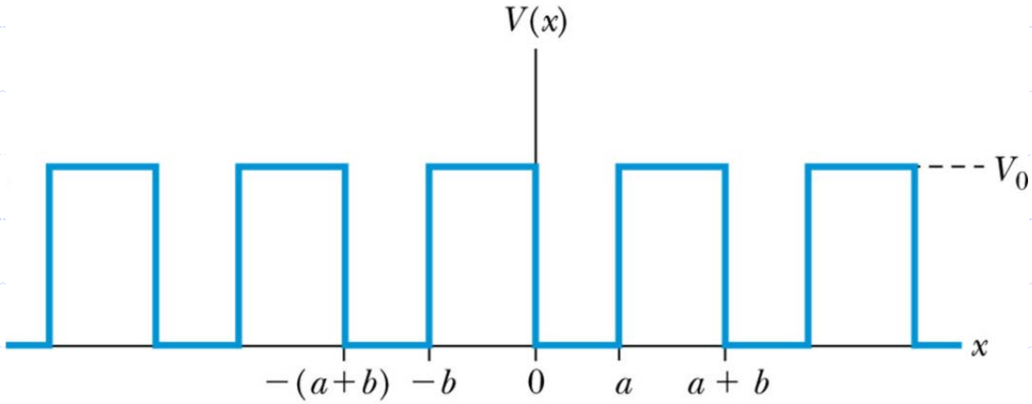
Band Theory

- The other approach to band theory solves the Schrodinger equation using a periodic potential to represent the Coulomb attraction of the positive ions
- In the Kronig-Penny model the periodic potential is taken to be a series of deep, narrow square wells



Band Theory

- We learned in class how to solve this problem
  - Write down the solutions in the two regions

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \text{ for region 1 (V = 0)}$$

$$\psi_2(x) = Ce^{k_2x} + De^{-k_2x} \text{ for region 2 (V = V}_0\text{)}$$

  - Apply boundary conditions
    - Wave function and its first derivative are continuous at the boundaries
- It turns out that there are other conditions to consider as well

Band Theory

- Bloch's theorem
  - Solutions to Schrodinger's equation for a periodic potential satisfy

$$\psi(x+L)=e^{iqL}\psi(x)$$

  - So we really just need to Schrodinger's equation for one cell
- A consequence of Bloch's theorem is that

$$|\psi(x)|^2=|\psi(x+L)|^2$$

- As the electron wave propagates through the crystal, its amplitude varies but its flux (probability) at periodic points does not
  - Remember the unexplained mean free path in the free electron model?

Band Theory

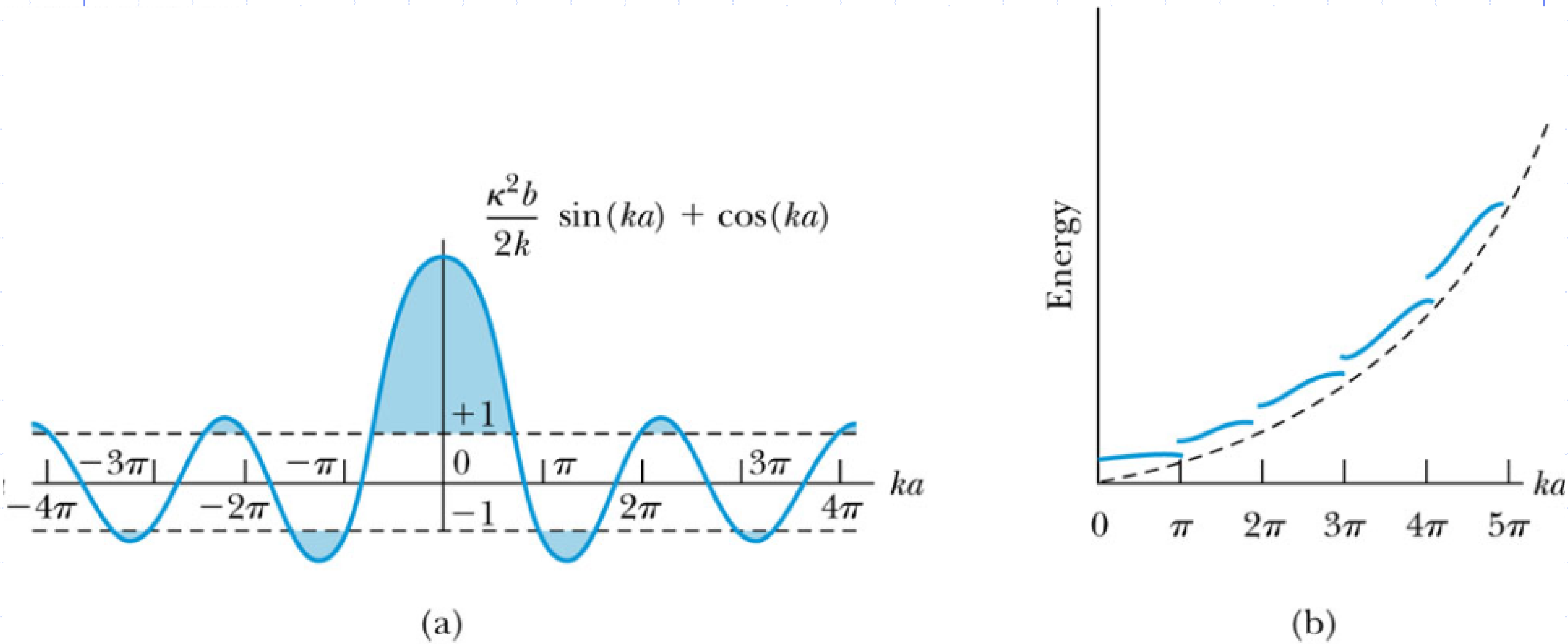
- Bloch's theorem provides two periodicity conditions the wavefunction must satisfy in addition to usual boundary condition
  - The solution is tedious so we will just quote the result

