PHOT 222: Quantum Photonics
LECTURE 16

Michaël Barbier, Spring semester (2024-2025)

OVERVIEW OF THE COURSE

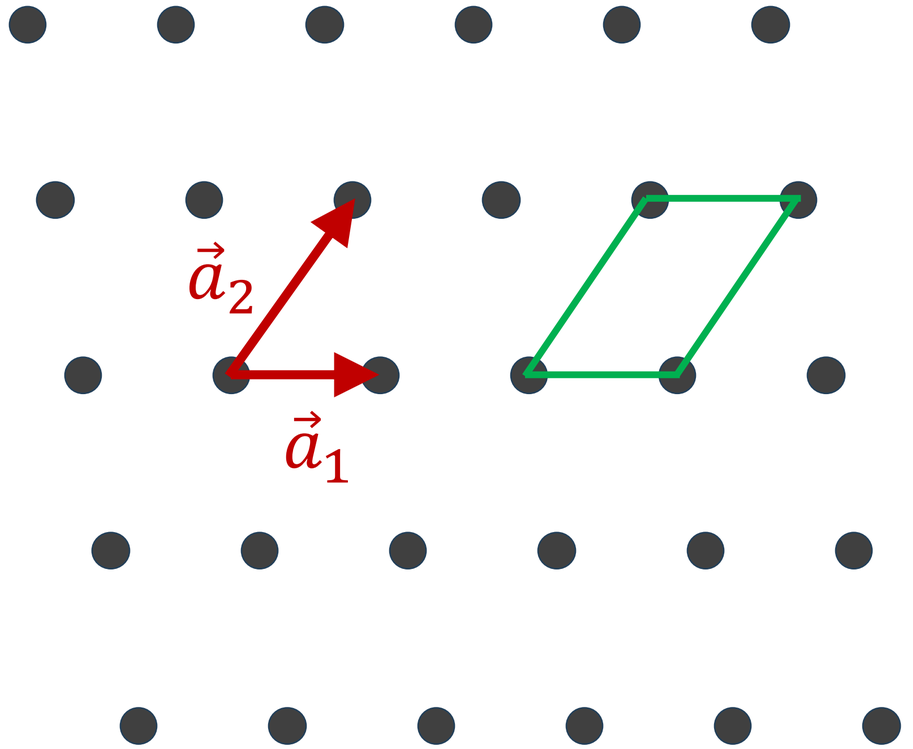
week	topic	Serway 9th	Young
Week 1	Relativity	Ch. 39	Ch. 37
Week 2	Waves and Particles	Ch. 40	Ch. 38-39
Week 3	Wave packets and Uncertainty	Ch. 40	Ch. 38-39
Week 4	The Schrödinger equation and Probability	Ch. 41	Ch. 39
Week 5	**Midterm exam 1**		
Week 6	Quantum particles in a potential	Ch. 41	Ch. 40
Week 7	Bayram		
Week 8	Harmonic oscillator	Ch. 41	Ch. 40
Week 9	Tunneling through a potential barrier	Ch. 41	Ch. 40
Week 10	**Midterm exam 2**		
Week 11	Bohr's hydrogen atom, absorption/emission spectra	Ch. 42	Ch. 41
Week 12	Quantum mechanical model of the hydrogen atom	Ch. 42	Ch. 41
Week 13	Exercises		
Week 14	Spin / Many-electron atoms	Ch. 42	Ch. 41
Week 15	Molecules	Ch. 43	Ch. 42
Week 16	**Crystalline materials & energy band structure**	**Ch. 43**	**Ch. 42**

Solids - Crystal structures

CRYSTAL STRUCTURE

- Crystal structure:
  - Longe-range order
  - Periodic repetition of same atoms
- Translation symmetry

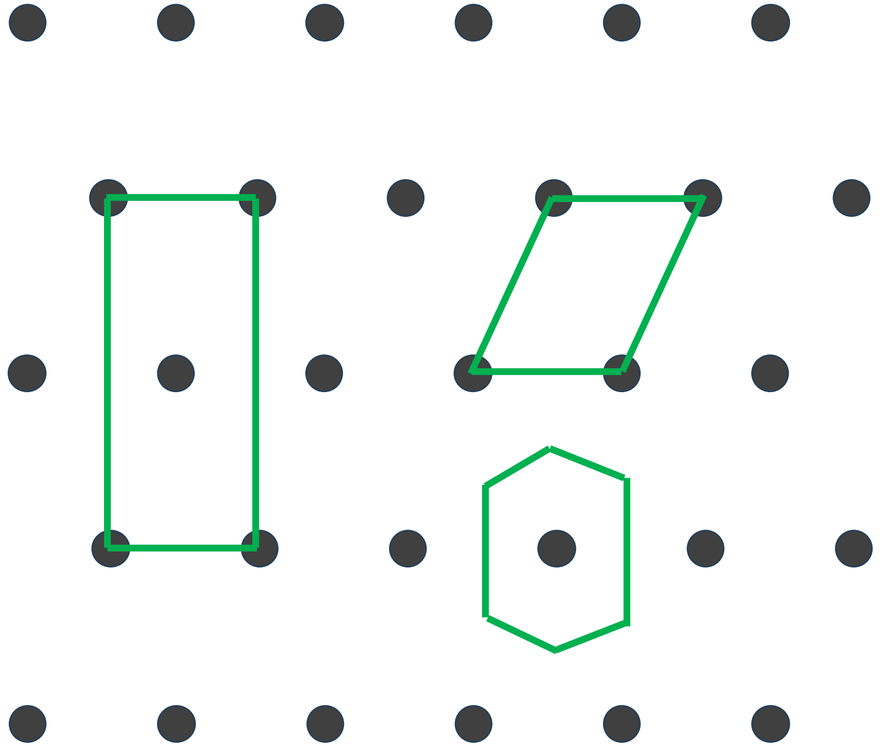
  Basis vectors $\vec{a}_1, \vec{a}_2, (\vec{a}_3)$
- **Unit cell**: a single repeated block
- **Primitive unit cell**: a unit cell with one lattice point



