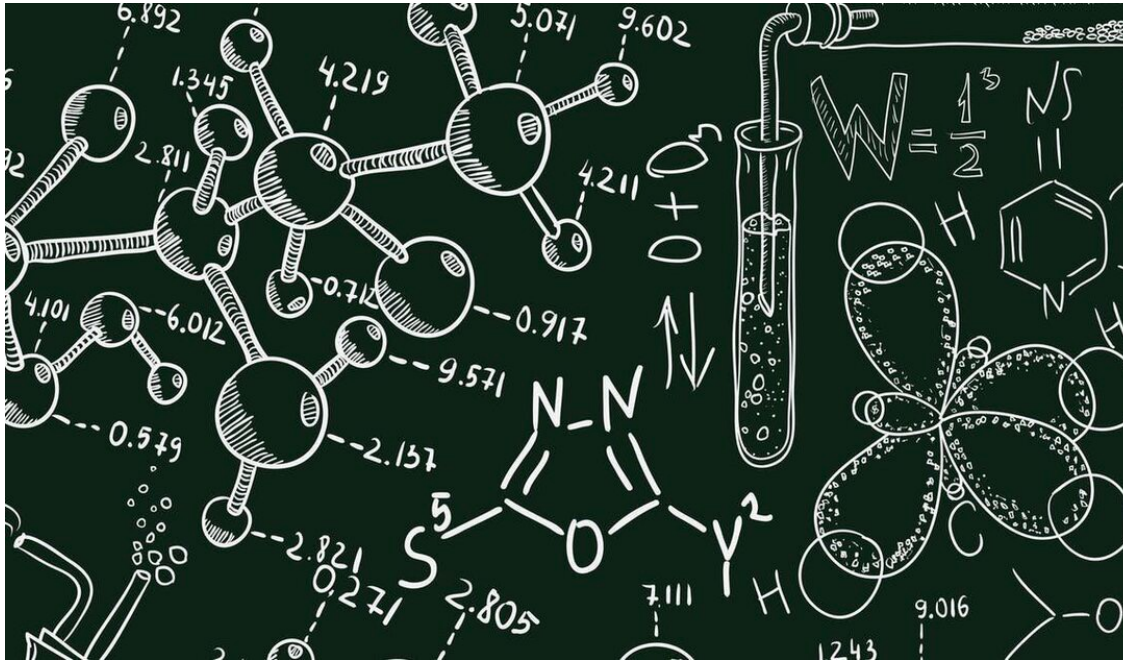
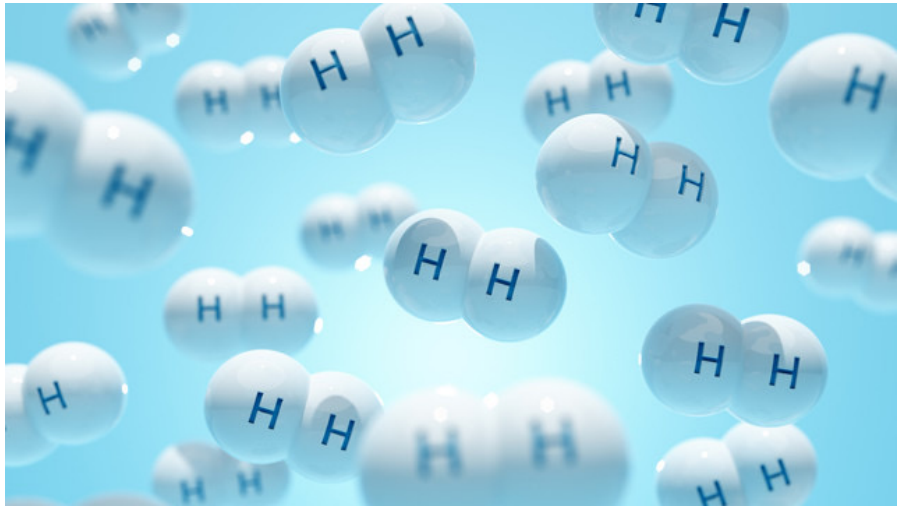
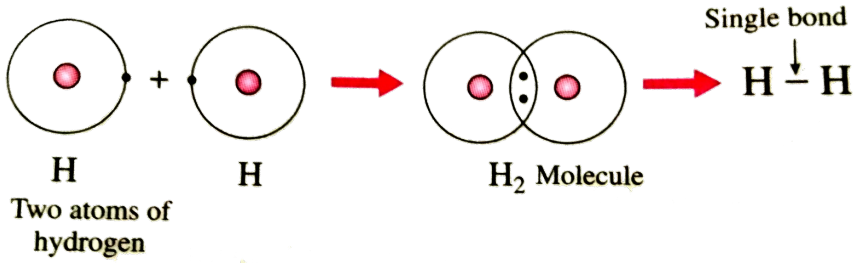
5. Bonding


6.892
5.071
9.602
1.345
4.219
2.811
4.211
4.101
6.012
0.712
0.917
9.571
0.579
2.137
2.821
0.271
2.805
7.111
9.016
1243
N-N
O
S
5
2