$$\frac{k_2^2 b}{2k_1}\sin k_1 a + \cos k_1 a = \cos qa$$

- The main point is that not values of k_1 and k_2 are allowed because the left hand side is restricted to +1/-1 by the right hand side
- A periodic potential (such as Kronig-Penny) leads to forbidden zones (band gaps) separating the bands of allowed energies

Band Theory

- A periodic potential leads to band gaps



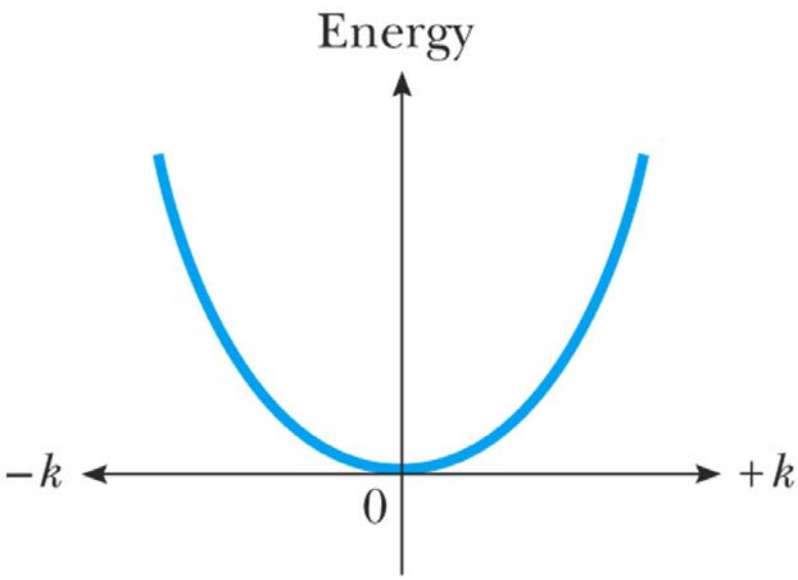
Band Theory

- Here is an equivalent way to see that electrons in a periodic lattice will have forbidden energy levels