CRYSTAL STRUCTURE

- Different unit cell possible
- Non-primitive unit cells: symmetry

→ Body-centered rectangular unit cell

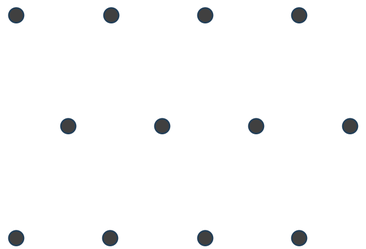


BRAVAIS LATTICE + BASIS

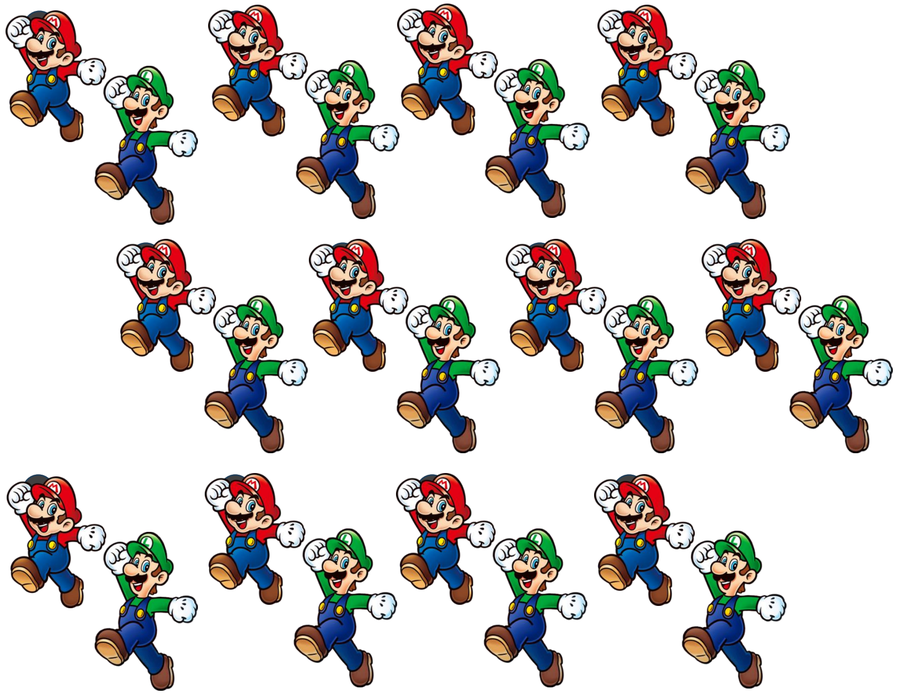
Basis

Atoms/molecule

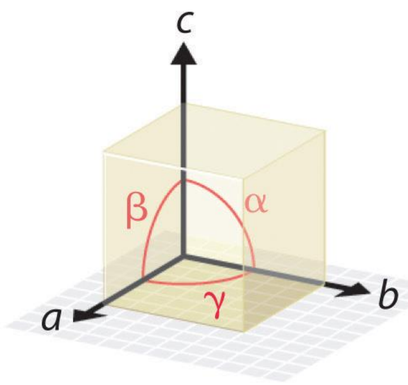
Lattice



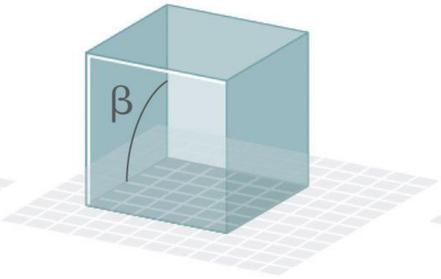
Crystal



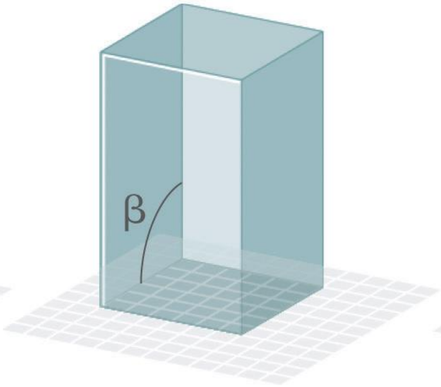
#7 TYPES OF 3D CRYSTAL SYSTEMS



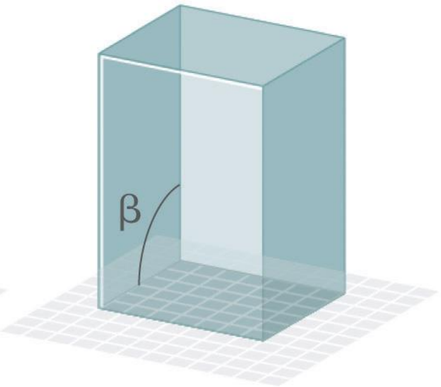
Edges and angles



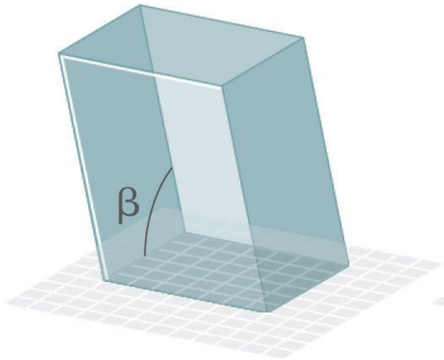
Cubic
$a = b = c$
$\alpha = \beta = \gamma = 90°$



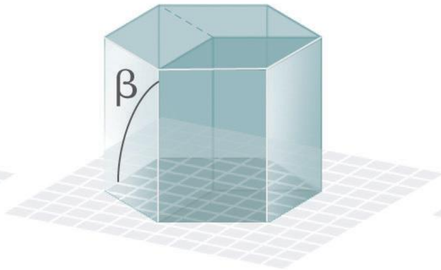
Tetragonal
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$



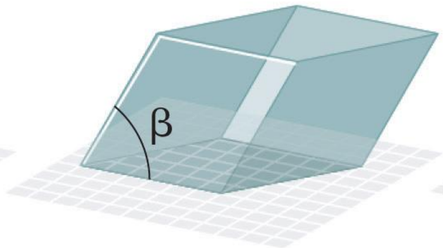
Orthorhombic
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$



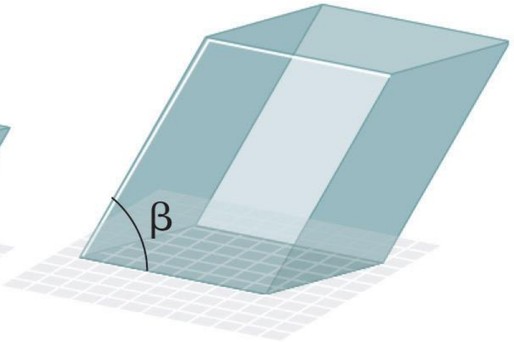
Monoclinic
$a \neq b \neq c$
$\alpha = \gamma = 90° \neq \beta$



