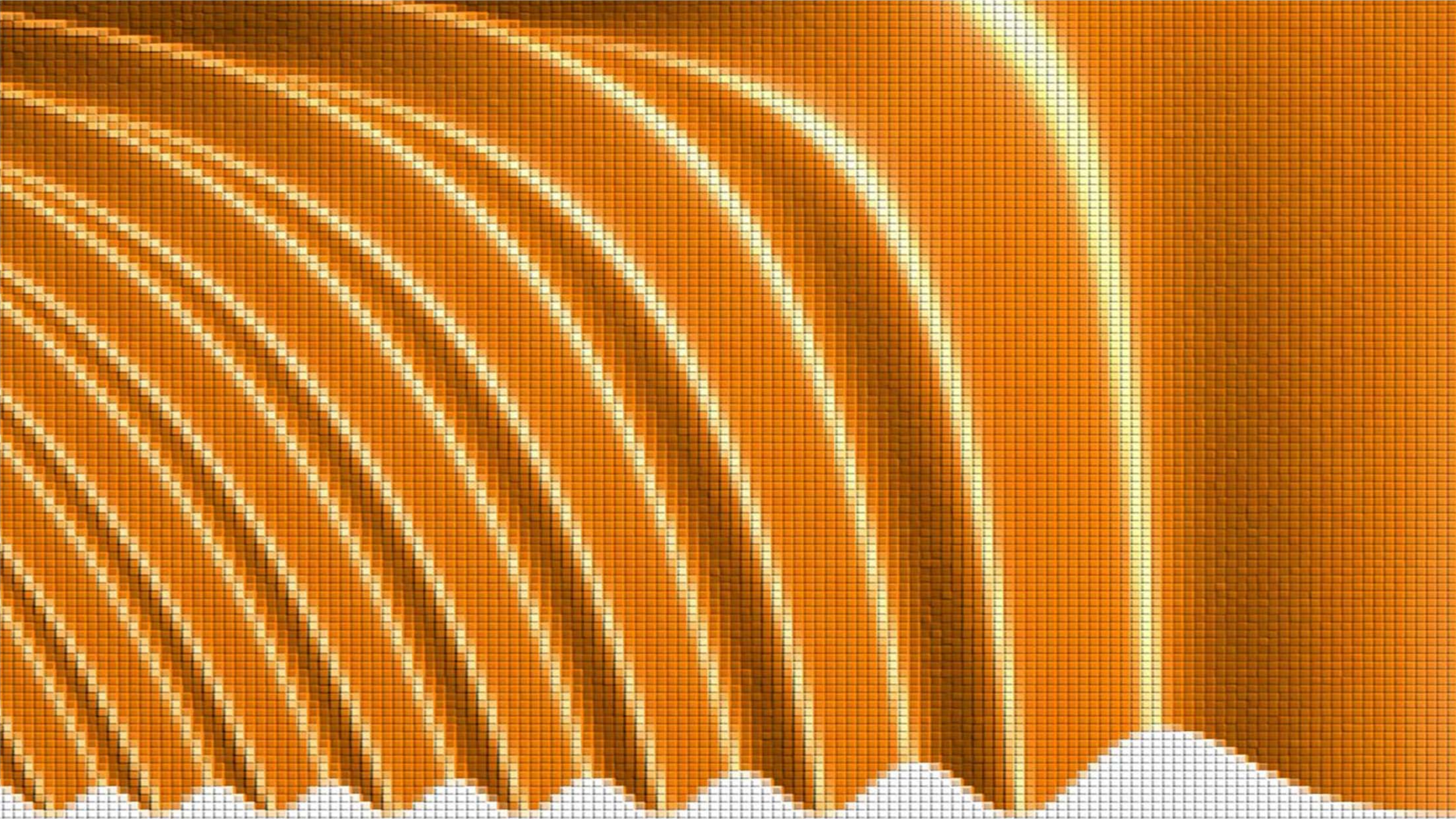
$$\equiv u_{-\mathbf{k}}(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r}) = \psi(-\mathbf{k},\mathbf{r})$$



Kramers degeneracy

- This equivalence of the energies for **k** and -**k** is known as
  - Kramers degeneracy
- Note that, once we include spin
  - these two states will have opposite spin
    - but often the spin makes no difference to the energy
- Hence bands often have minima or maxima at $k = 0$