$$\psi(x) = Ae^{i(kx-\omega t)}$$

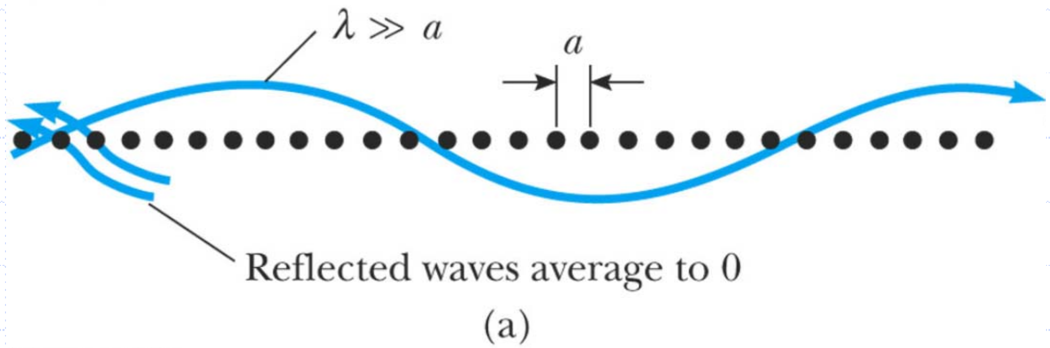
$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

- First consider a free electron
  - A plot of E versus k is continuous



Band Theory

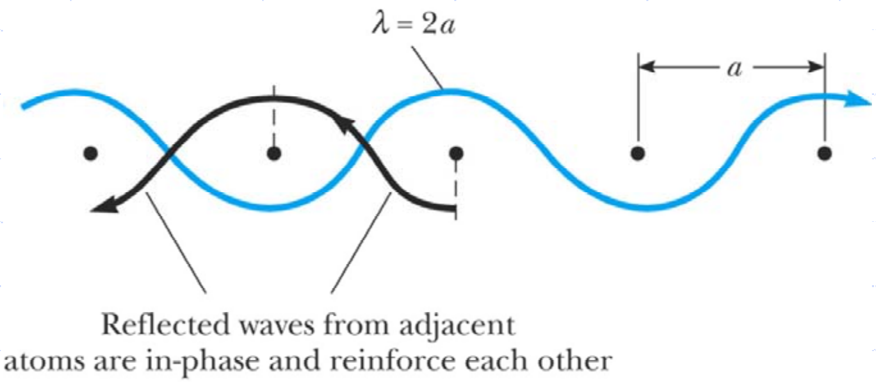
- Now consider an electron wave with small k (large λ) incident on a periodic lattice
  - Waves reflected from each ion will be slightly out of phase and will cancel if there are many reflections (scatterings)
  - Thus the electron moves through the lattice like a free particle (long mean free path)



Band Theory

- Now consider an electron wave with larger k (smaller λ=2a) incident on a periodic lattice
  - In this case, the reflections from adjacent atoms will be in phase
  - More generally there will be constructive interference in the reflected waves for

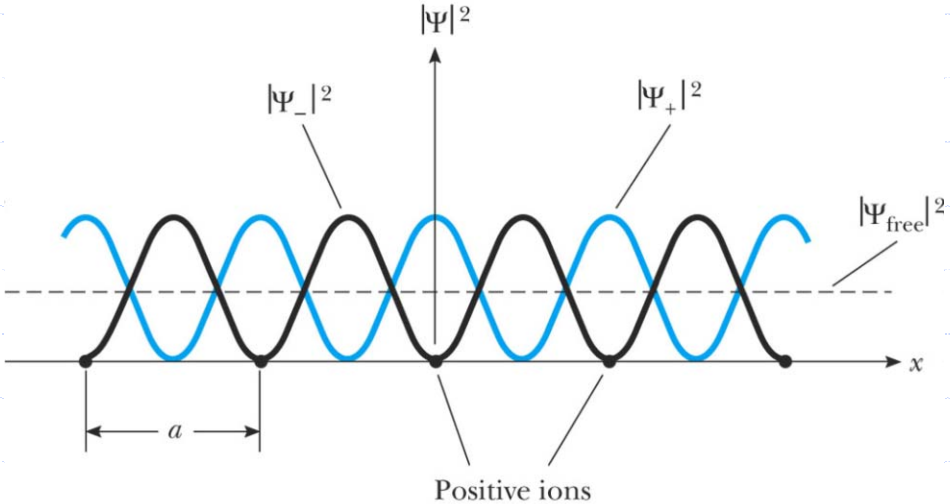
$$n\lambda = \pm 2a \text{ or equivalently } k = \pm\frac{n\pi}{a}$$



(b)