Hexagonal
$a = b \neq c$
$\alpha = \beta = 90°, \gamma = 120°$



Rhombohedral
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$

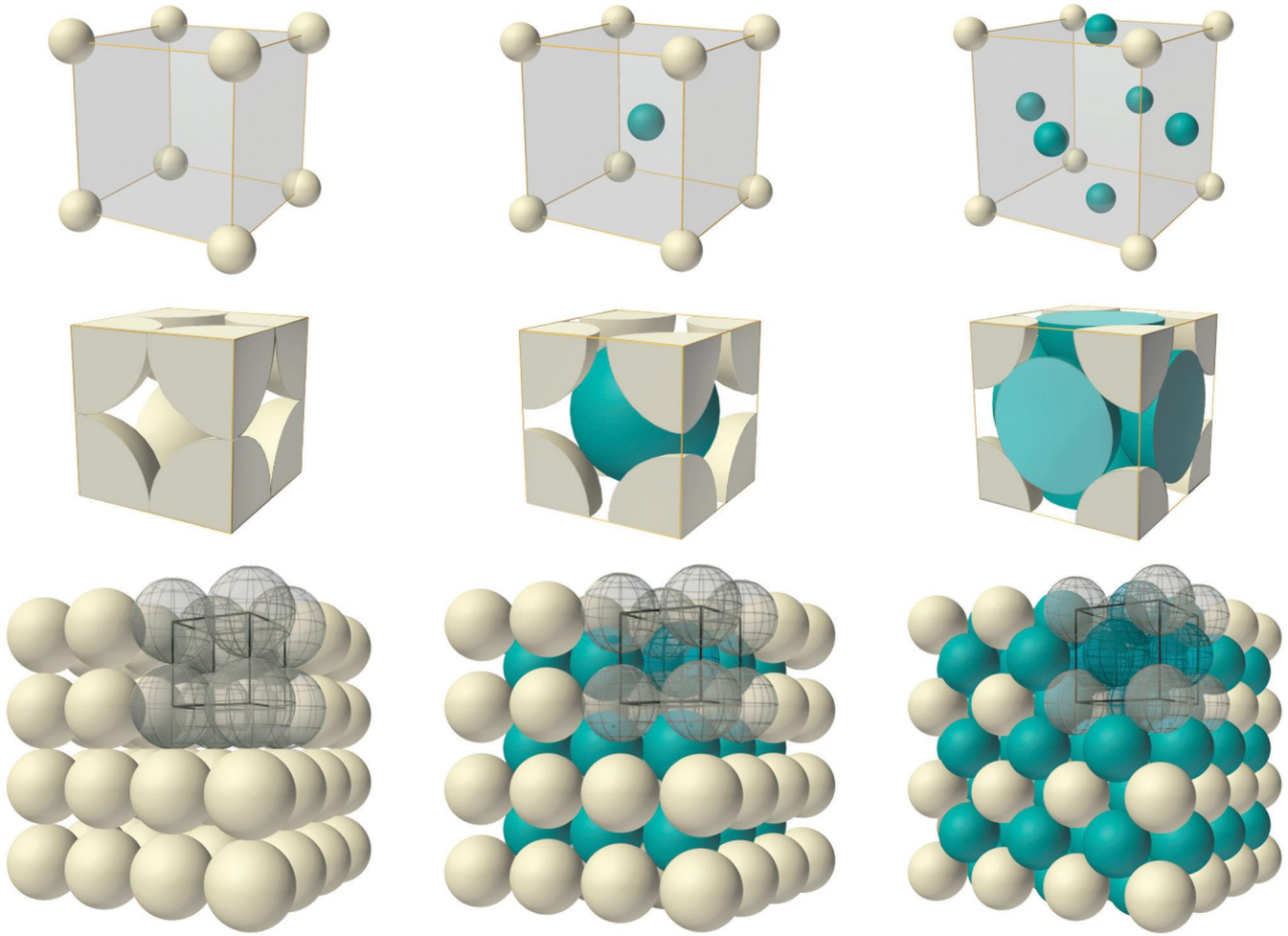


Triclinic
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

Adapted from LibreTexts - Chemistry

3D CRYSTAL BRAVAIS LATTICES

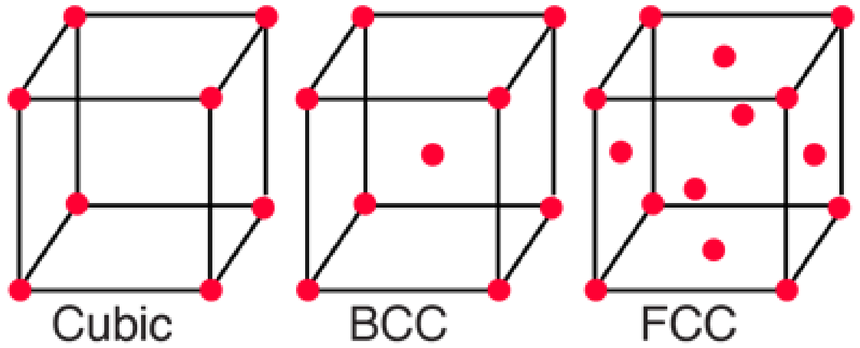
- Crystal system + symmetry
- 14 Bravais lattices in 3D
- Example - Cubic system has 3 Bravais lattices:
  - Simple cubic
  - Body-centered cubic
  - Face-centered cubic

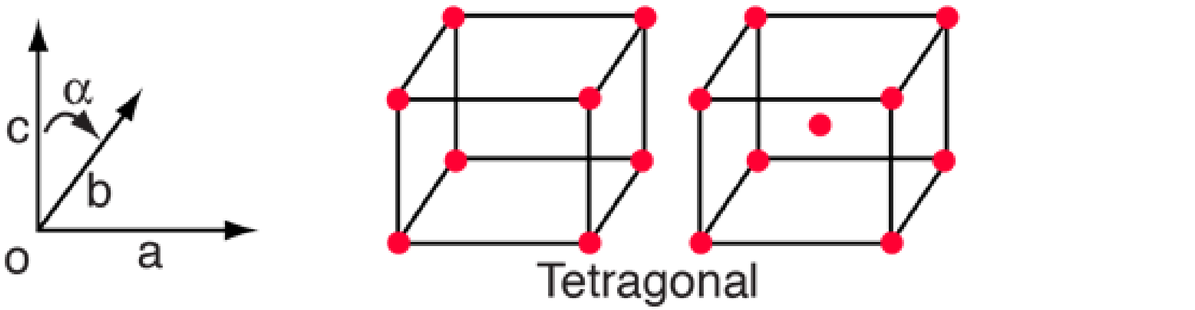


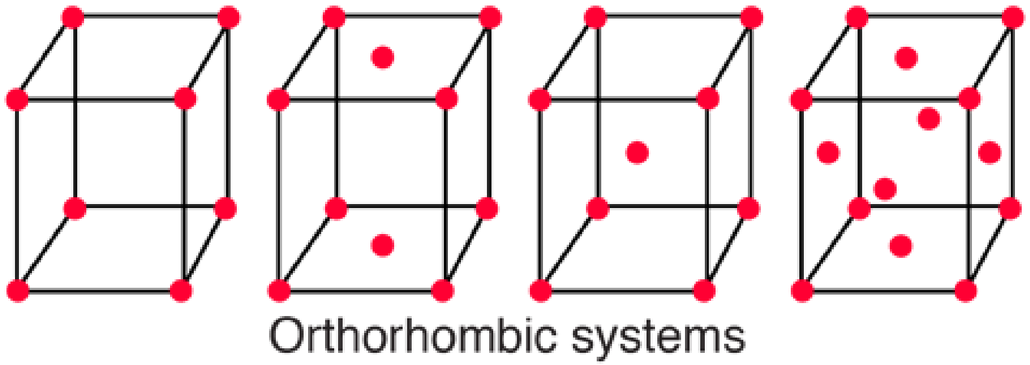
(a) Simple cubic (b) Body-centered cubic (c) Face-centered cubic

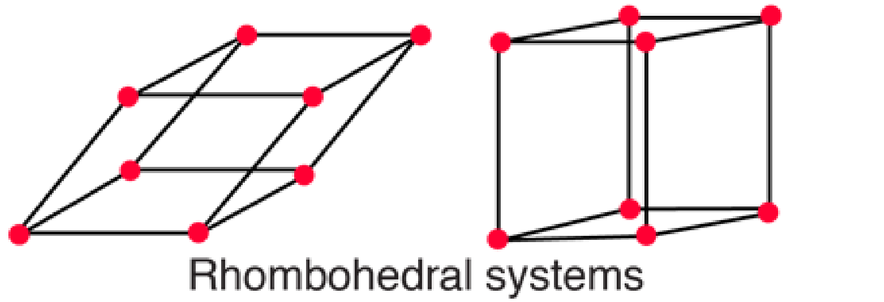
Adapted from LibreTexts - Chemistry

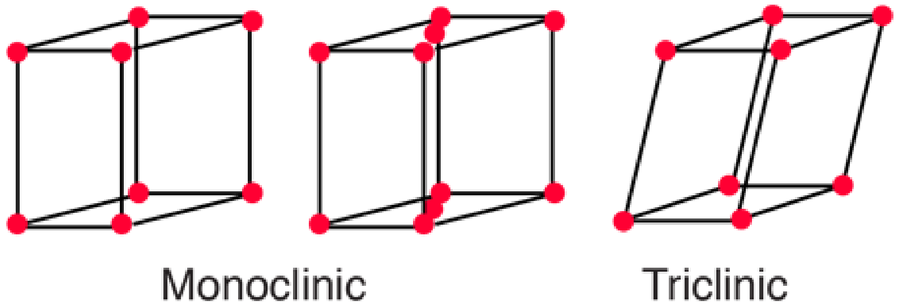
#14 3D CRYSTAL BRAVAIS LATTICES







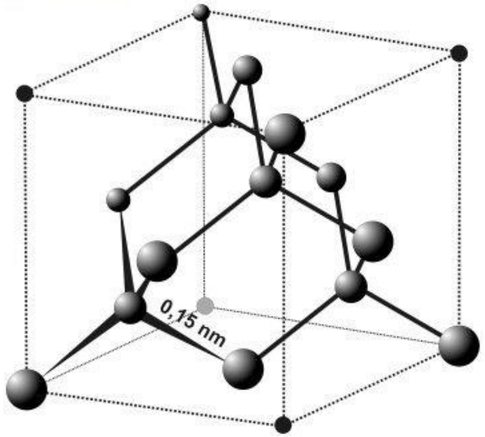


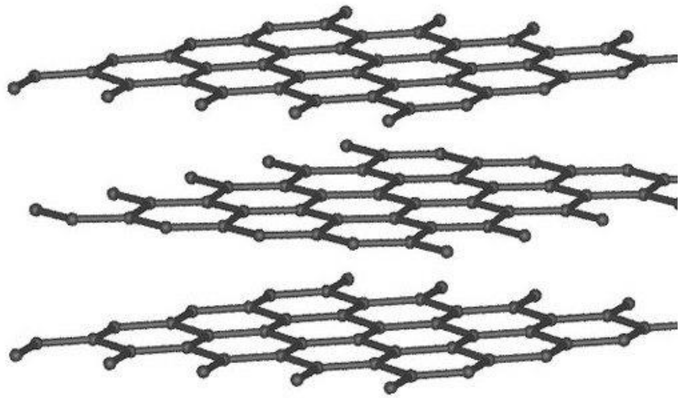


Adapted from Hyperphysics

BONDS IN CRYSTALLINE MATERIALS

- Different types of bonds
  - Ionic bonds
  - Covalent bonds
  - Vanderwaals bonds
  - Hydrogen bonds