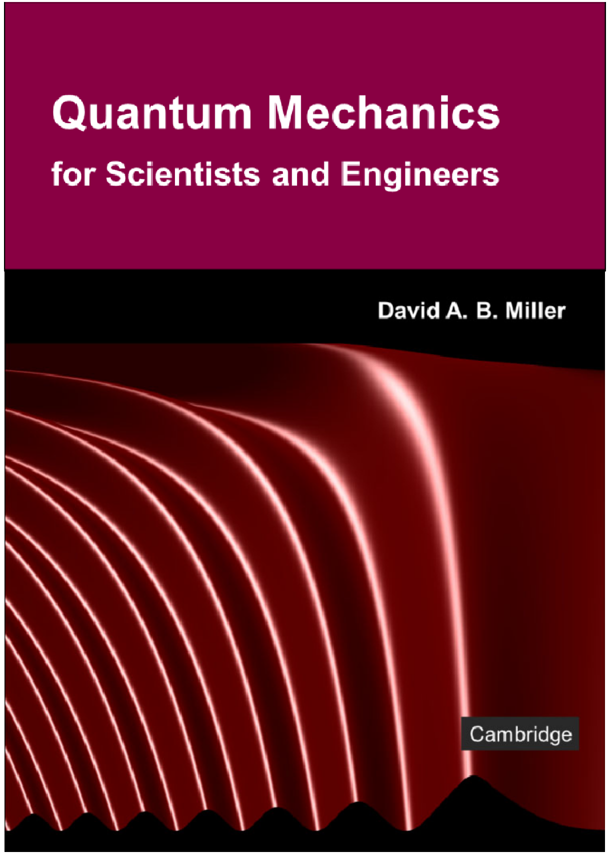


29 Band structures

Slides: Lecture 29c Semiconductors, insulators and metals

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.5



Band structures

Semiconductors, insulators and metals

Quantum mechanics for scientists and engineers

David Miller

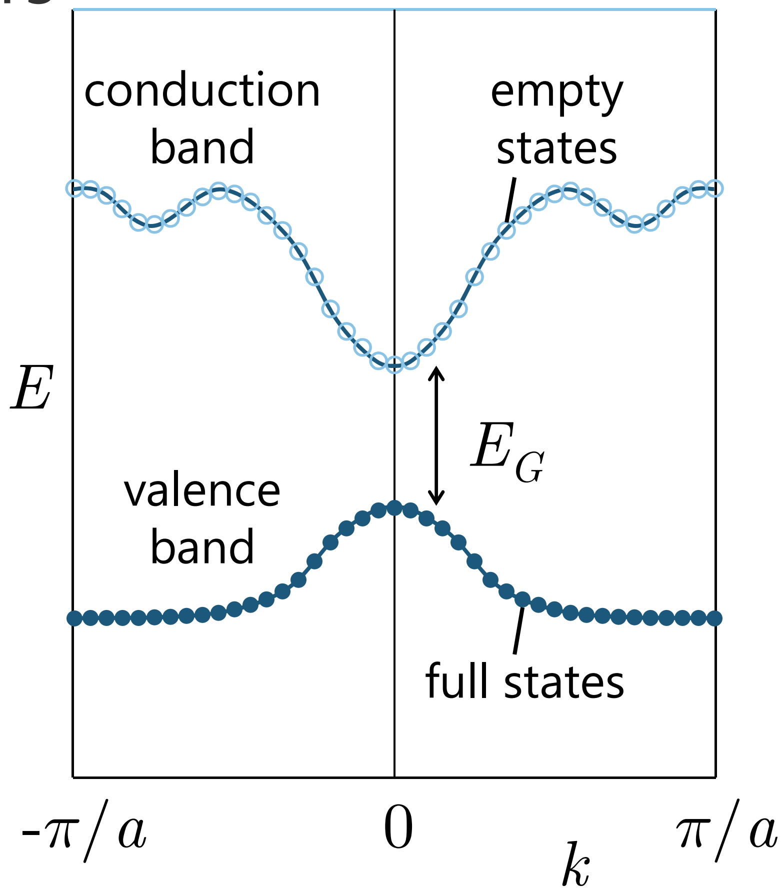
Semiconductors and insulators

Semiconductors and insulators

- have an (almost) completely full band
  - the valence band

separated by a "bandgap" energy E_G

- from an (almost) completely empty band
  - the conduction band



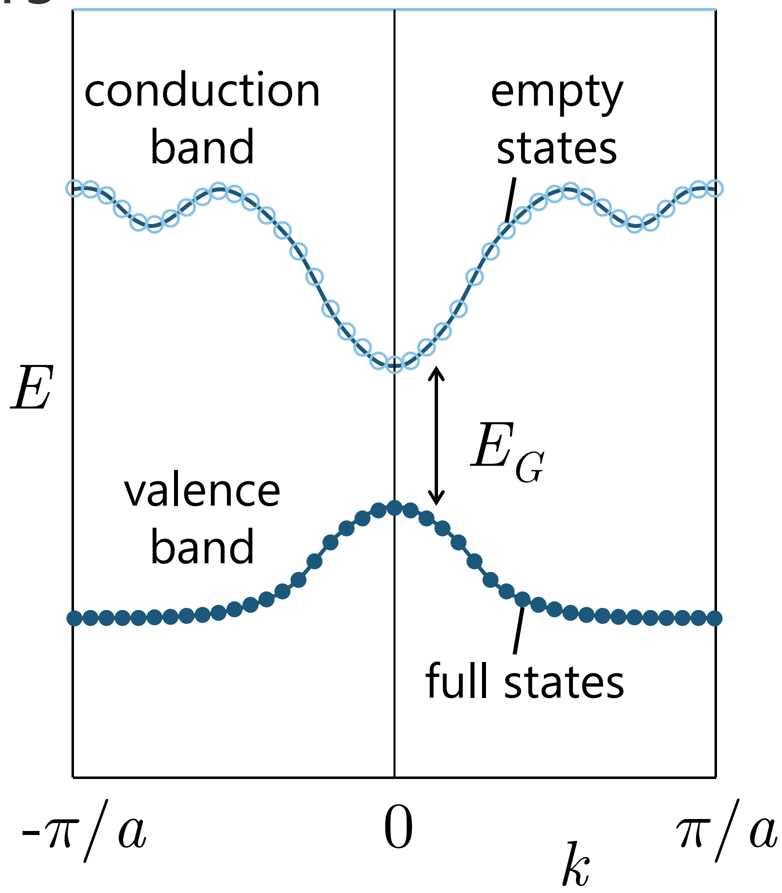
Semiconductors and insulators

Note that

- an empty band does not conduct electricity
  - There are no mobile electrons

Also

- a full band does not conduct electricity
  - The electrons cannot change states within the band
    - because all the states are full



Semiconductors and insulators

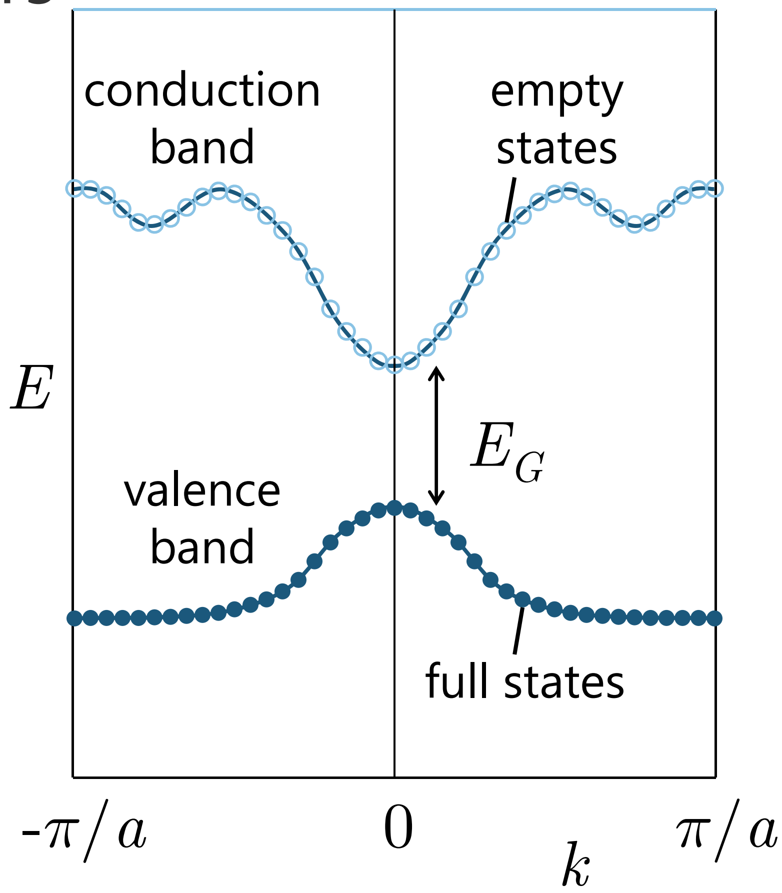
The difference between semiconductors and insulators is primarily that