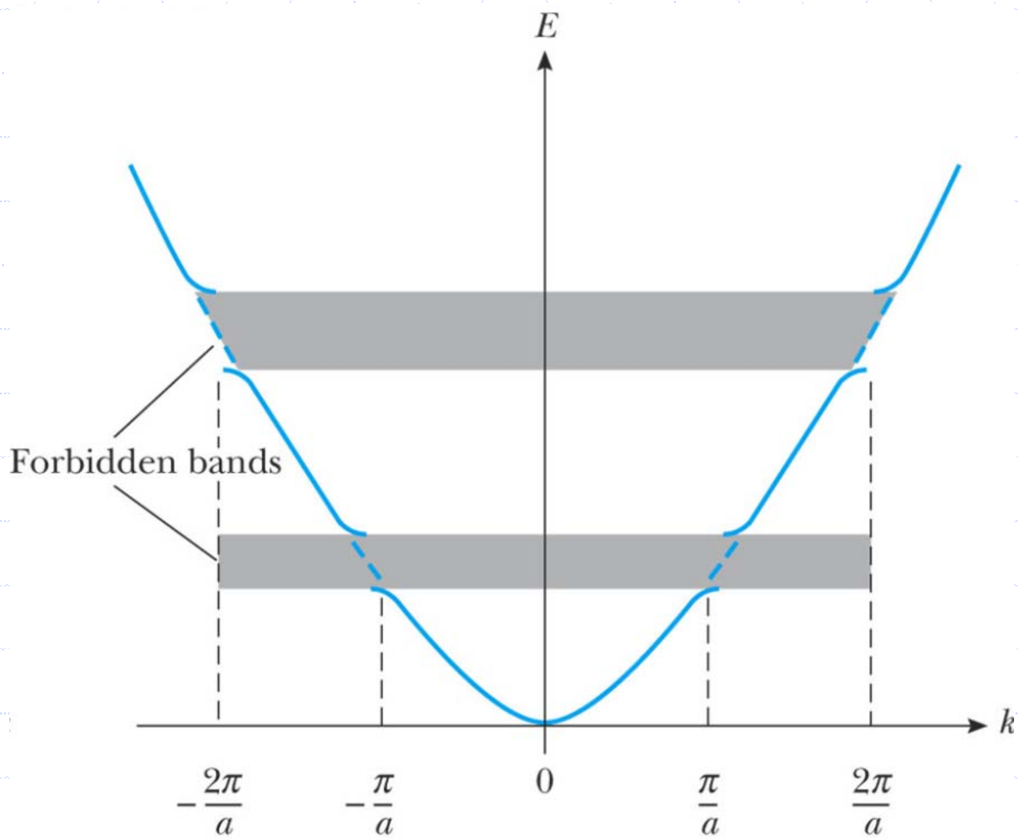
Band Theory

- For k=±nπ/a, there will be the incident electron wave traveling to the left and the reflected electron wave traveling to the right
  - The two traveling waves can be added or subtracted to form two possible standing waves Ψ_+ and Ψ_-
  - The Ψ_+ wave will have a slightly lower energy because the electron probability is closer to the lattice ions



Band Theory

- The difference in energy between these two standing waves leads to a discontinuity in energy at k=±nπ/a as found with the more formal Kronig-Penny approach