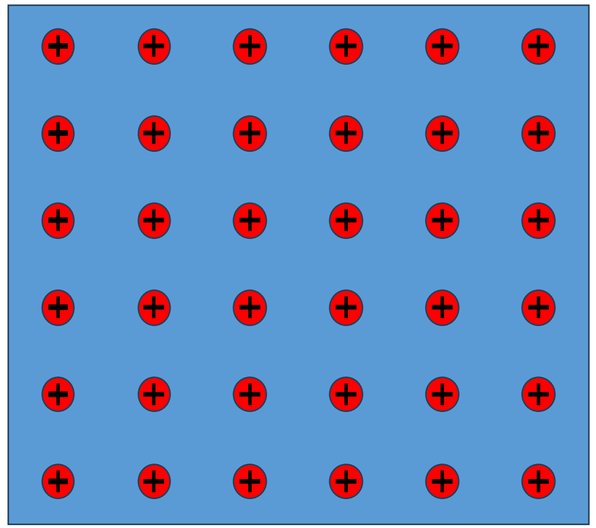




Metals – Free electron model

METALS: FREE-ELECTRON MODEL

- In metals orbitals of valence electrons have a large overlap
- Metals share electrons



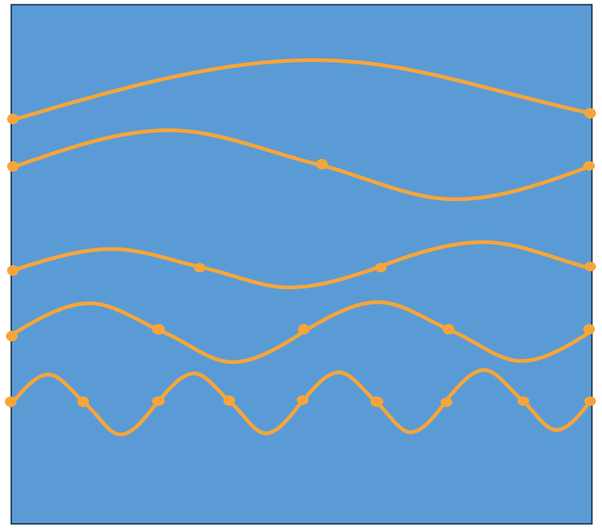
- Electrons are moving nearly free

⟹ Particle in a box

$$E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

METALS: FREE-ELECTRON MODEL

- In metals orbitals of valence electrons have a large overlap
- Metals share electrons

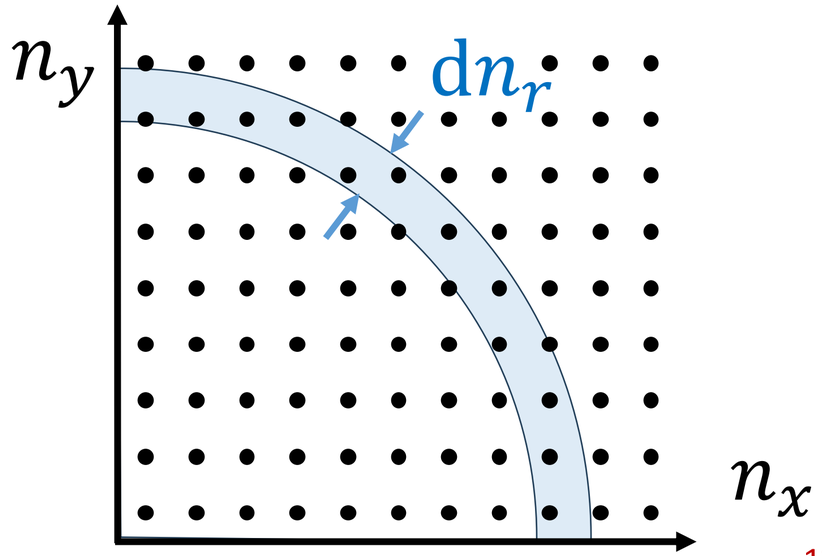


- Electrons are moving nearly free

➡ Particle in a box

$$E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

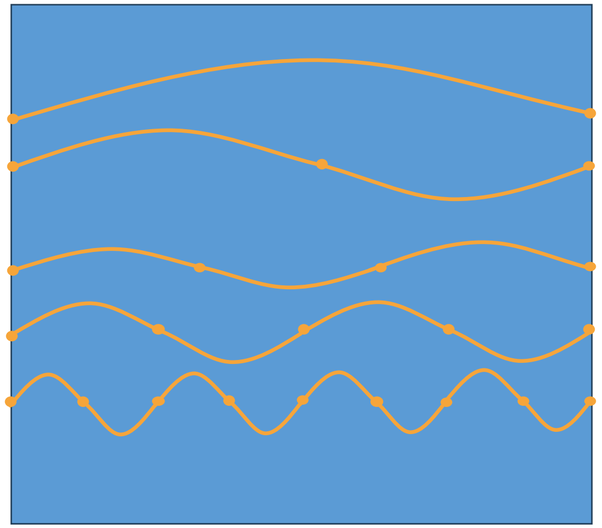
$$\psi_{n_x,n_y,n_z} = \sqrt{\frac{8}{L^3}}\,\sin\left(\frac{n_x\pi x}{L}\right)\,\sin\left(\frac{n_y\pi y}{L}\right)\,\sin\left(\frac{n_z\pi z}{L_z}\right)$$



FREE-ELECTRON MODEL: DENSITY OF STATES

- Number of states increases with energy

$$E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$



- For larger radius $n_r = \sqrt{n_x^2 + n_y^2 + n_z^2}$ more states

- Density of States $g(E)$:

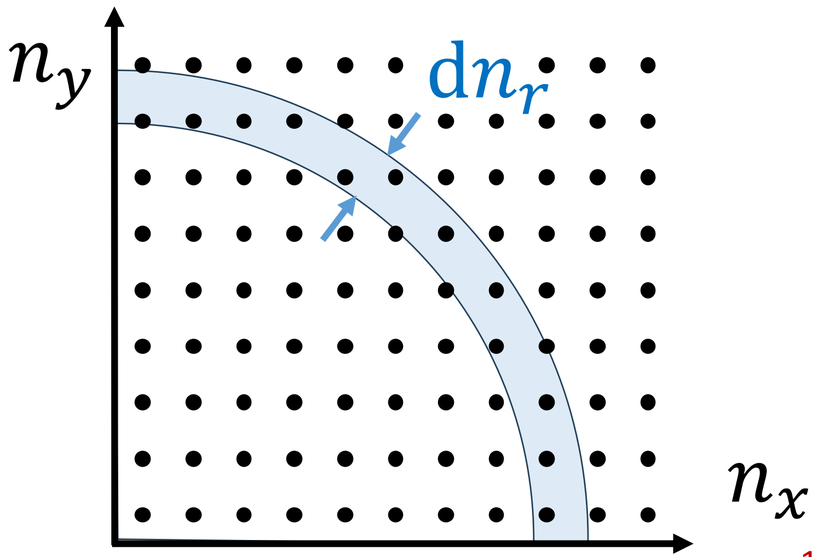
$$g(E) = \frac{dn}{dE}$$

Volume sphere

$$n(E) = \frac{1}{8}\left(\frac{4}{3}\pi n_r^3\right)2 = \frac{\pi n_r^3}{3} = \frac{(2m)^{\frac{3}{2}}L^3E^{\frac{3}{2}}}{3\pi^2\hbar^3}$$