Hydrogen molecule





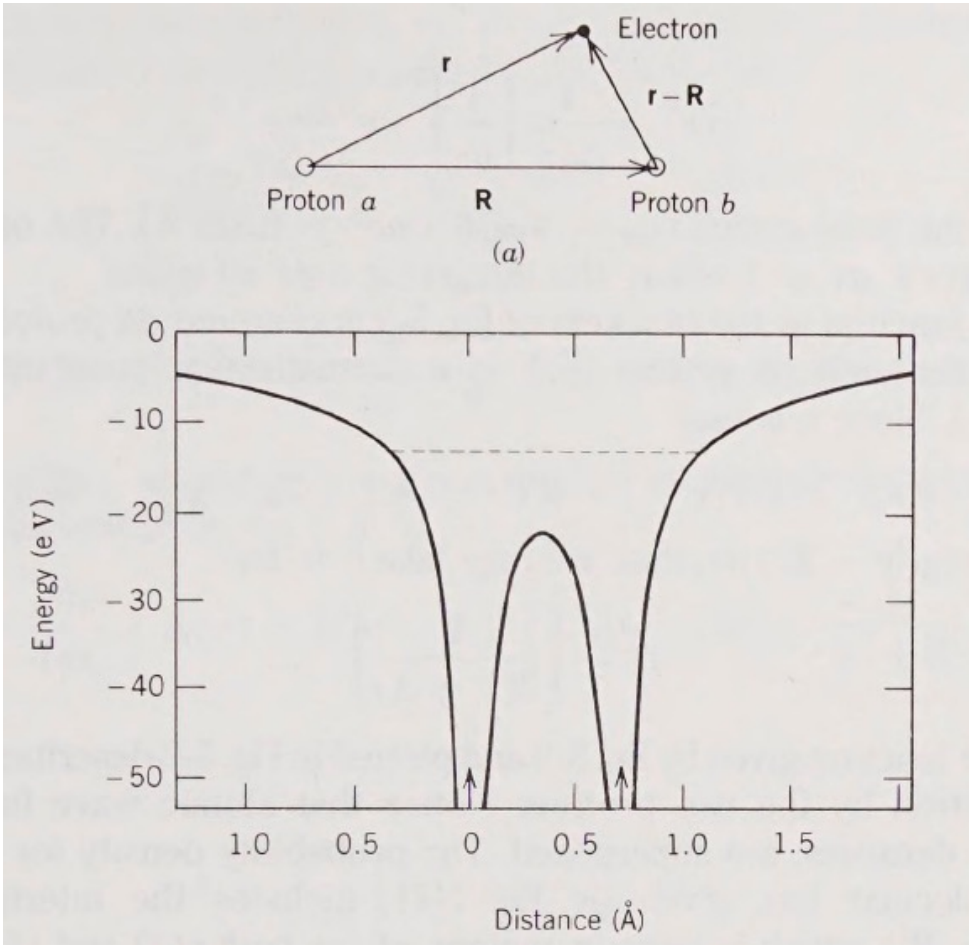
Schroedinger's equation

$$H\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

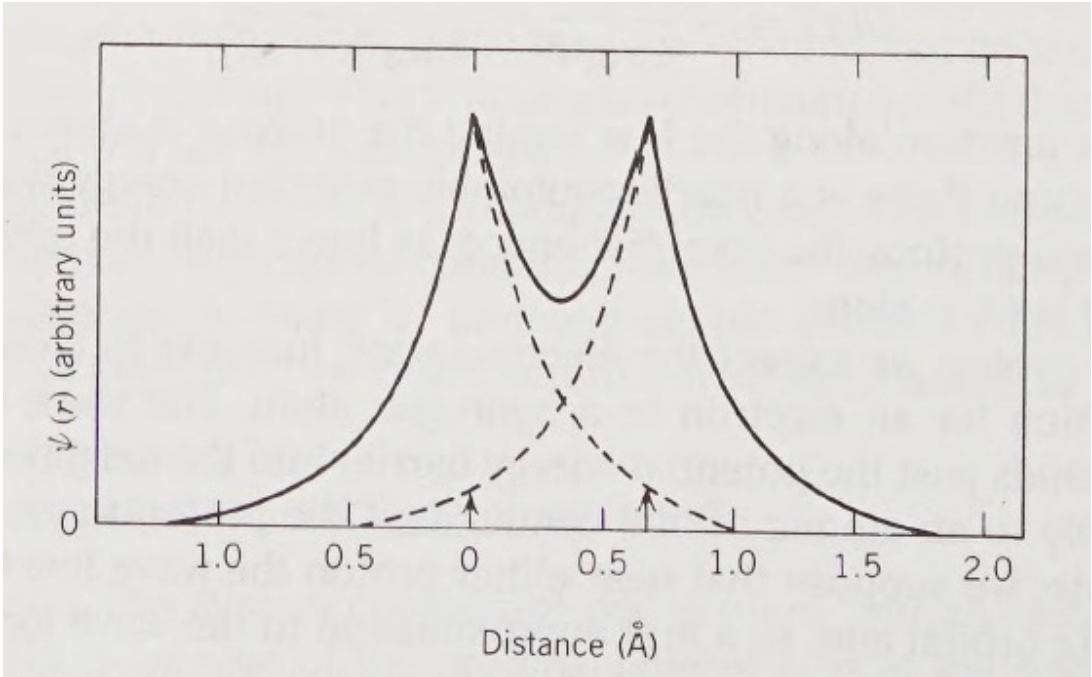
Time evolution

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2} + U(x)\Psi(x) = E\Psi(x)$$

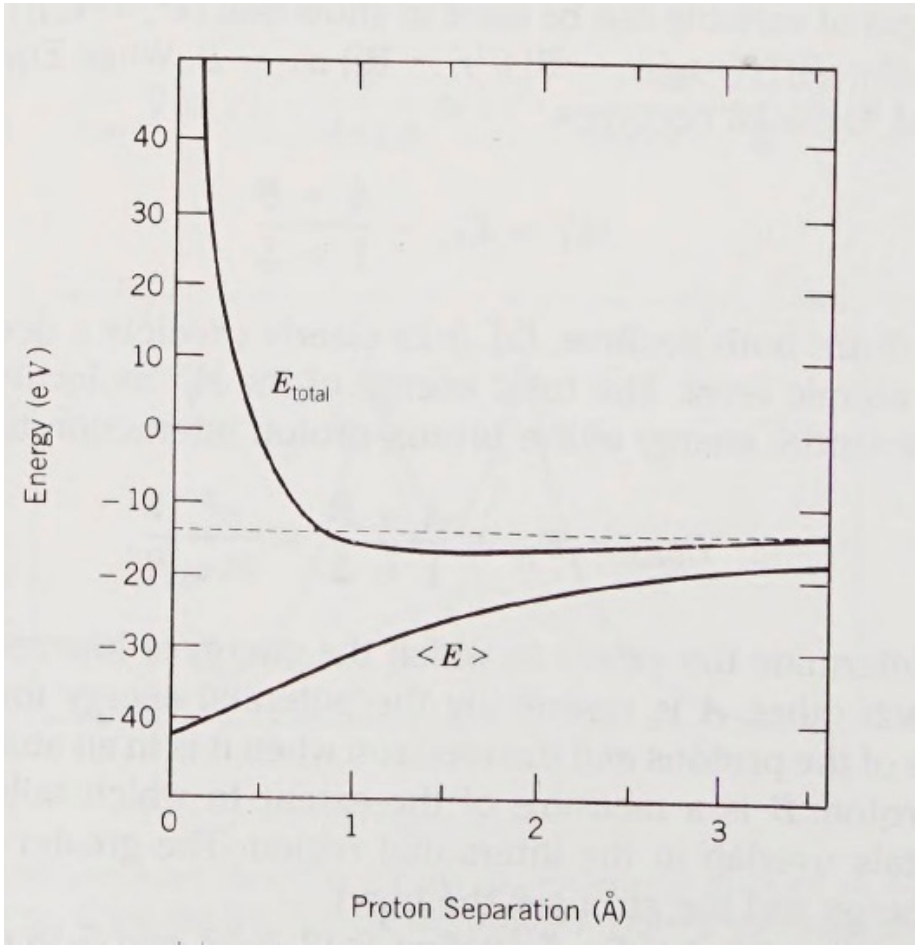
Time independent equation



Molecular H_2 ion

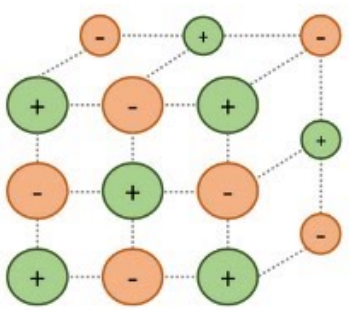


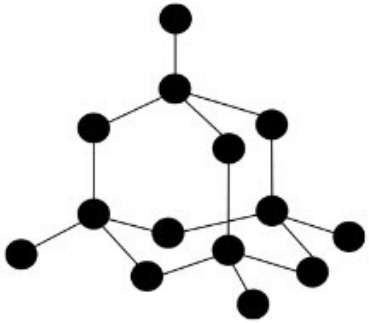
Bonding wave function

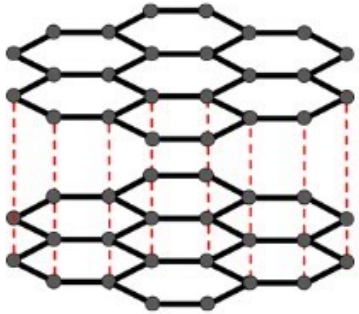

40
30
20
10
0
−10
−20
−30
−40
Energy (eV)
E_{total}
$< E >$
0
1
2
3
Proton Separation (Å)