insulators have such a large bandgap energy

that there is negligible thermal excitation of electrons

from the valence band

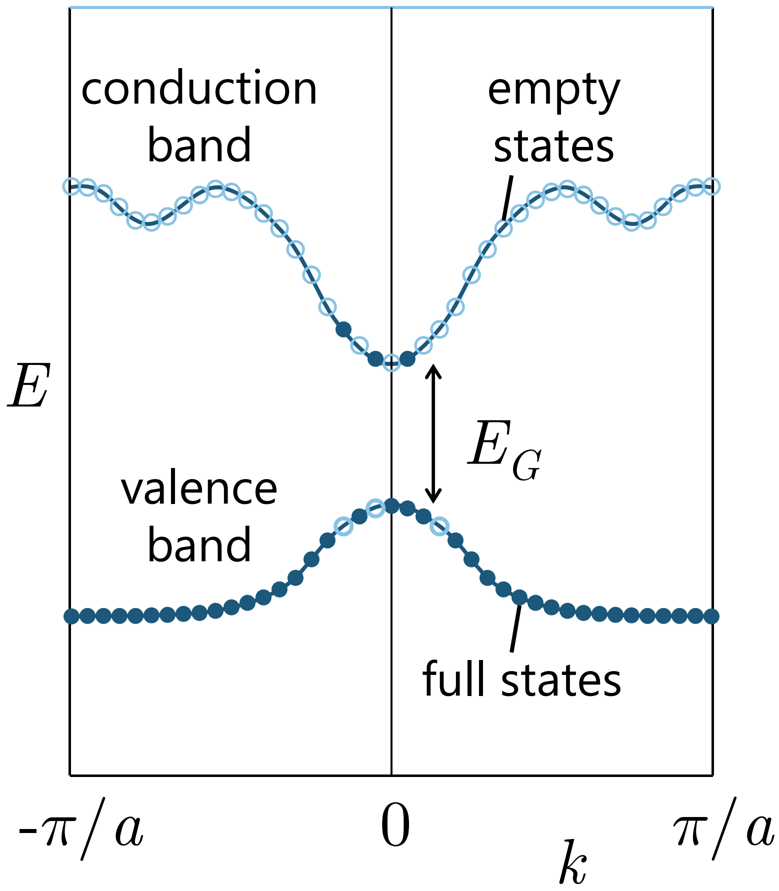
to the conduction band



Semiconductors

At finite temperatures in a semiconductor

- a small number of electrons are excited
  - from the valence band
    - to the conduction band



Semiconductors

These electrons in the
conduction band

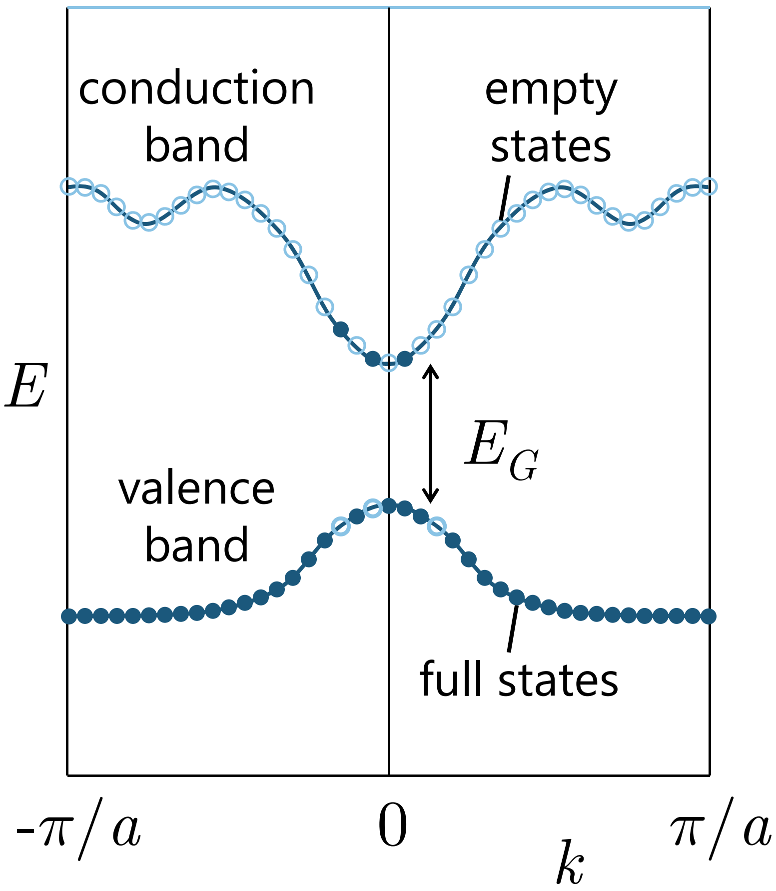
and

absences of electrons or "holes"
in the valence band

can conduct electricity within their bands

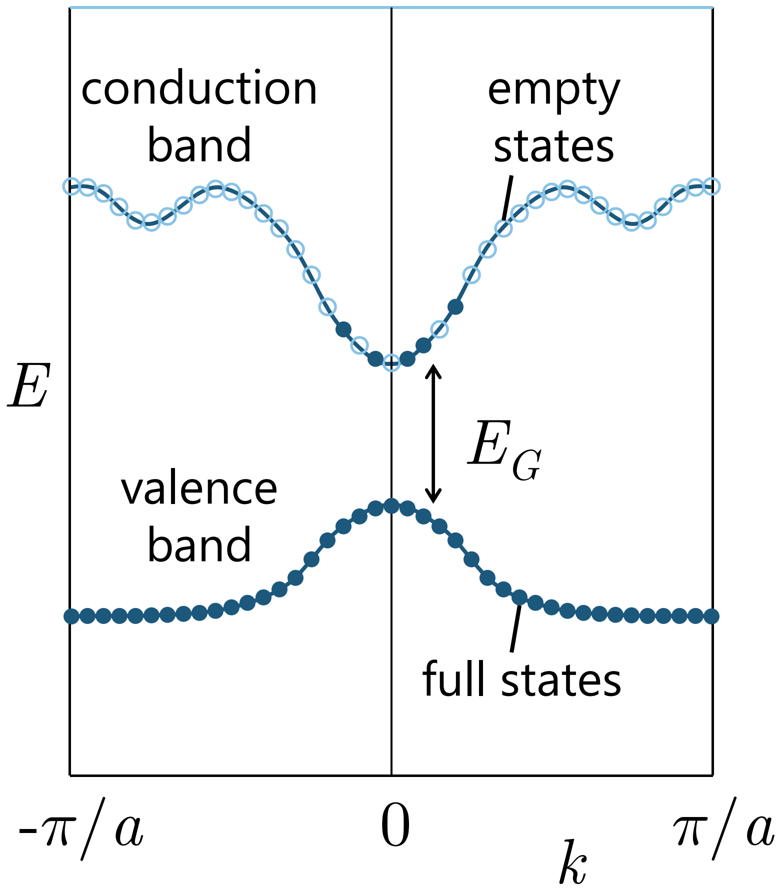
So semiconductor materials conduct electricity weakly