1/8 of sphere

spin



FREE-ELECTRON MODEL: DENSITY OF STATES

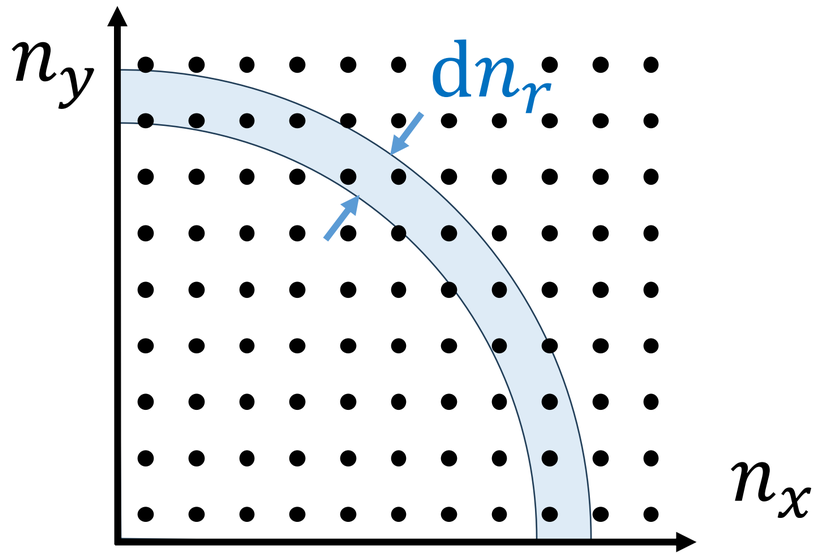
- Number of states increases with energy

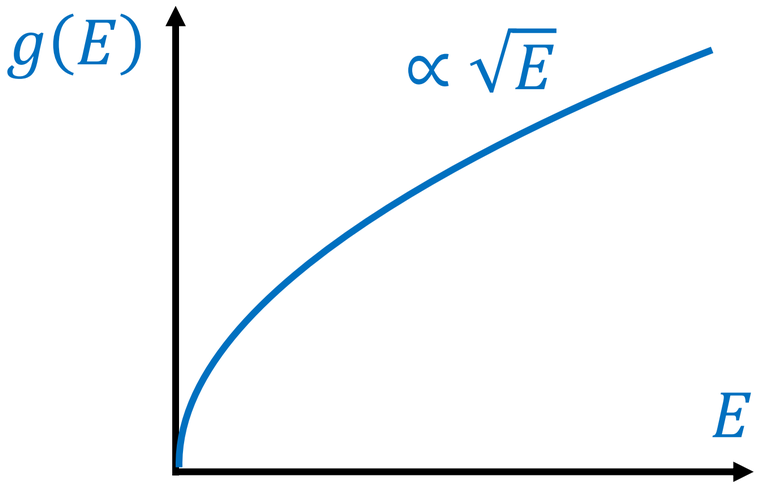
$$n(E) = \frac{1}{8}\left(\frac{4}{3}\pi n_r^3\right)2 = \frac{\pi n_r^3}{3} = \frac{(2m)^{\frac{3}{2}}L^3E^{\frac{3}{2}}}{3\pi^2\hbar^3}$$

- Density of States $g(E)$:

$$g(E) = \frac{dn}{dE} = \frac{(2m)^{\frac{3}{2}}VE^{\frac{1}{2}}}{2\pi^2\hbar^3}$$

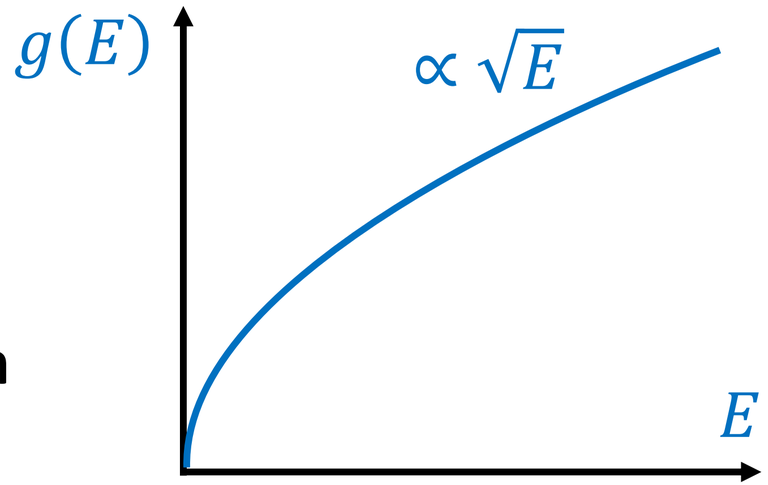
- How do the electrons fill the states?





FREE-ELECTRON MODEL: FERMI-DIRAC DISTRIBUTION

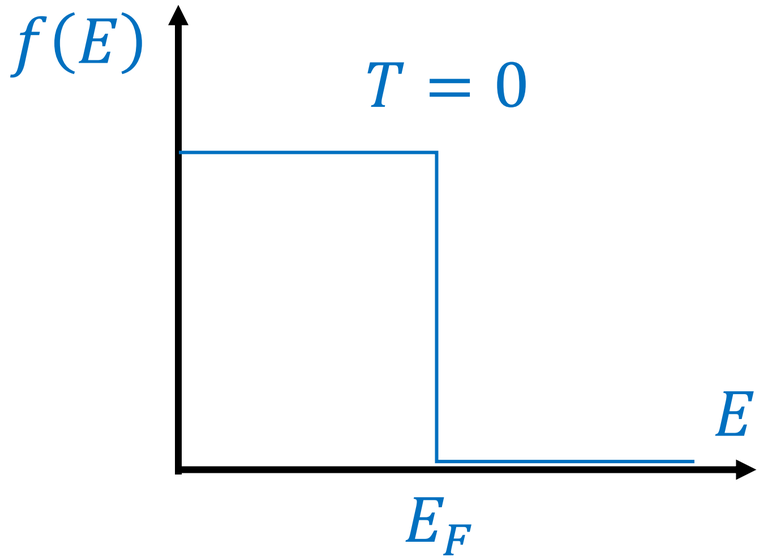
- Density of States: $g(E) = \frac{dn}{dE} = \frac{(2m)^{\frac{3}{2}} V E^{\frac{1}{2}}}{2\pi^2 \hbar^3}$



- Probability electron fill states: **Fermi-Dirac distribution**
  - **Classically:** Maxwell-Boltzmann $e^{-E/k_B T}$
  - Exclusion principle not satisfied
  - Electrons are indistinguishable

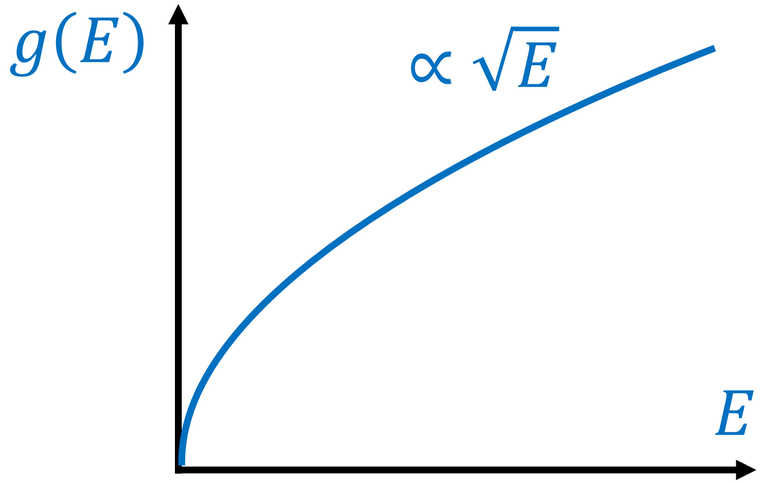
$$f(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1}$$