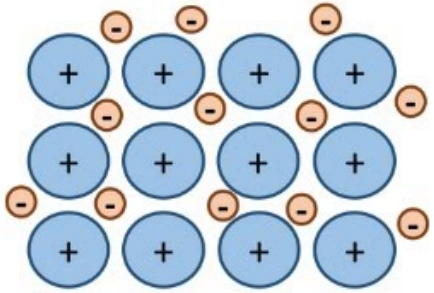
Energy

Ionic, covalent, van der Waals and metallic bonding

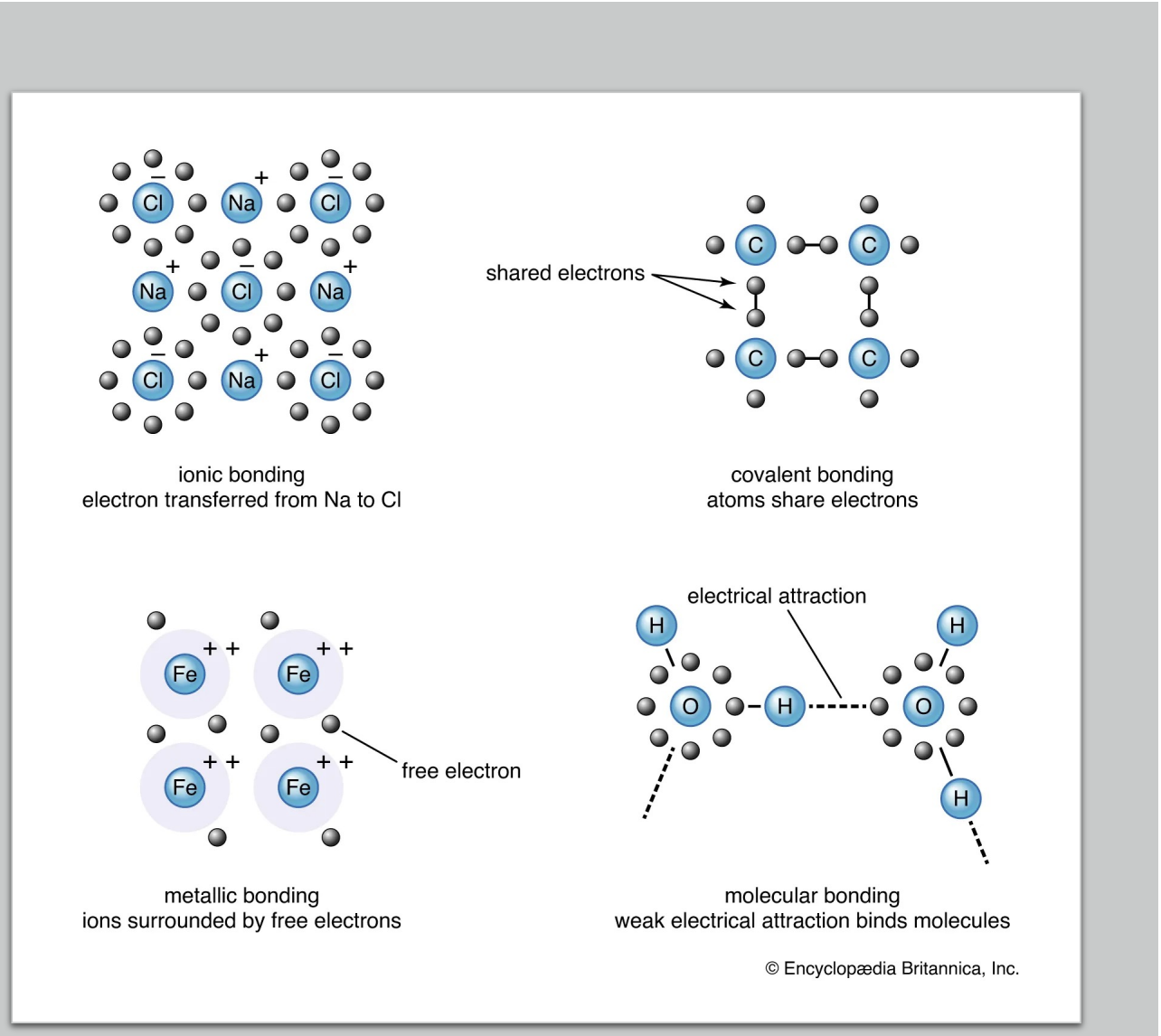




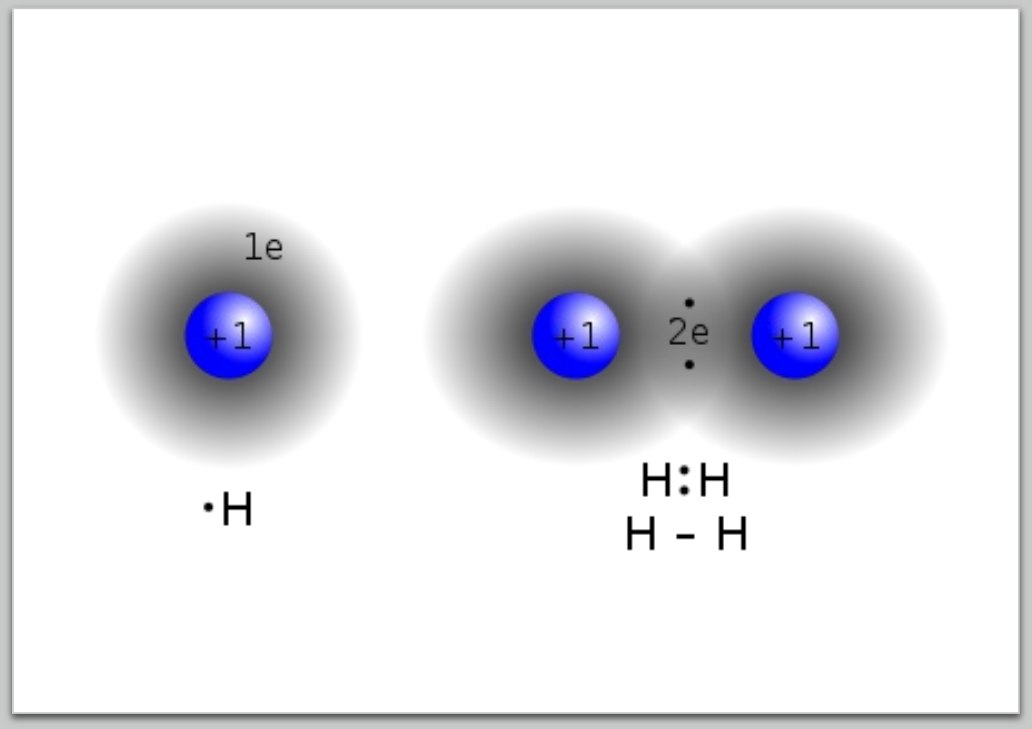