hence the name



Doping semiconductors

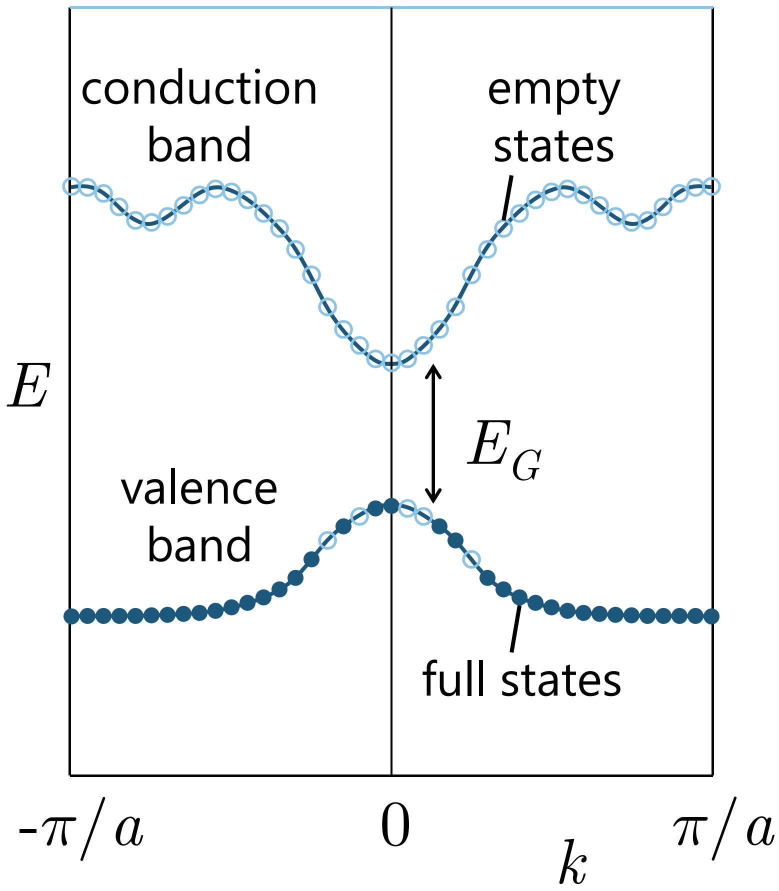
- Substituting a few atoms with more electrons
  - e.g., a Group V element like phosphorus in a Group IV semiconductor like silicon
  - known as n-type doping
  - makes the material conduct more
  - using these additional electrons



Doping semiconductors

Substituting a few atoms with fewer electrons

- e.g., a Group III element like boron in a Group IV semiconductor like silicon
  - known as p-type doping
- makes the material conduct more
  - using these additional "holes"



Direct gap semiconductor

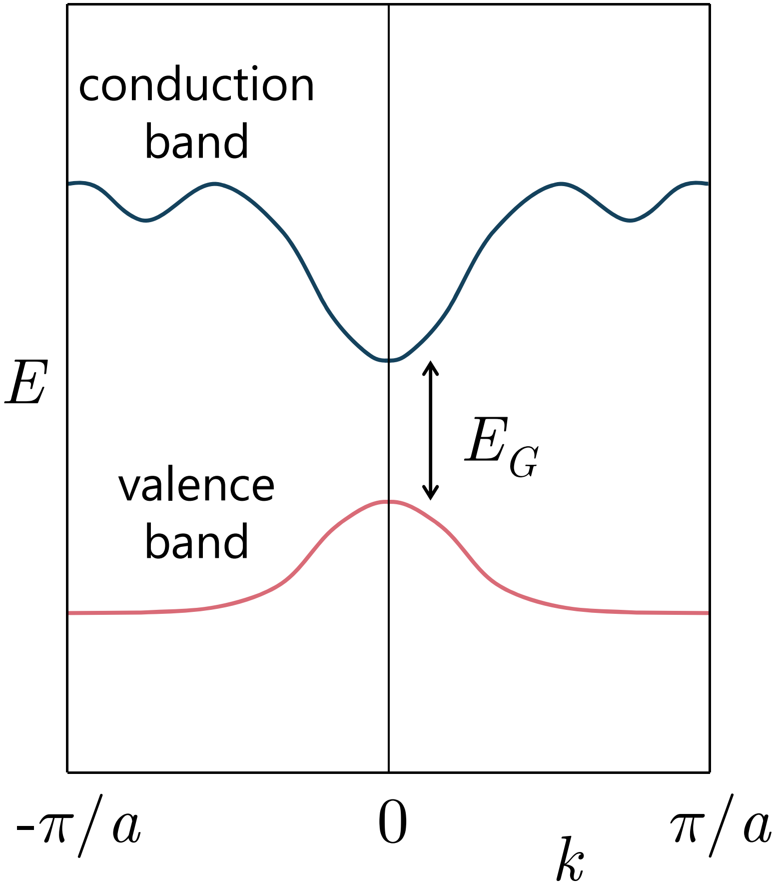
If the lowest minimum in the conduction band

lies directly above

the highest maximum in the valence band

the semiconductor is said to have a

"direct gap"