where E_F is the **Fermi-energy**



FREE-ELECTRON MODEL: FERMI-DIRAC DISTRIBUTION

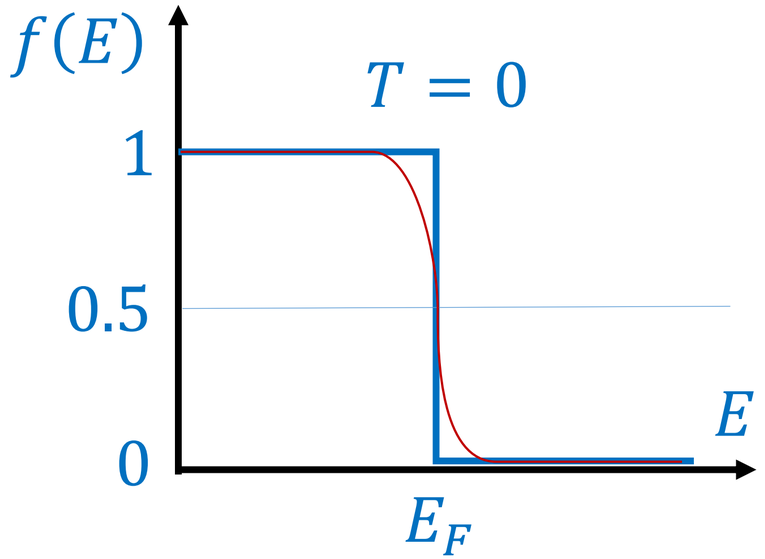
- **Density of States**: $g(E) = \frac{(2m)^{\frac{3}{2}} V E^{\frac{1}{2}}}{2\pi^2 \hbar^3}$



- **Fermi-Dirac distribution:** $f(E) = \frac{1}{e^{(E-E_F)/k_B T}+1}$
  - E_F is the Fermi-energy
  - Fermi-Dirac distribution **at $T = 0$ Kelvin**:

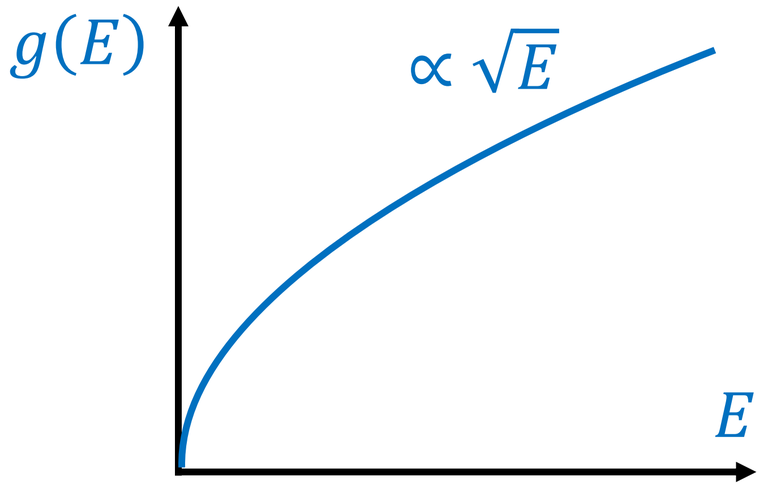
    States below E_F are filled: $f(E < E_F) = 1$
    States above E_F are empty: $f(E > E_F) = 0$

  - Finite temperature **$T > 0$ Kelvin:** smoother



FREE-ELECTRON MODEL: FERMI-DIRAC DISTRIBUTION

- **Density of States**: $g(E) = \frac{(2m)^{\frac{3}{2}} V E^{\frac{1}{2}}}{2\pi^2 \hbar^3}$



- **Fermi-Dirac distribution:** $f(E) = \frac{1}{e^{(E-E_F)/k_B T}+1}$
  - E_F is the Fermi-energy
  - Fermi-Dirac distribution **at $T = 0$ Kelvin**:

    States below E_F are filled: $f(E < E_F) = 1$
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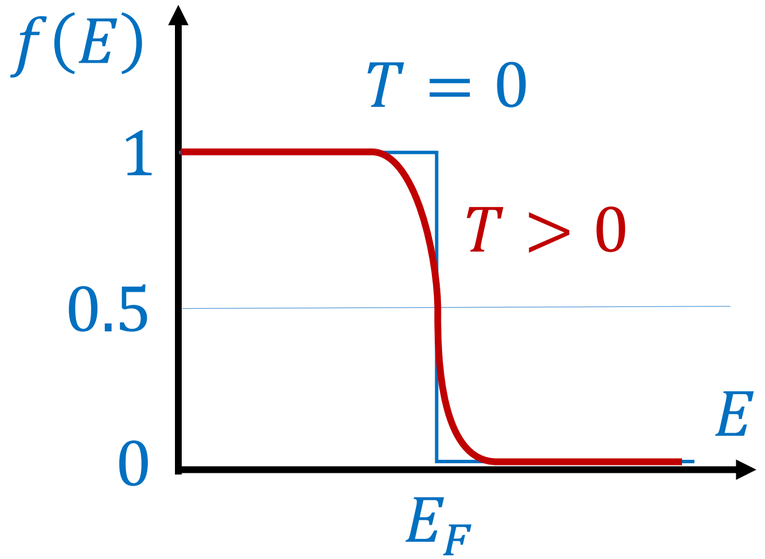


FREE-ELECTRON MODEL: ELECTRON DENSITY

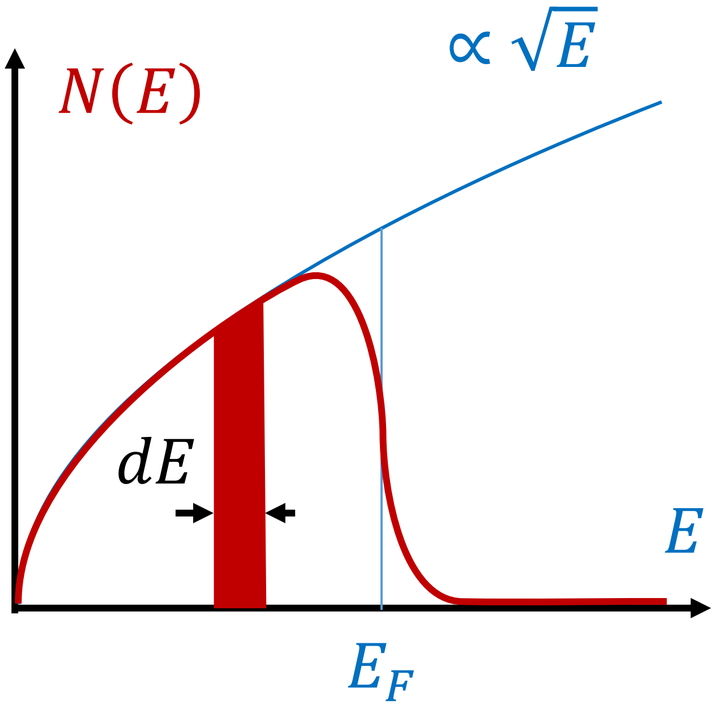
- **Density of States**: $g(E) = \frac{(2m)^{\frac{3}{2}} V E^{\frac{1}{2}}}{2\pi^2 \hbar^3}$

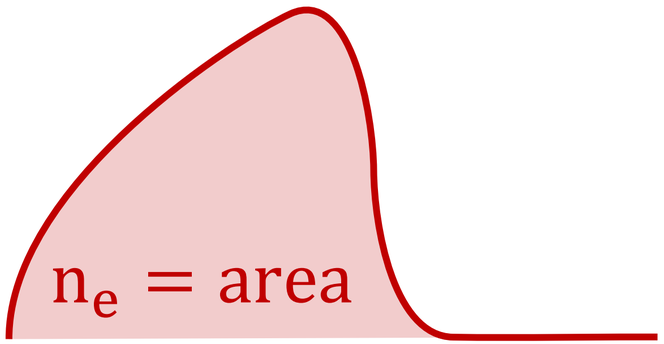
- **Fermi-Dirac distribution:** $f(E) = \frac{1}{e^{(E-E_F)/k_B T}+1}$