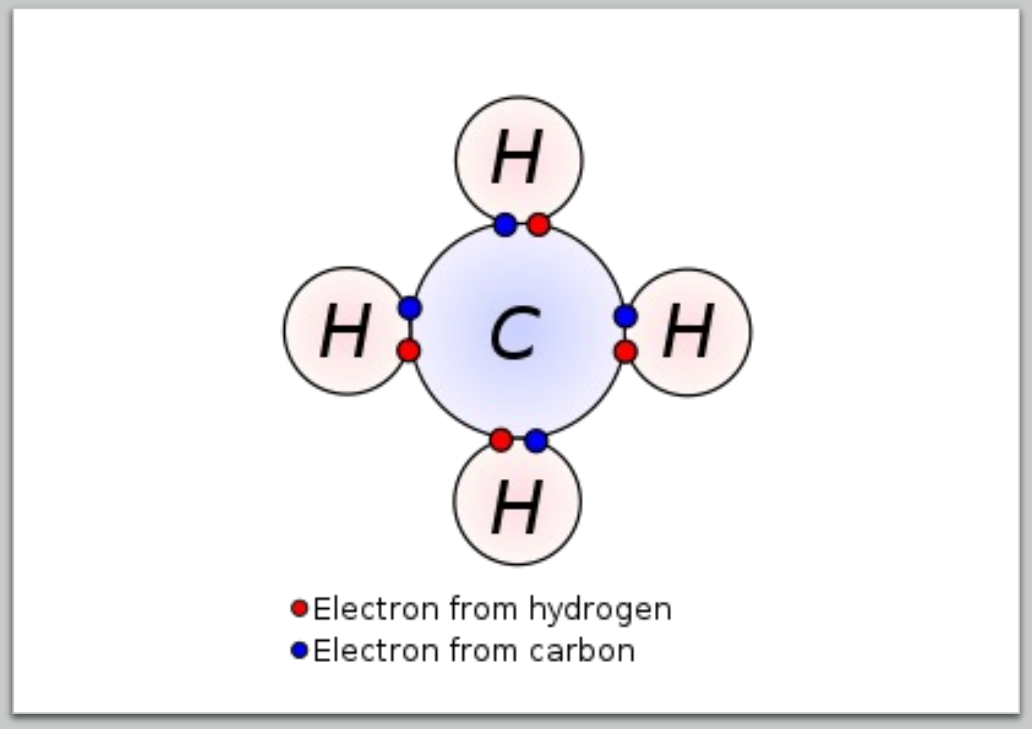


Bonding mechanisms

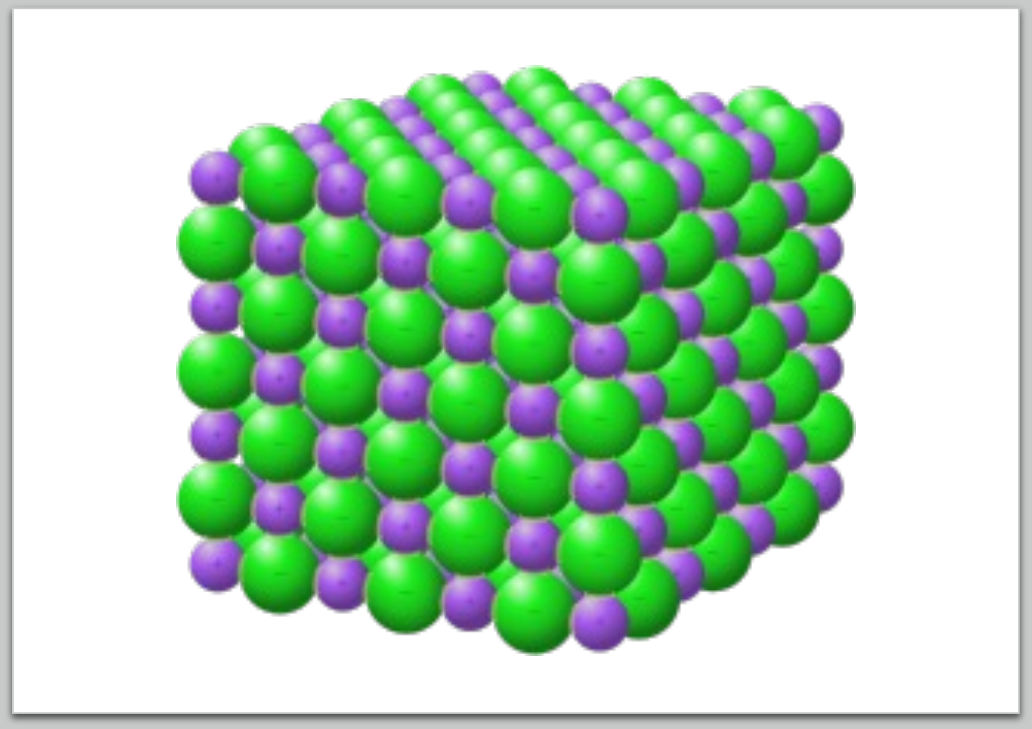


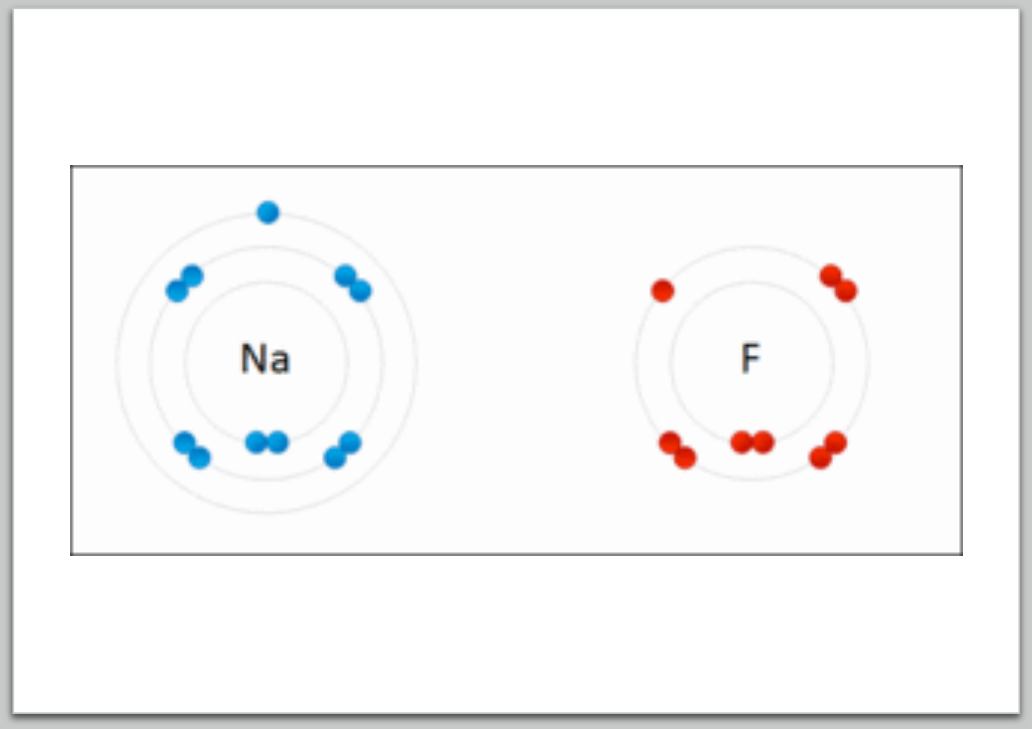
Covalent bonding



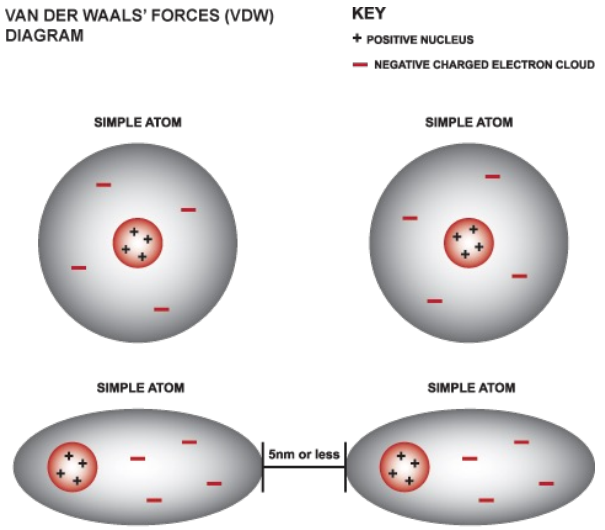