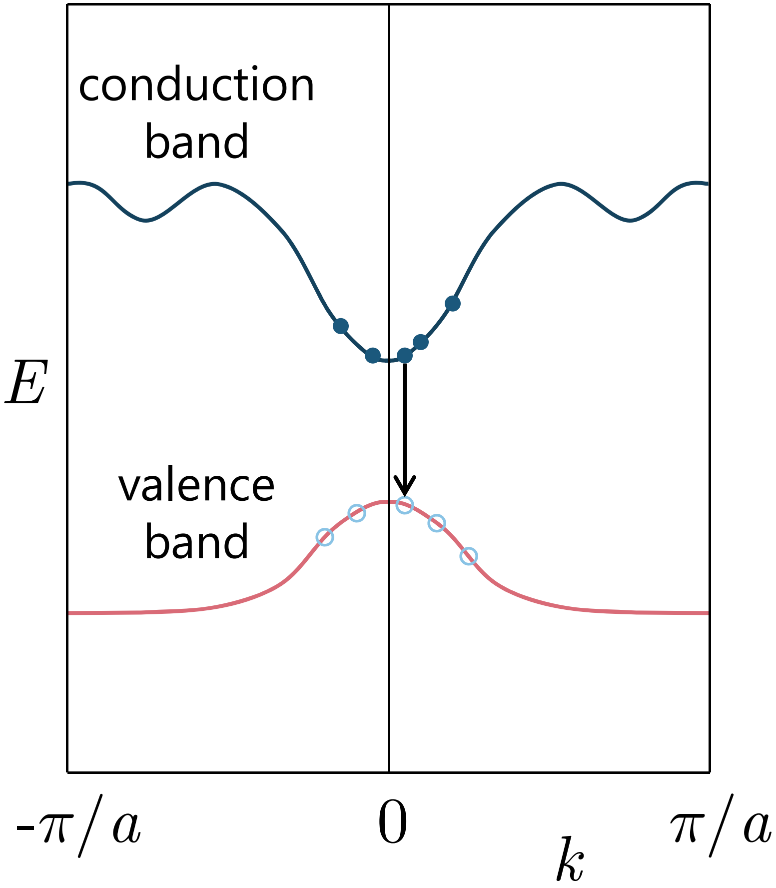


Direct gap semiconductor

Direct gaps are important for light emitters

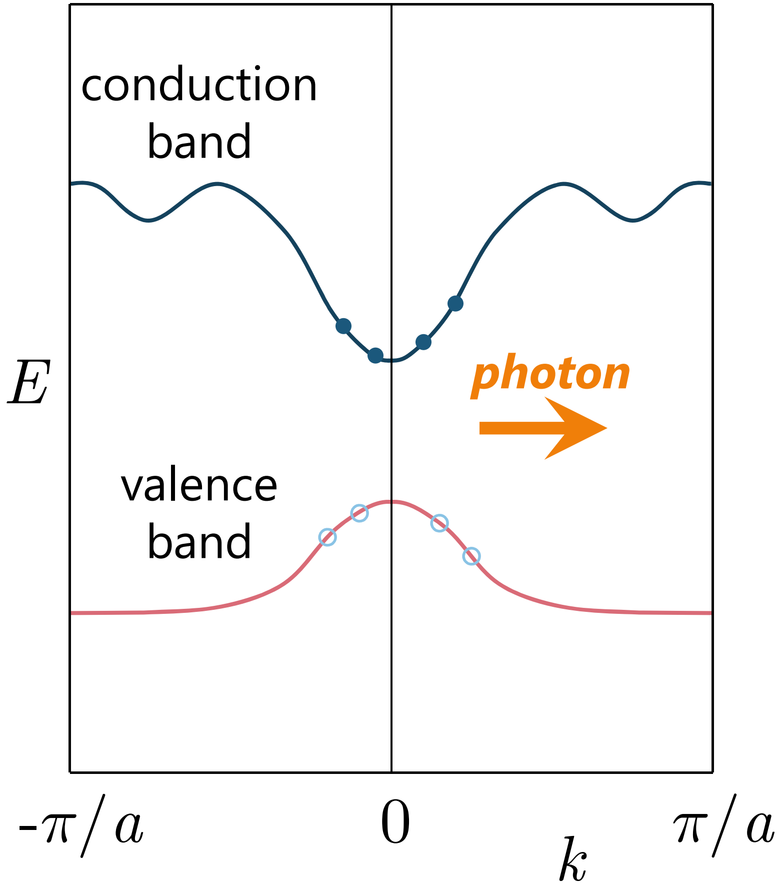
- Electrons "pumped" into the conduction band gather in the lowest minimum
- "Holes" pumped into the valence band gather in the highest maximum

An electron can fall "vertically" to fill in a hole beneath it



Direct gap semiconductor

- Direct gaps are important for light emitters
  - Electrons "pumped" into the conduction band gather in the lowest minimum
  - "Holes" pumped into the valence band gather in the highest maximum
- An electron can fall "vertically" to fill in a hole beneath it
  - emitting light



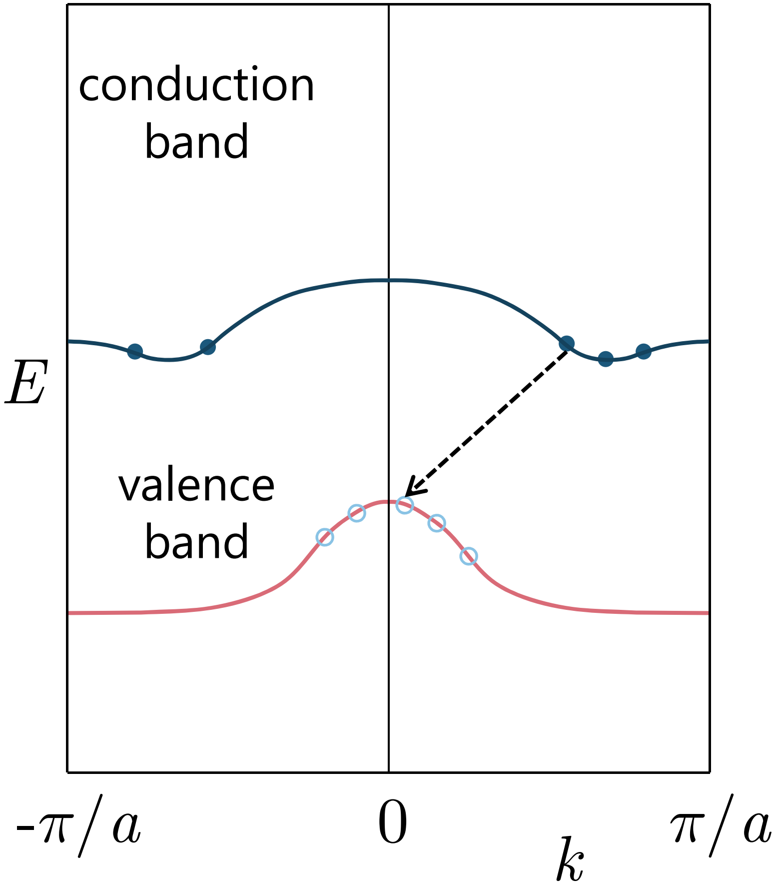
Indirect gap semiconductor

In an indirect gap semiconductor

- e.g., silicon, germanium
  - the lowest conduction band minimum (or minima) is not directly above the highest valence band maximum