- Electron density (per energy & volume) $N(E)$**:**

$$N(E)\, dE = f(E) g(E)\, dE$$

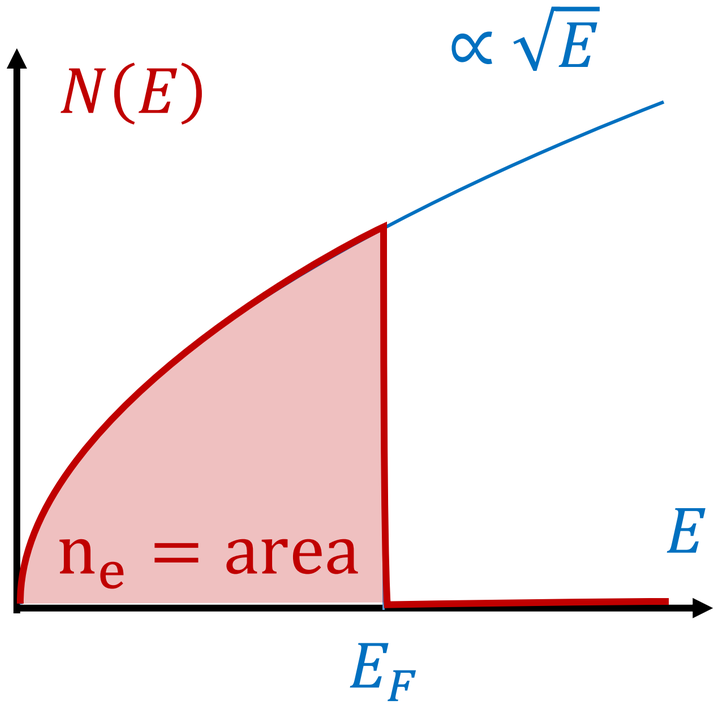
- Electrons (per volume): $\mathrm{n_e} = \int_0^\infty N(E)\, dE$





FREE-ELECTRON MODEL: FERMI-ENERGY FOR METALS

$$N(E) = f(E)g(E) = \frac{1}{e^{(E-E_F)/k_BT}+1} \times \frac{(2m)^{\frac{3}{2}}E^{\frac{1}{2}}}{2\pi^2\hbar^3}$$



- Electrons (per volume): $\mathrm{n_e} = \int_0^\infty N(E)\, dE$
- Find Fermi-energy from $\mathrm{n_e}$ at zero temperature

$$\mathrm{n_e} = \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\int_0^{E_F}\sqrt{E}\, dE = \frac{2}{3}\frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}E_F^{3/2}$$

$$\Rightarrow \quad E_F(0) = \frac{\mathrm{h}^2}{2\mathrm{m}}\left(\frac{3\mathrm{n_e}}{8\pi}\right)^{2/3}$$

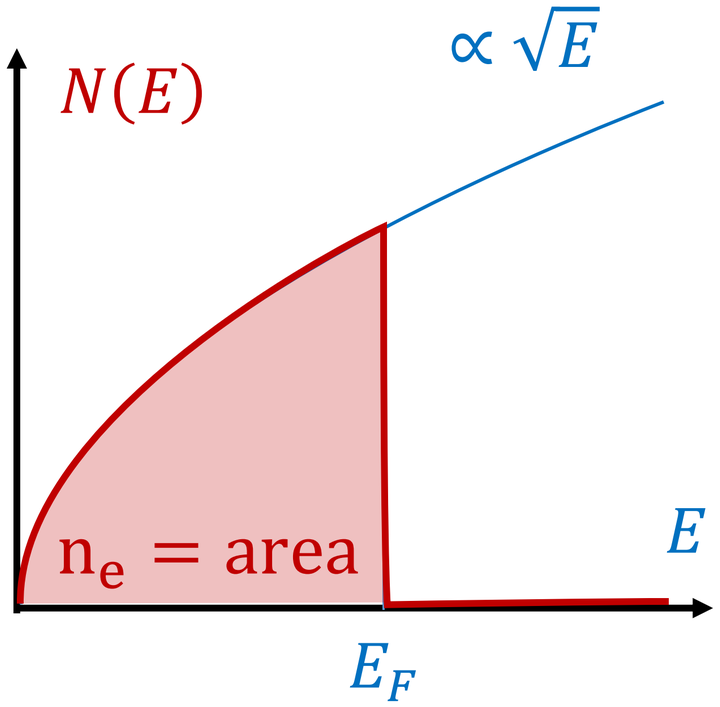
FREE-ELECTRON MODEL: FERMI-ENERGY FOR METALS

$$E_F(0) = \frac{h^2}{2m}\left(\frac{3n_e}{8\pi}\right)^{2/3}$$

- Derive concentration of electrons n_e from number of atoms and valence electrons

Metal	n_e (in $10^{28}\ m^{-3}$)	Fermi energy (eV)
Li	4.70	4.72
Na	2.65	3.23
K	1.40	2.12
Cu	8.46	7.05
Ag	5.85	5.48
Au	5.90	5.53

Values in the table can be found in our textbook: Serway & Jewett, 9th ed.

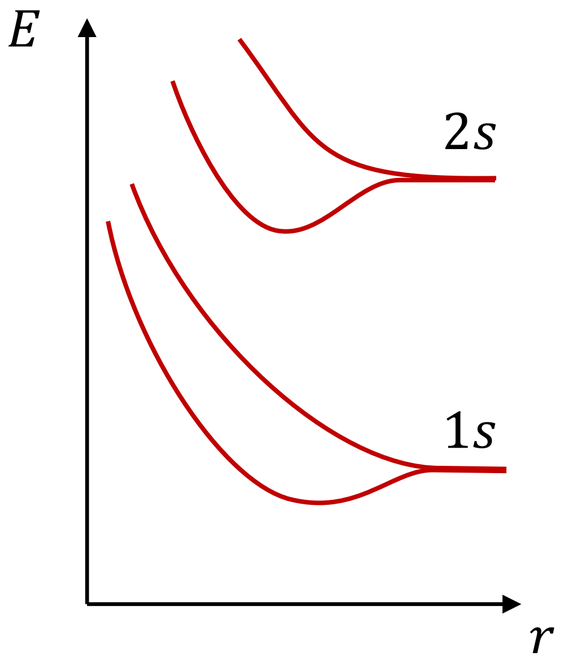


Energy bandstructure

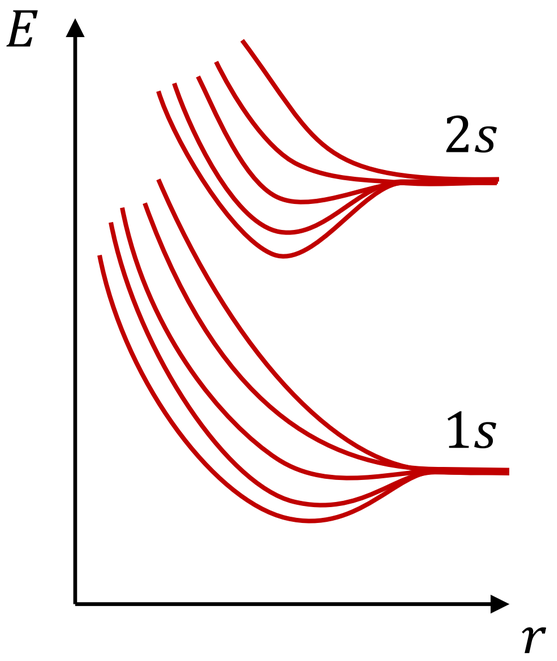
ENERGY BANDS

- Atoms close to each other have overlapping orbitals
- Splitting of their energy levels