Ionic bonding

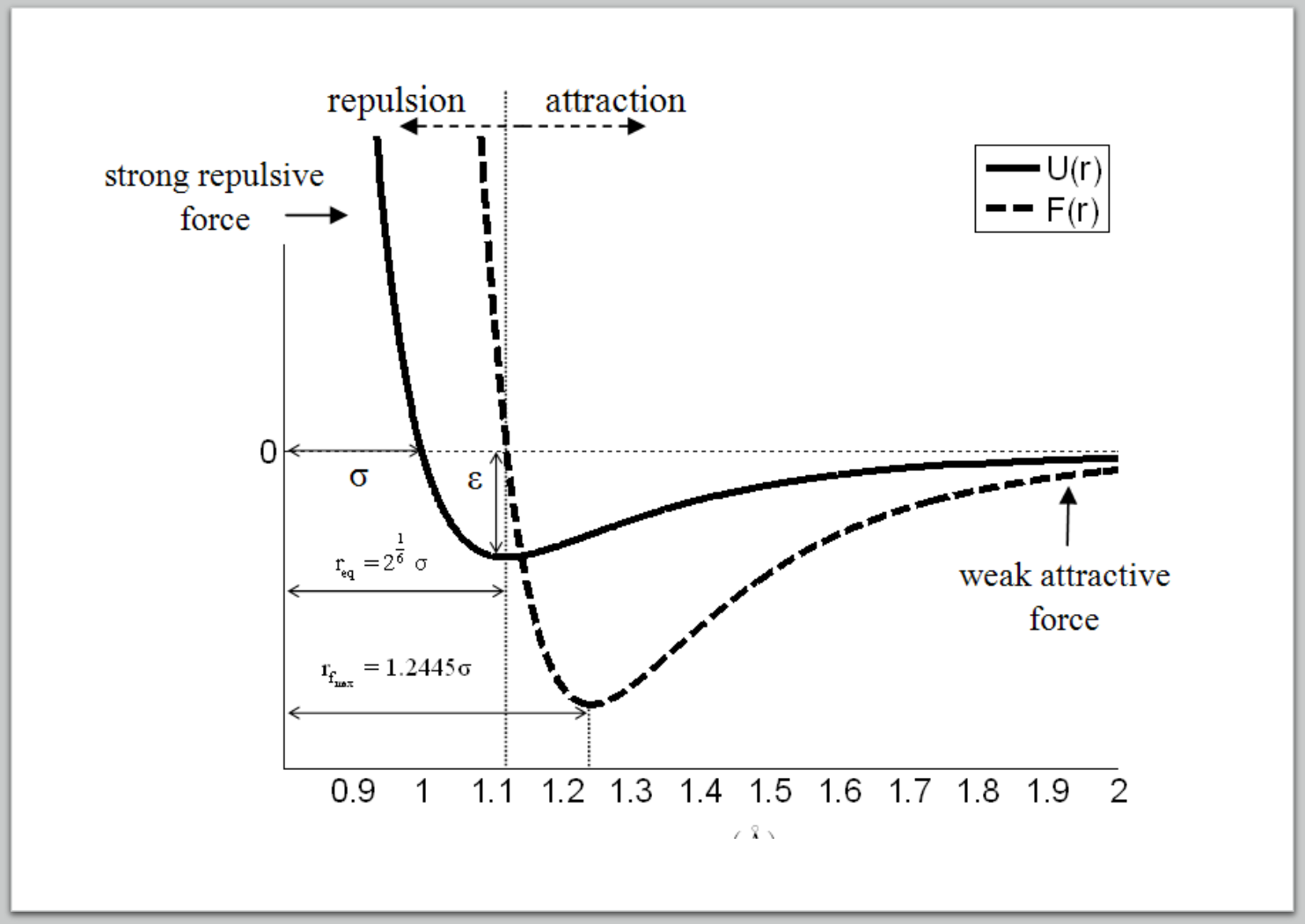




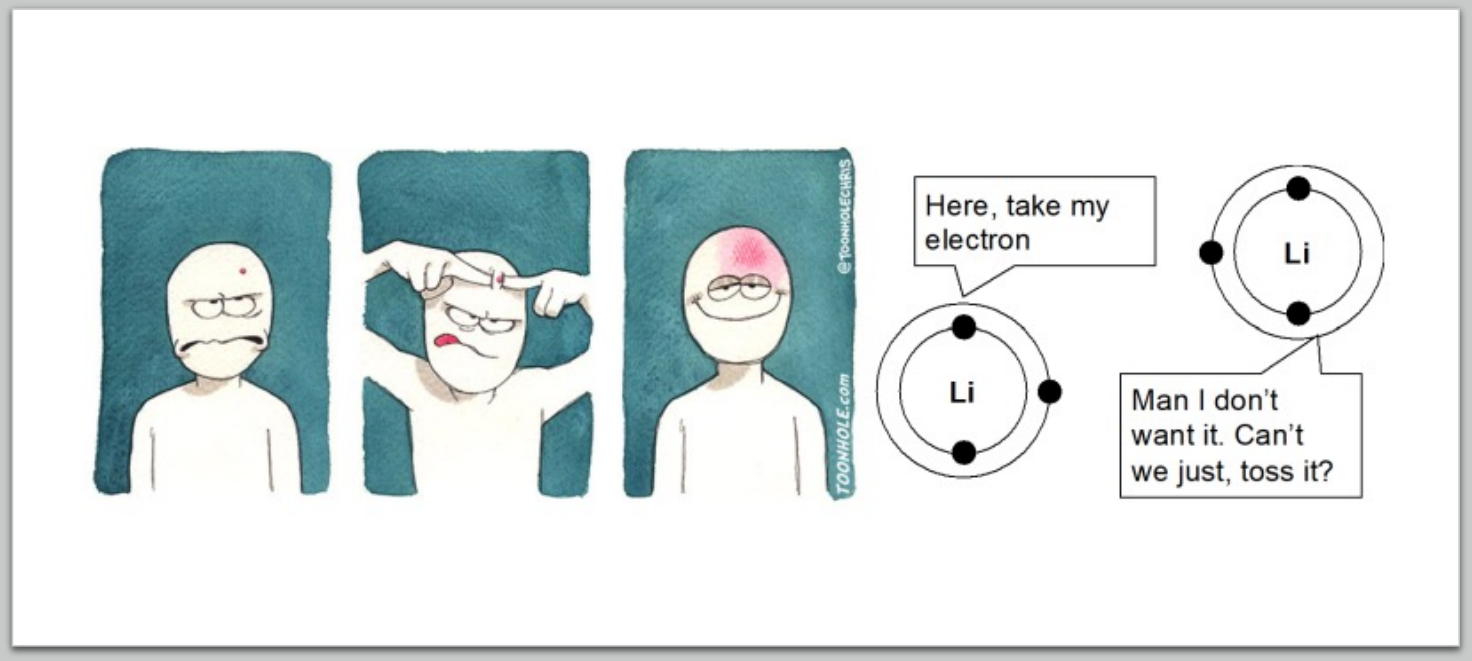
Van der Waals bonding



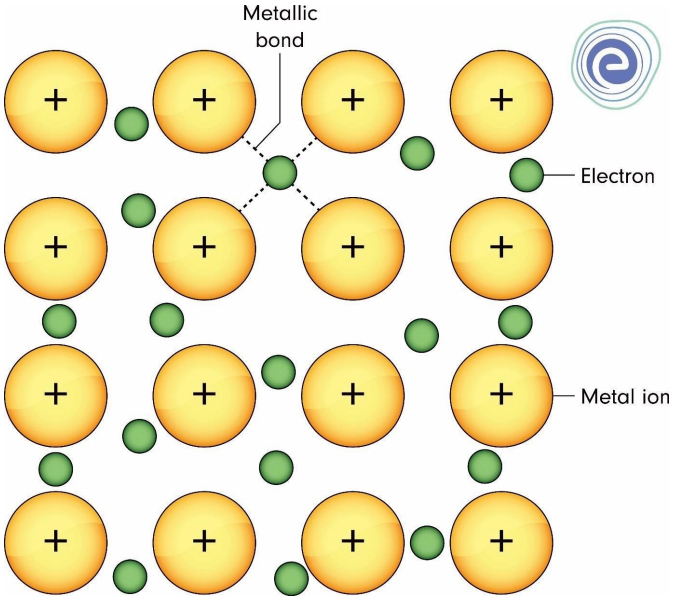
Lennard-Jones potential