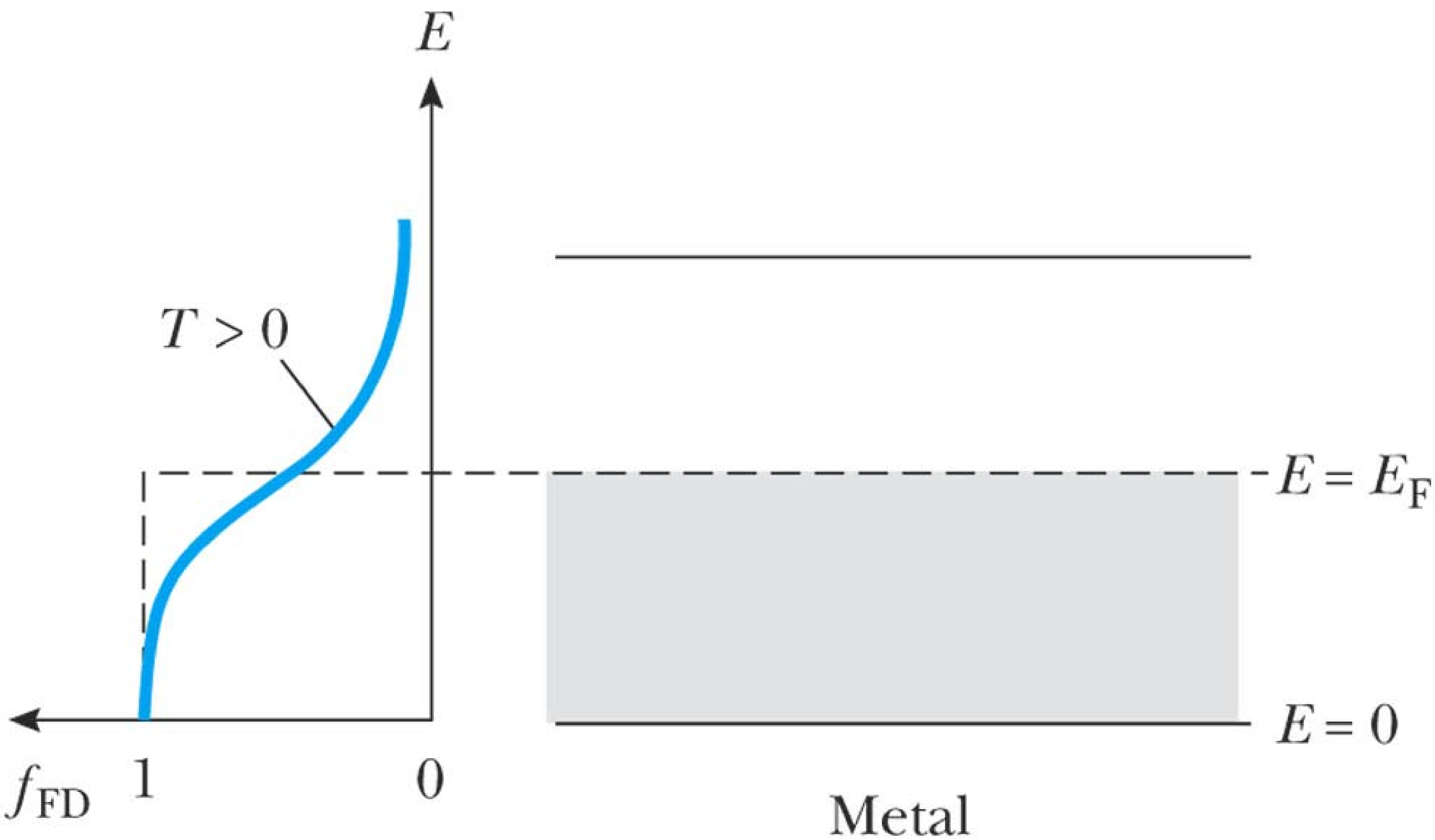


Band Theory

- Now that we have established the existence of bands and gaps, we can qualitatively explain the differences between metals, semiconductors, and insulators
- The position and occupation of the highest band or two of the solid determine the conductivity