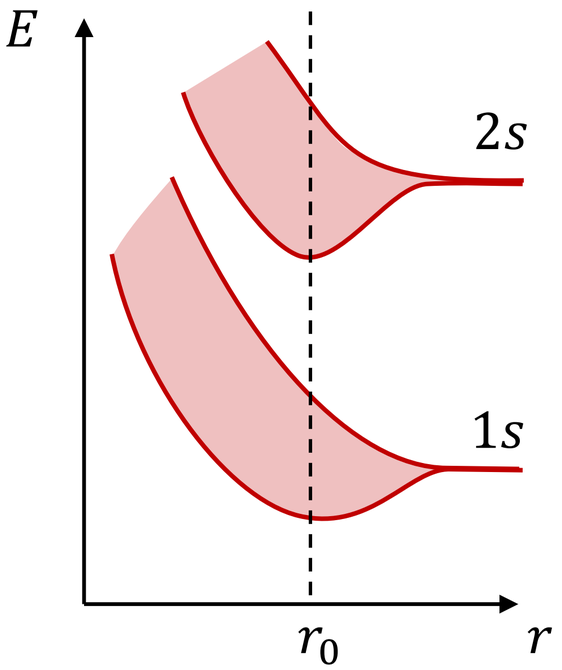
Distance defines the energy levels



$N = 5$ atoms results in 5 energy levels



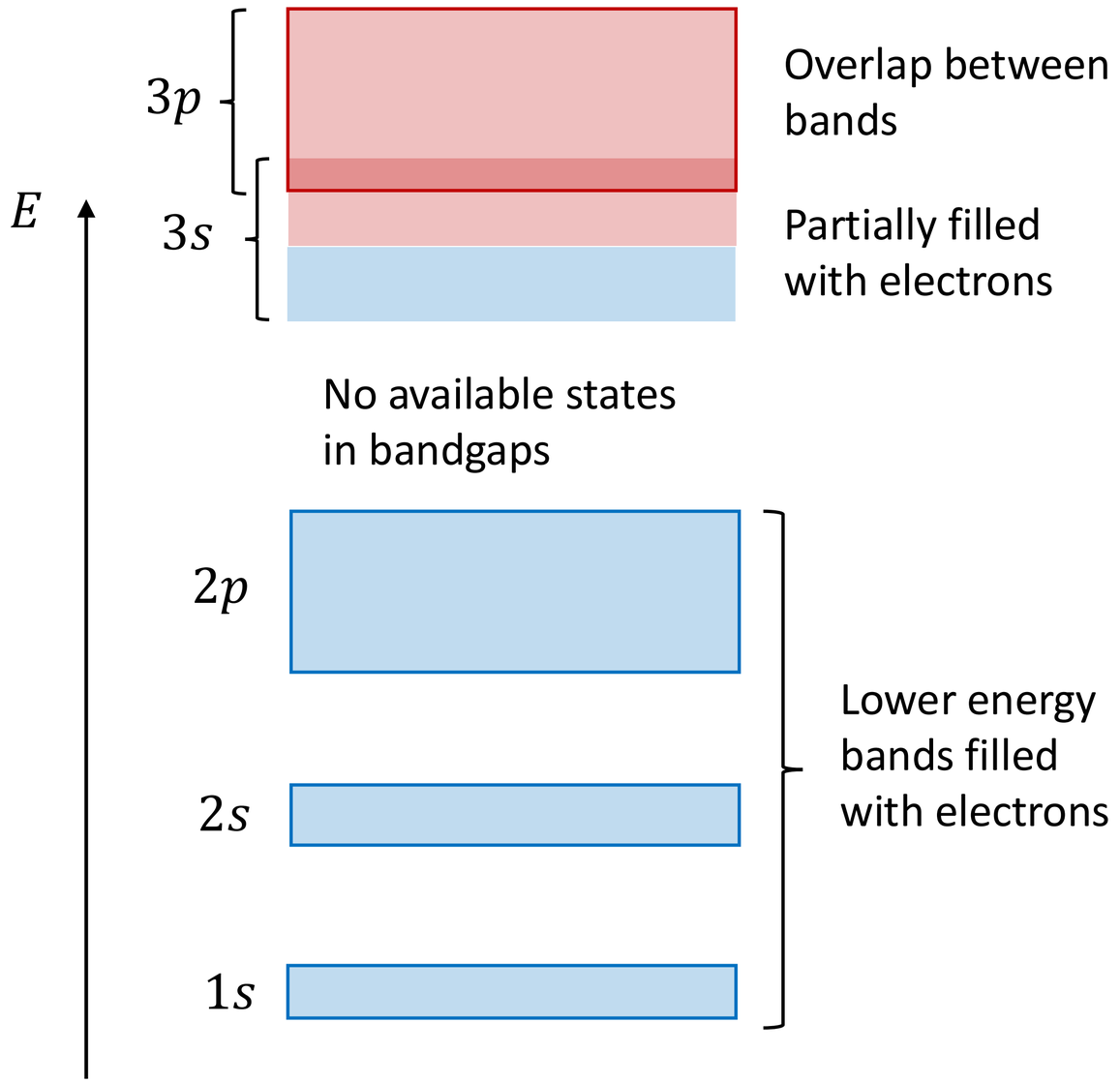
$N \gg 1$ atoms results in dense energy bands



ENERGY BANDS

- Atoms close to each other have overlapping orbitals
- Overlap of orbitals results in splitting their energy levels
- N atoms results in N $\times$ splitting
- For macroscopic materials N is on the order of 10^{23} atoms per cubic centimeter

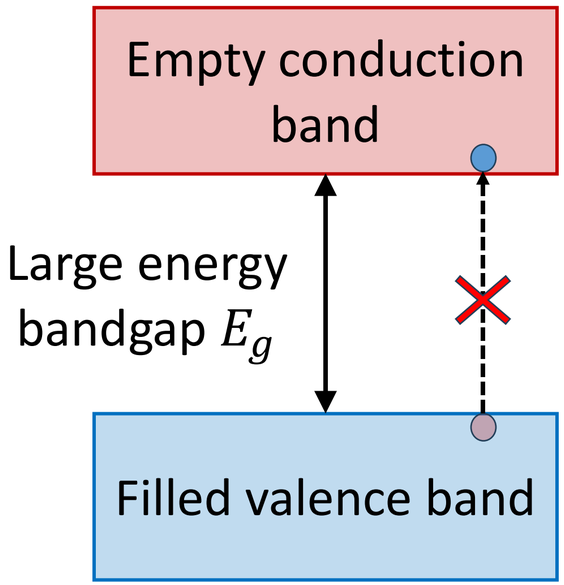
Many energy levels become indistinguishable and form a continuum **energy band**



ENERGY BANDSTRUCTURE TYPES

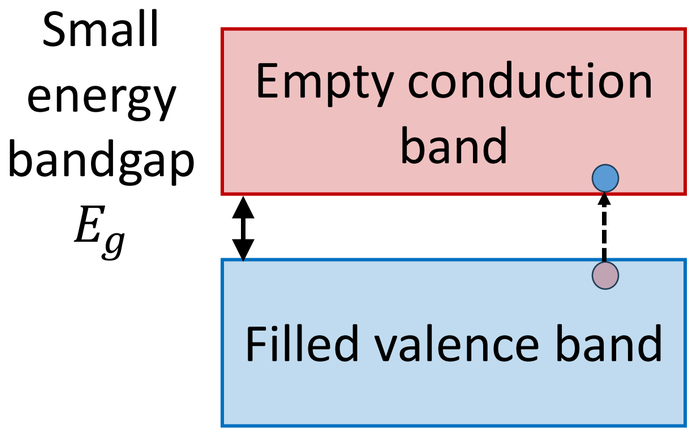
Insulators

- Empty conduction band at $\mathrm{T} = 0\ \mathrm{K}$
- Large E_g prevents excitation to conduction band



Semiconductors

- Empty conduction band at $\mathrm{T} = 0\ \mathrm{K}$
- Small E_g allows limited conduction at $\mathrm{T} > 0\ \mathrm{K}$



Conductors

- Electrons in the conduction band at $\mathrm{T} = 0\ \mathrm{K}$
- High conductivity