Metallic bonding



Metallic bonding




Aluminum


Copper

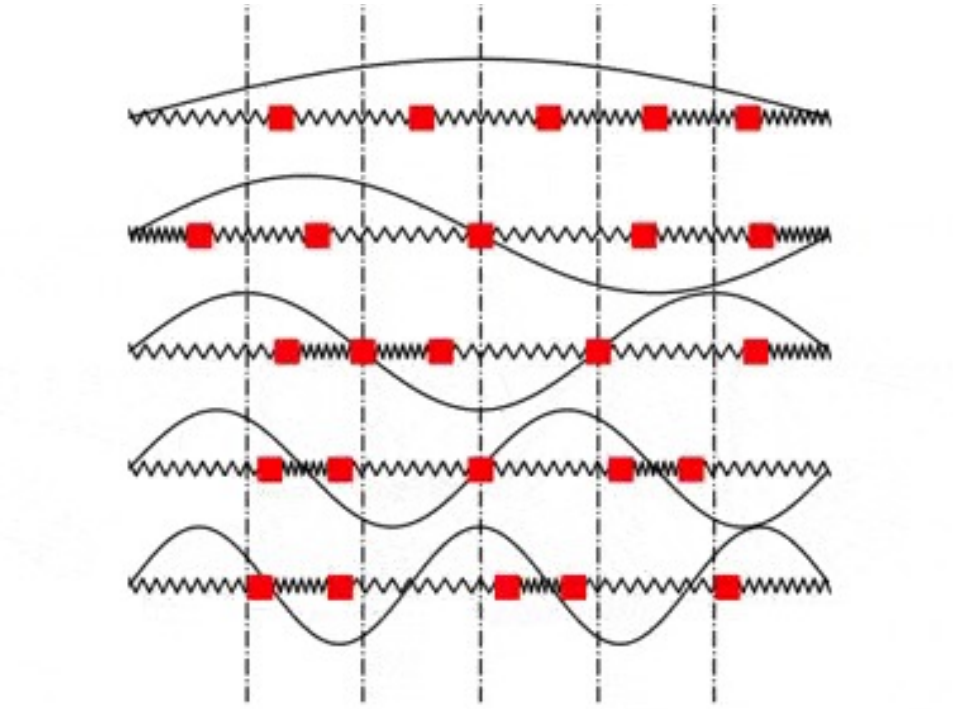

Brass


Magnesium

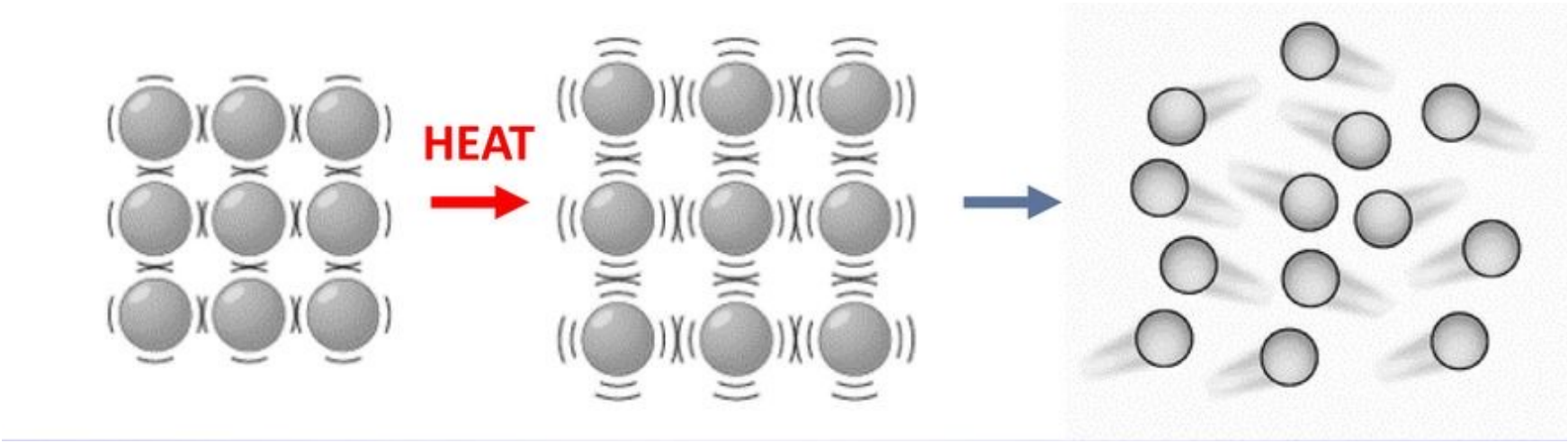

Titanium


Tungsten

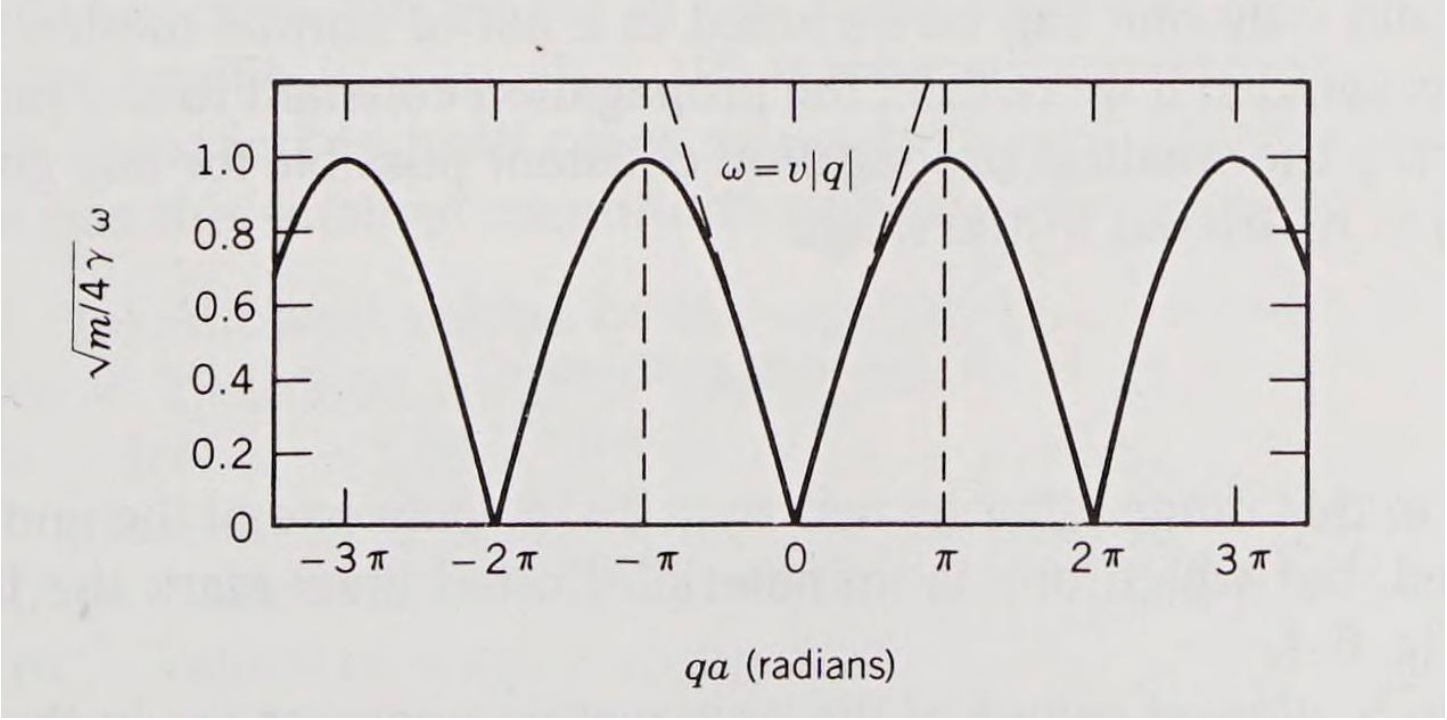