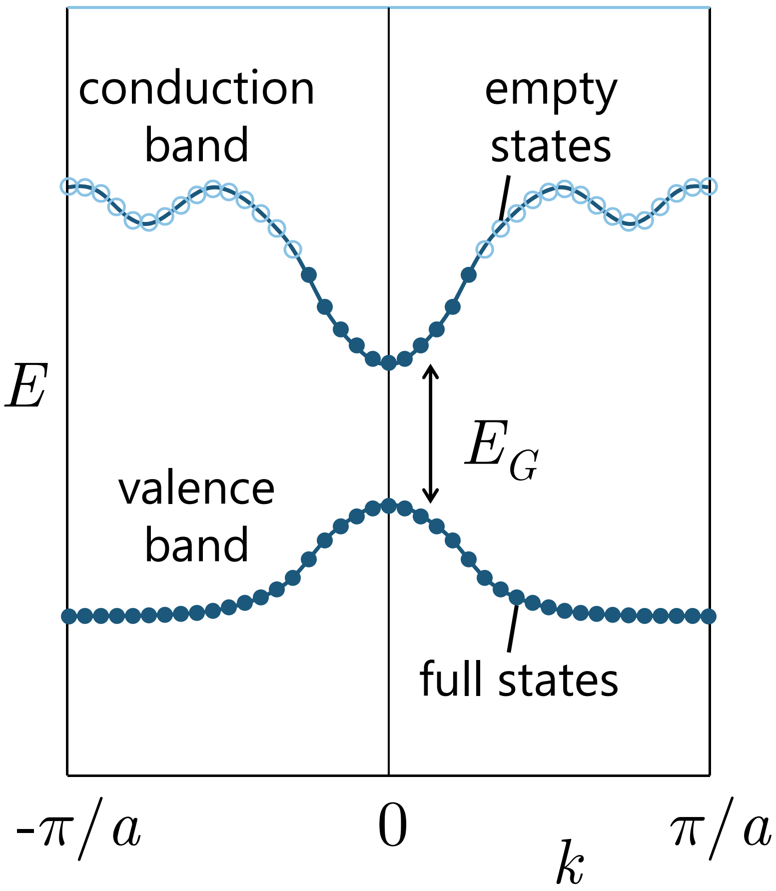
Light emission is weak

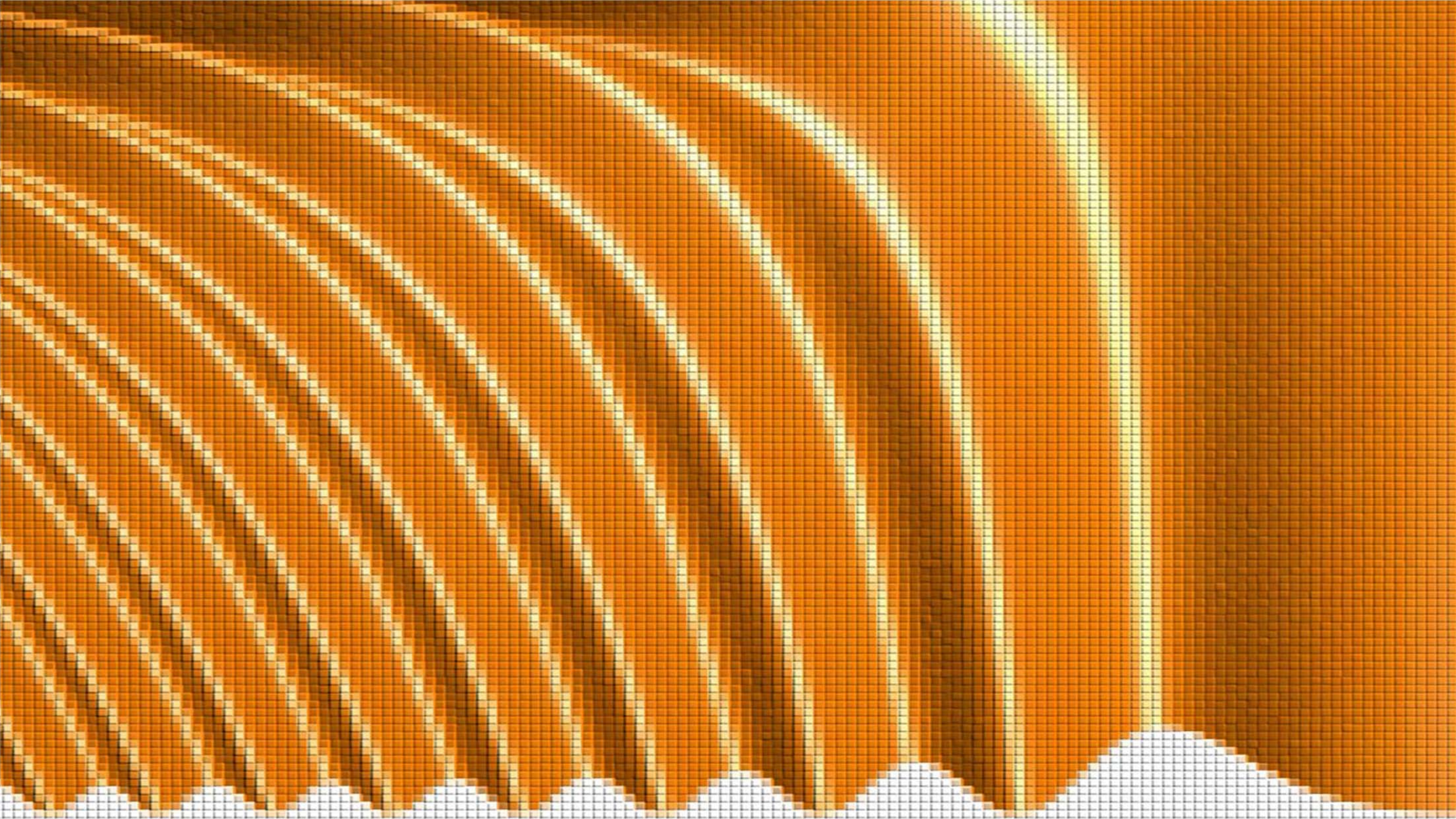
- "non-vertical" transitions by emission of photons are weak



Metals

- Because of the number of electrons in the metal atoms
  - the lowest conduction band is partially full of electrons
    - e.g., half-full
      - even at zero temperature
- Hence metals conduct electricity well



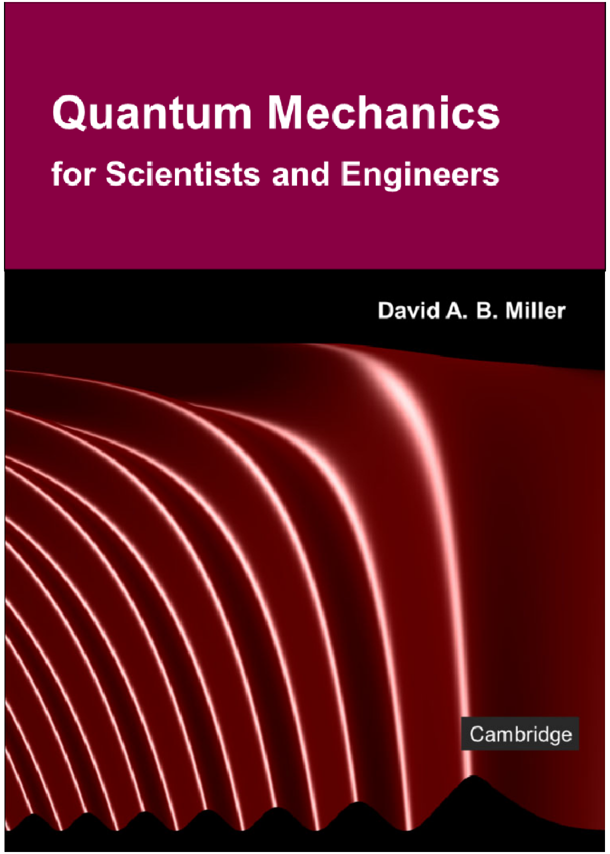


29 Band structures

Slides: Lecture 29d Band structures in 3D

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.5



Band structures

Band structures in 3D

Quantum mechanics for scientists and engineers

David Miller

Brillouin zone in 3D

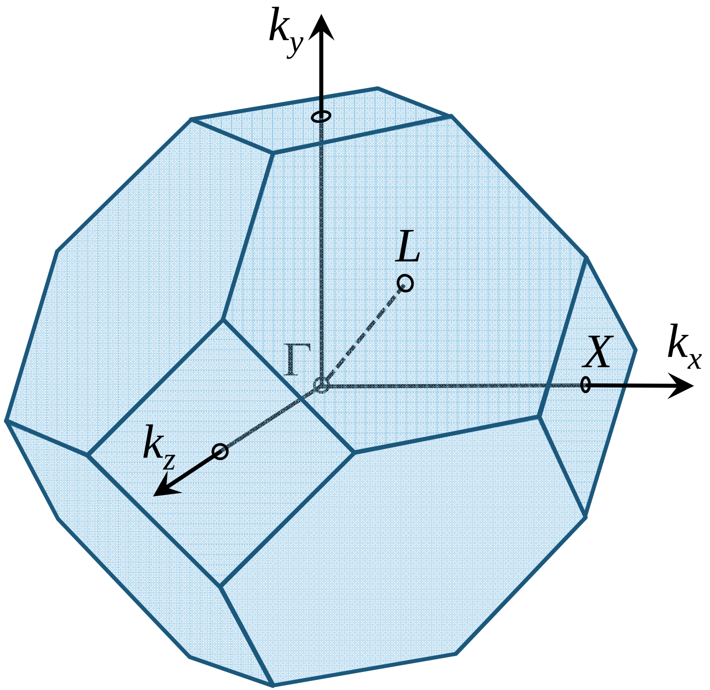
This Brillouin zone for the diamond or zinc-blende lattice