Band Theory

- Metals



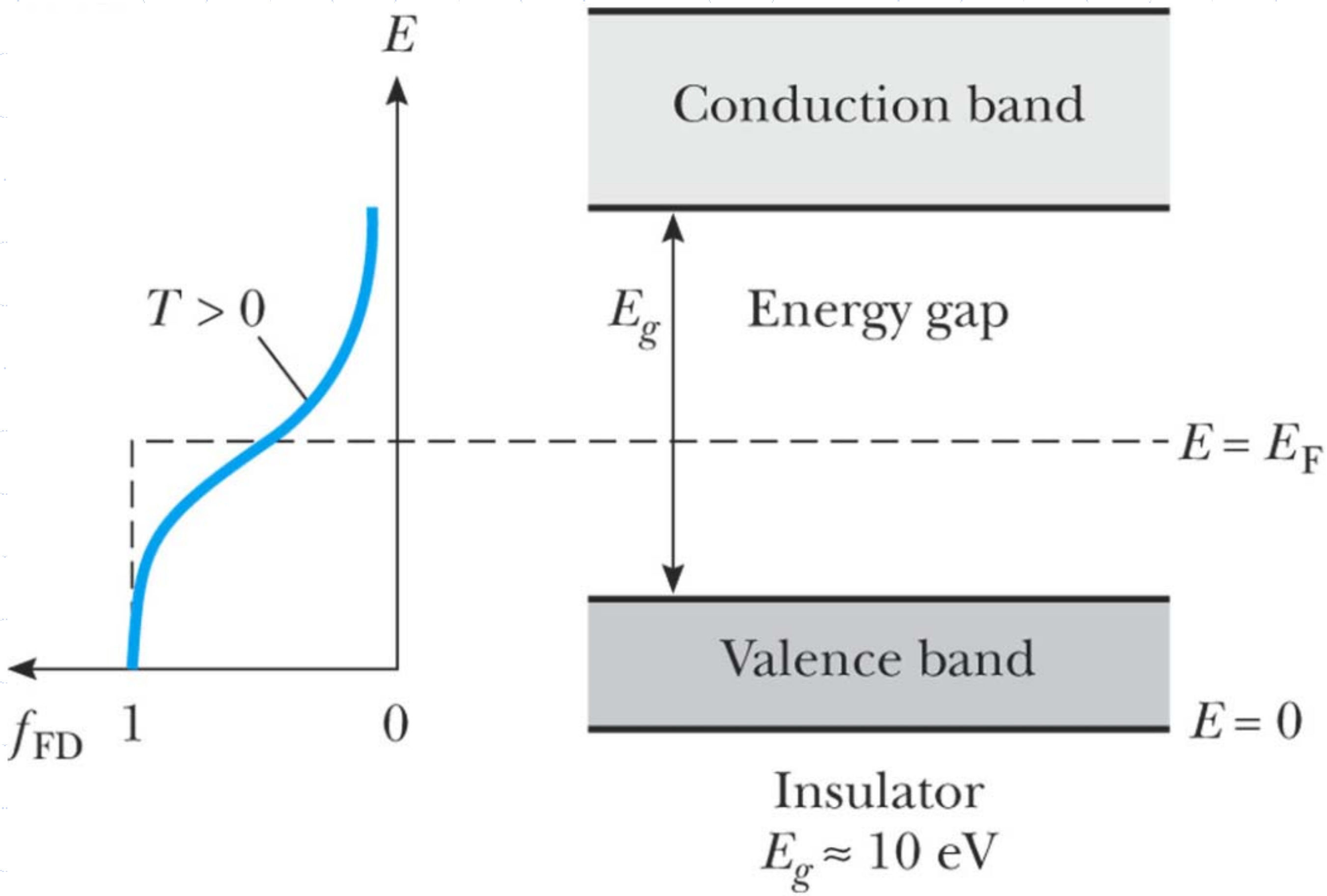
Band Theory

➢ Metals

- The Fermi energy E_F is inside the conduction band
  - e.g. in Na, E_F lies in the middle of the band
- At T=0, all levels in the conduction band below E_F are filled with electrons while those above E_F are empty
- For T>0, some electrons can be thermally excited to energy levels above E_F, but overall there is not much difference from the T=0 case
- However electrons can be easily excited to levels above E_F by applying a (small) electric field to the metal
- Thus metals have high electrical conductivity