6. Vibraçoes atómicas



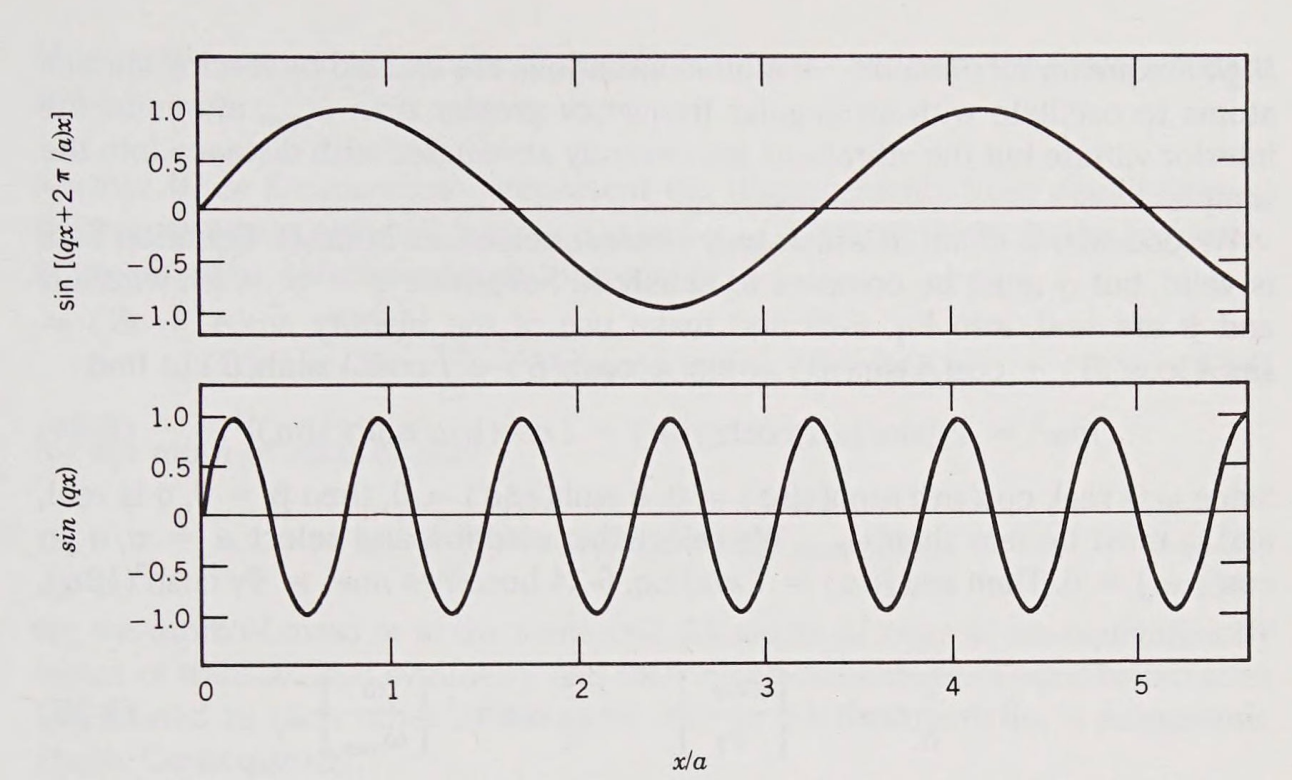
Vibrations



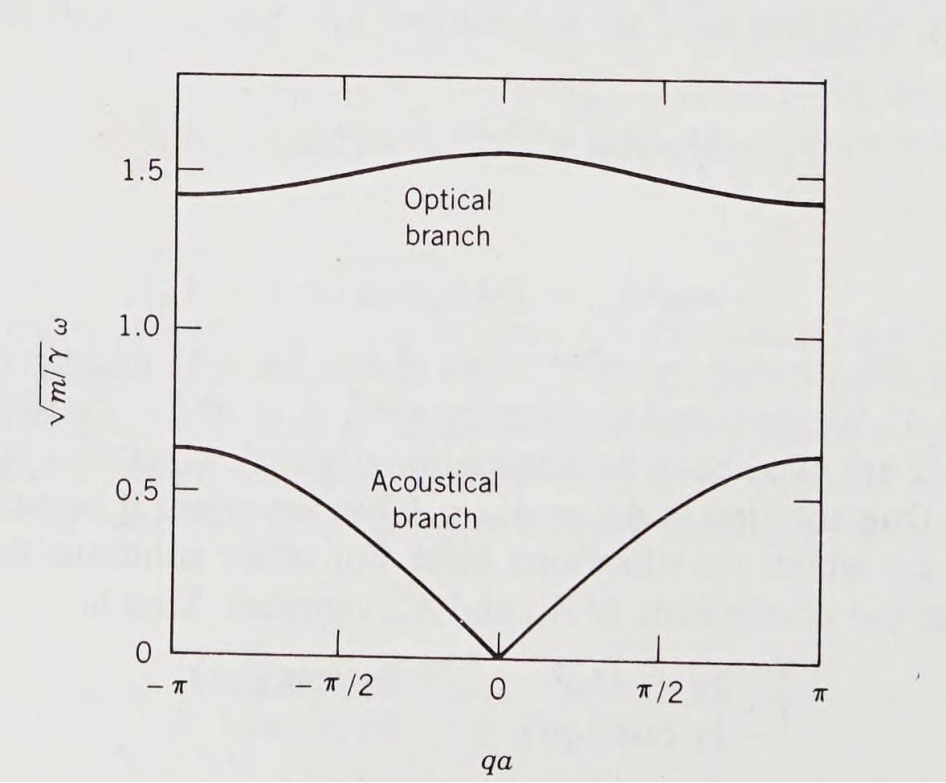
Dispersion relation: 1d lattice



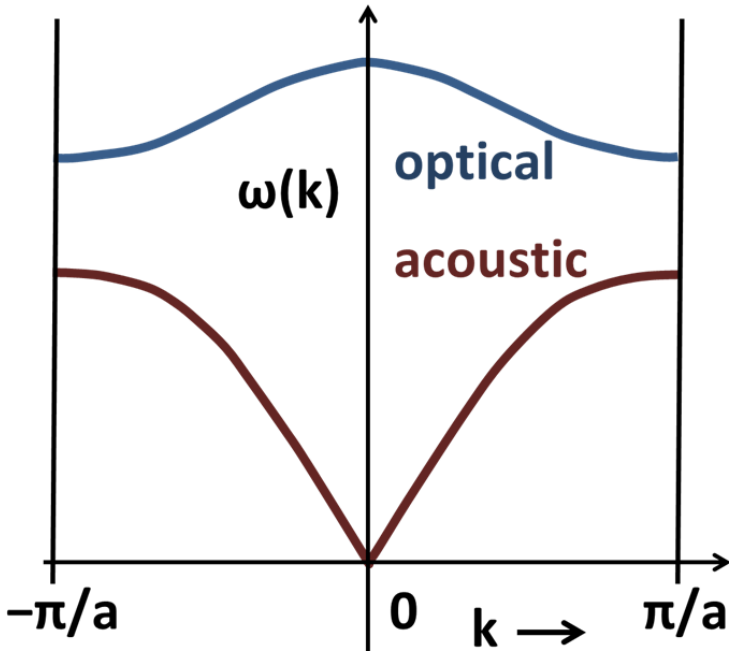