- is itself a 3D object
  - in k-space (or reciprocal space)

Two important directions are

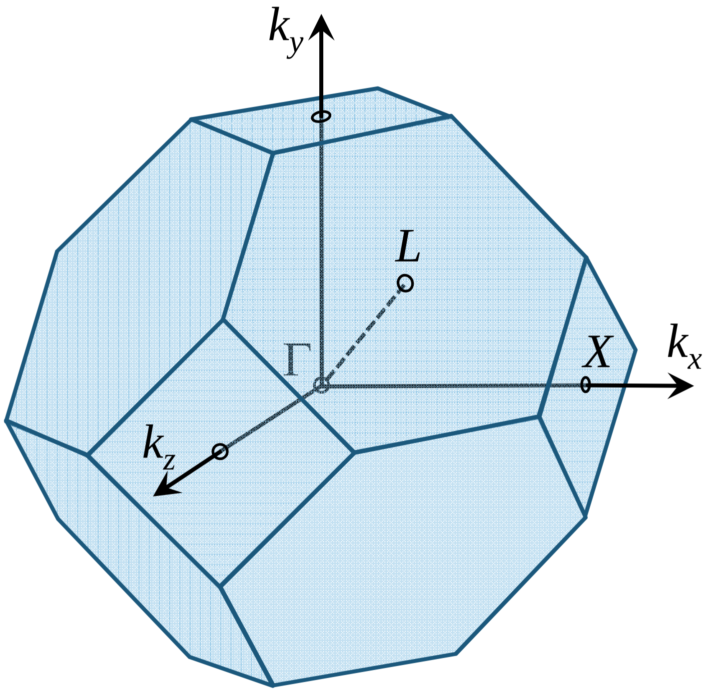
- X – along one of the x, y, or z coordinate directions
- L – along one of the cube space diagonals

The center is the Γ (gamma) point



Band structures for 3D crystals

- At least as a first useful representation of band structure
  - typically the band structure is calculated only along a few directions
    - such as along the lines from the Γ point (at the center of the Brillouin zone)
      - to the X point and the L point



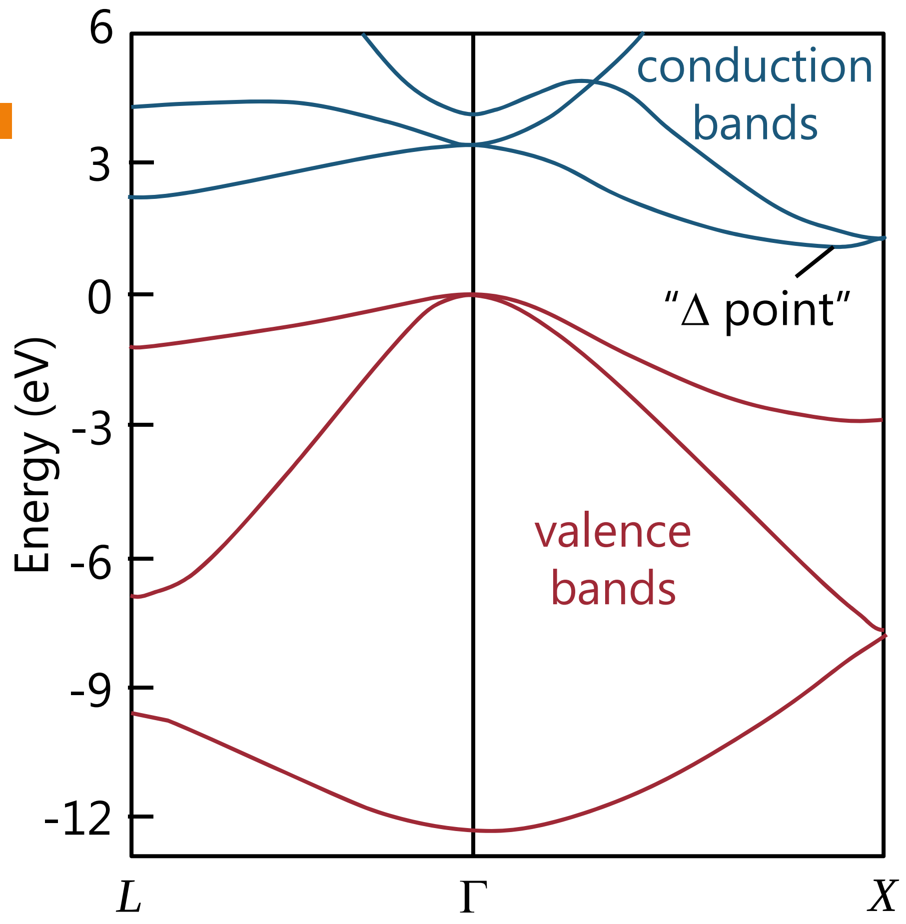
Si band structure

Sketch of major valence and conduction bands

- with the conduction band minimum at the Δ point

By Kramers degeneracy

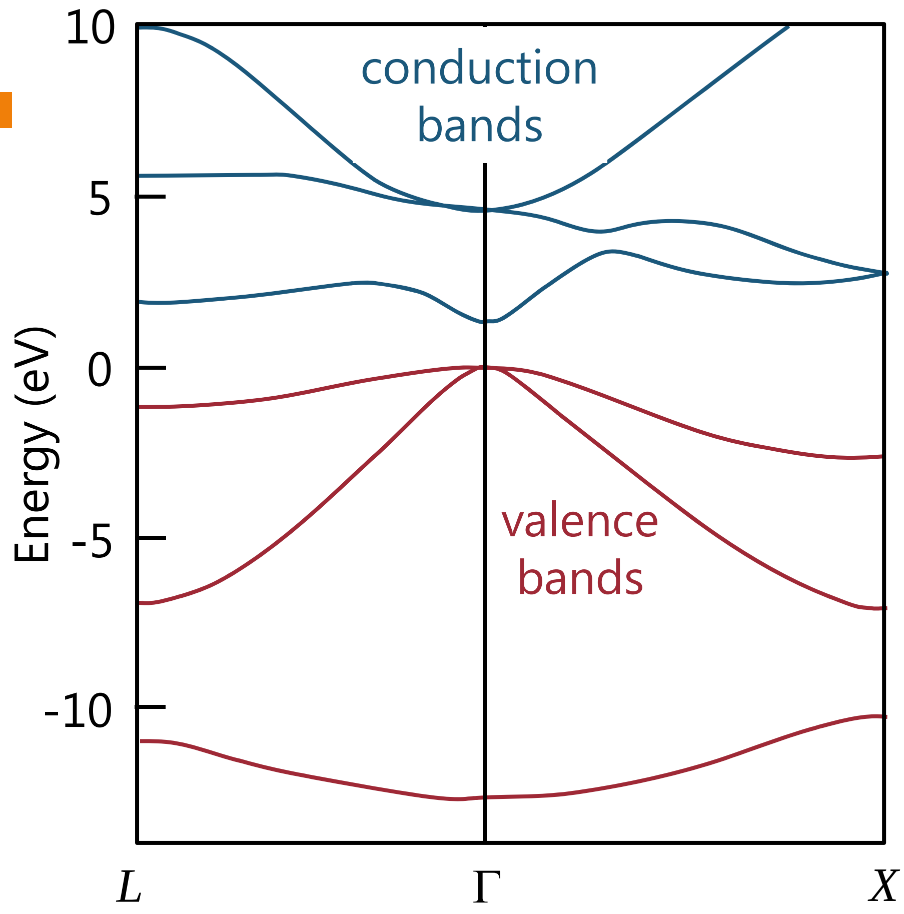
- we need only show one half of the band structure
  - so we can use the other half of the figure
    - for the band structure in another direction