Band Theory

- Insulators



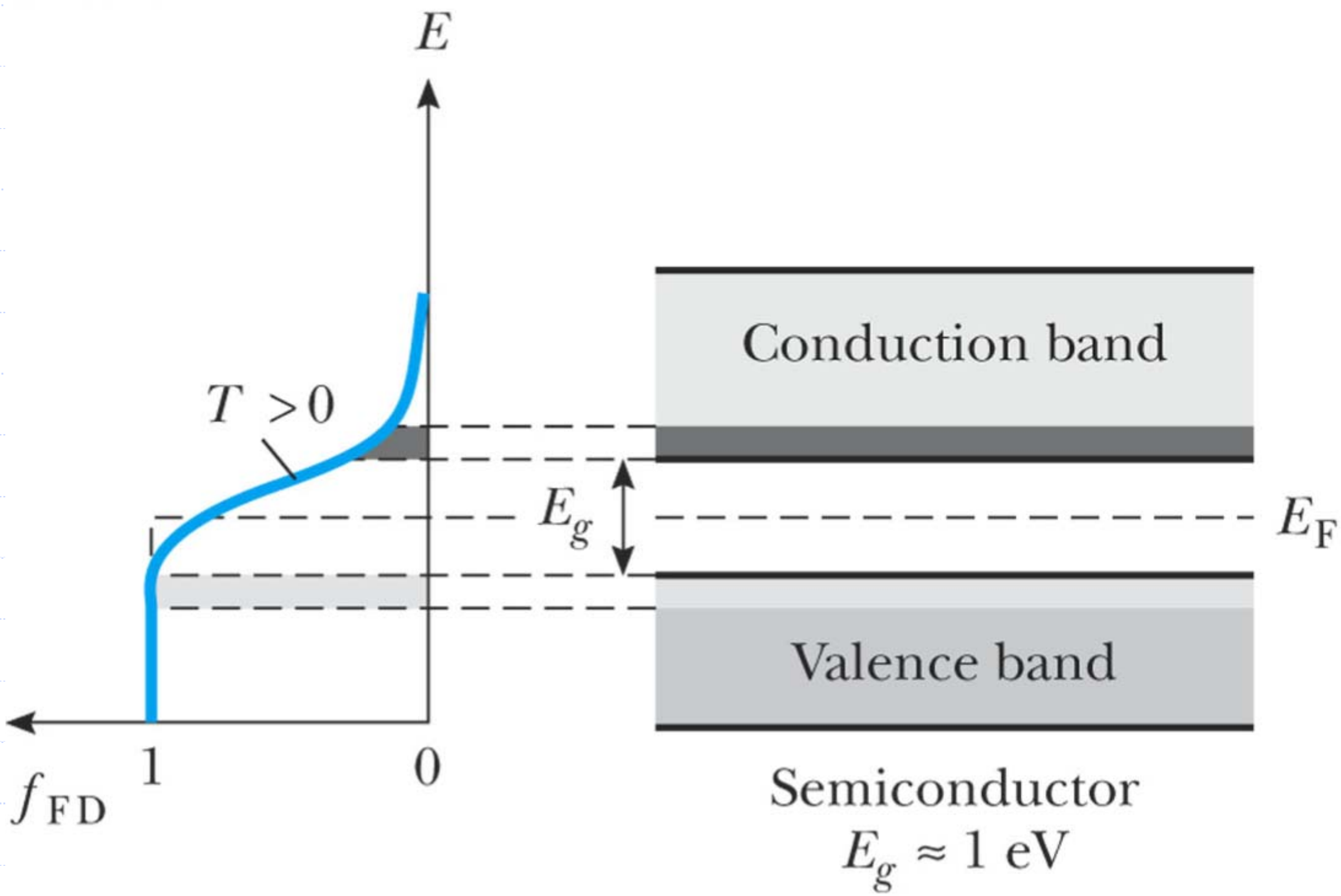
Band Theory

➢Insulators

- Here the Fermi energy E_F is at the midpoint between the valence band and the conduction band
- At T=0, the valence band is filled and the conduction band is empty
- However the band gap energy E_g between the two is relatively large (~ 10 eV) (compared to $k_B T$ at room temperature e.g.)
- Thus there are very few electrons in the conduction band and the electrical conductivity is low

Band Theory

- Semiconductors



Band Theory

Semiconductors

- Again the Fermi energy E_F is midway between the valence band and the conduction band
- At T=0, the valence band is filled and the conduction band is empty
- However for semiconductors the band gap energy is relatively small (1-2 eV) so appreciable numbers of electrons can be thermally excited into the conduction band
- Hence the electrical conductivity of semiconductors is poor at low T but increases rapidly with temperature