after K. S. Sieh and P. V. Smith, Phys. Status Solidi (b) **129**, 259 (1985)

GaAs band structure

- Sketch of major valence and conduction bands
  - with the conduction band minimum at the Γ point
- Note that GaAs is a direct gap semiconductor
  - unlike Si
    - which is indirect

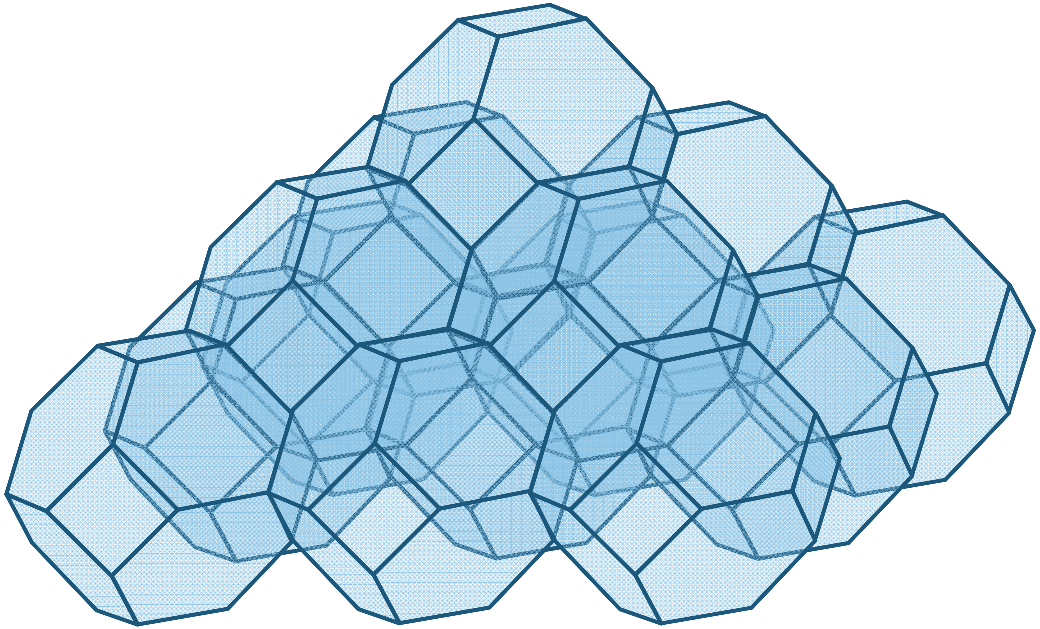


after M. Rohlfing, P. Krüger and J. Pollmann, Phys. Rev. B **48**, 17791 (1993)

Extended zones in 3D

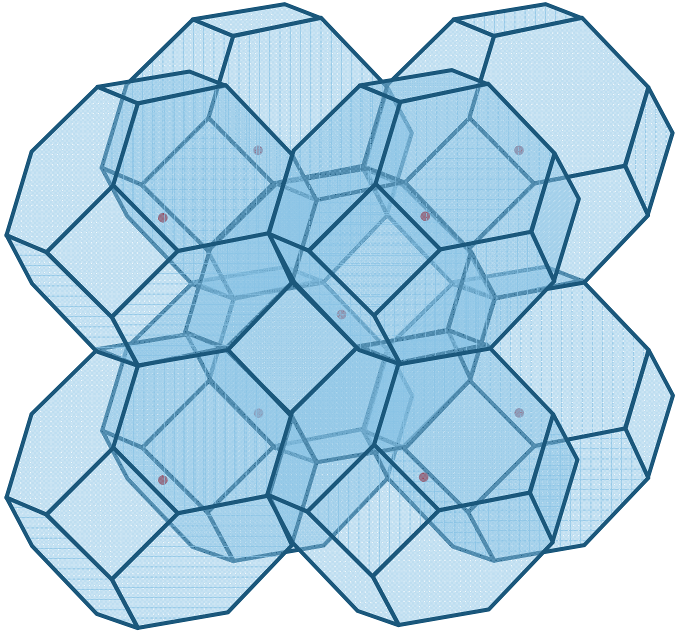
In 3D
- additional Brillouin zones repeat the same band structure

These zones form "unit cells" in k-space
- filling all k-space (reciprocal space)



Extended zones in 3D

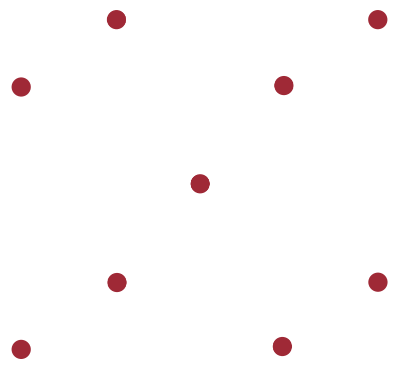
Marking the same “reciprocal lattice point” in each cell



Extended zones in 3D

Marking the same "reciprocal lattice point" in each cell

and erasing the "unit cells" (Brillouin zone shapes) themselves for clarity



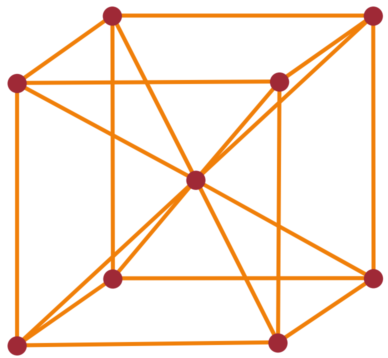
Extended zones in 3D

Marking the same “reciprocal lattice point” in each cell

and erasing the “unit cells” (Brillouin zone shapes) themselves for clarity

and adding guide lines

shows these extended Brillouin zones give a body centered cubic “reciprocal lattice”



Extended zones in 3D

This particular reciprocal lattice
with one mathematical lattice
point for each Brillouin zone
is typically the one meant
when talking about
"the reciprocal lattice"

The vectors in k-space between
these lattice points are called
reciprocal lattice vectors