Band Theory

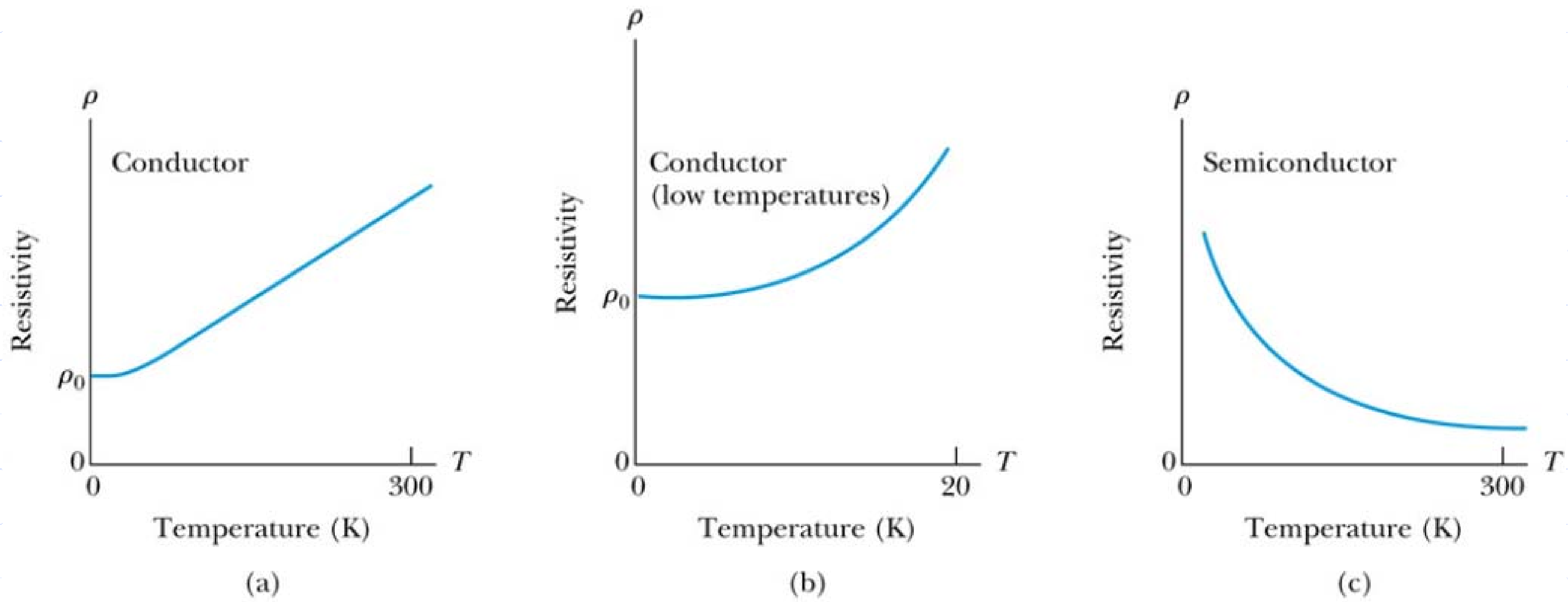
- Semiconductor band gap energies

Table 11.2 Energy Gaps for Selected Semiconductor Materials at $T = 0$ K and $T = 300$ K

	E_g (eV)	
Material	**$T = 0$ K**	**$T = 300$ K**
Si	1.17	1.11
Ge	0.74	0.66
InSb	0.23	0.17
InAs	0.43	0.36
InP	1.42	1.27
GaP	2.32	2.25
GaAs	1.52	1.43
GaSb	0.81	0.68
CdSe	1.84	1.74
CdTe	1.61	1.44
ZnO	3.44	3.2
ZnS	3.91	3.6

Band Theory

- There are striking differences between conductors and semiconductors



- Recall R=ρL/A

Band Theory

- At this point we could begin to study semiconductor devices such as diodes, LED's, and transistors
  - However we are out of class periods
- To conclude, I'll list some of the outstanding questions in condensed matter physics*
  - Since that is the field to which we have most recently been applying quantum mechanics
- For outstanding questions in particle physics you can ask Prof. Varnes

  - * Not my own

10 Questions in Condensed Matter Physics

- Are there new classes or states of matter?
  - Superconductors, Bose-Einstein condensates, …
- What is the origin of high temperature superconductivity?
  - Are there room temperature superconductors?
- What universal principles can be found studying condensed matter
  - Phase transitions, symmetry breaking, …

10 Questions in Condensed Matter Physics

- Can a practical quantum computer be built?
  - Qubits are used instead of bits
- How can we explain the behavior of glasses?
  - Glasses are frozen liquids
- How do we describe matter away from equilibrium
  - Understanding chaos
- Can statistical mechanics be applied to a living cell?

10 Questions in Condensed Matter Physics

- How do singularities form in matter and spacetime?
  - How do vertices form in a crumpled sheet of paper?
- What physics principles govern the flow of granular material?
  - Sand, snow, powders, …
- What are the physical principles of biological self-organization?
  - How does pattern and structure arise in complex systems?

10 Questions in Condensed Matter Physics

- None of these questions will appear on the final!
- Good luck and thanks for a lively semester