N normal modes: 1d lattice

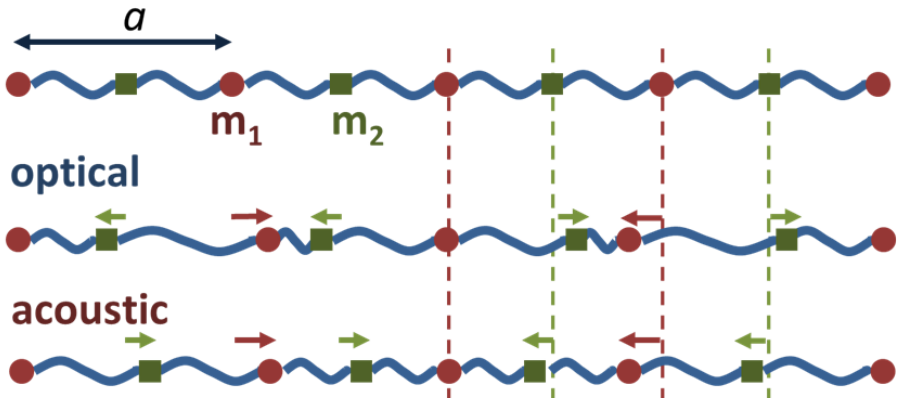


1d lattice with basis of two atoms

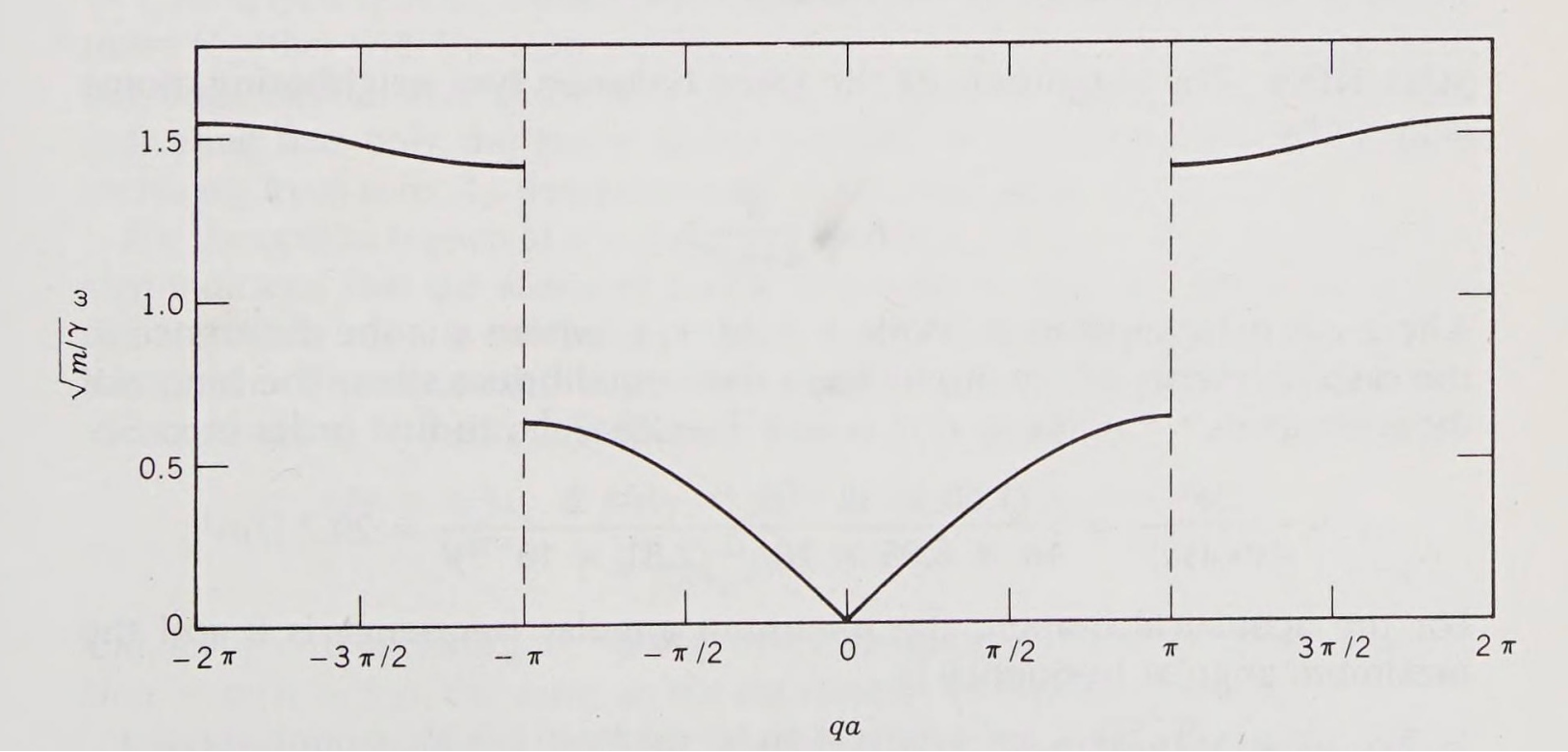


1d lattice with basis of two atoms

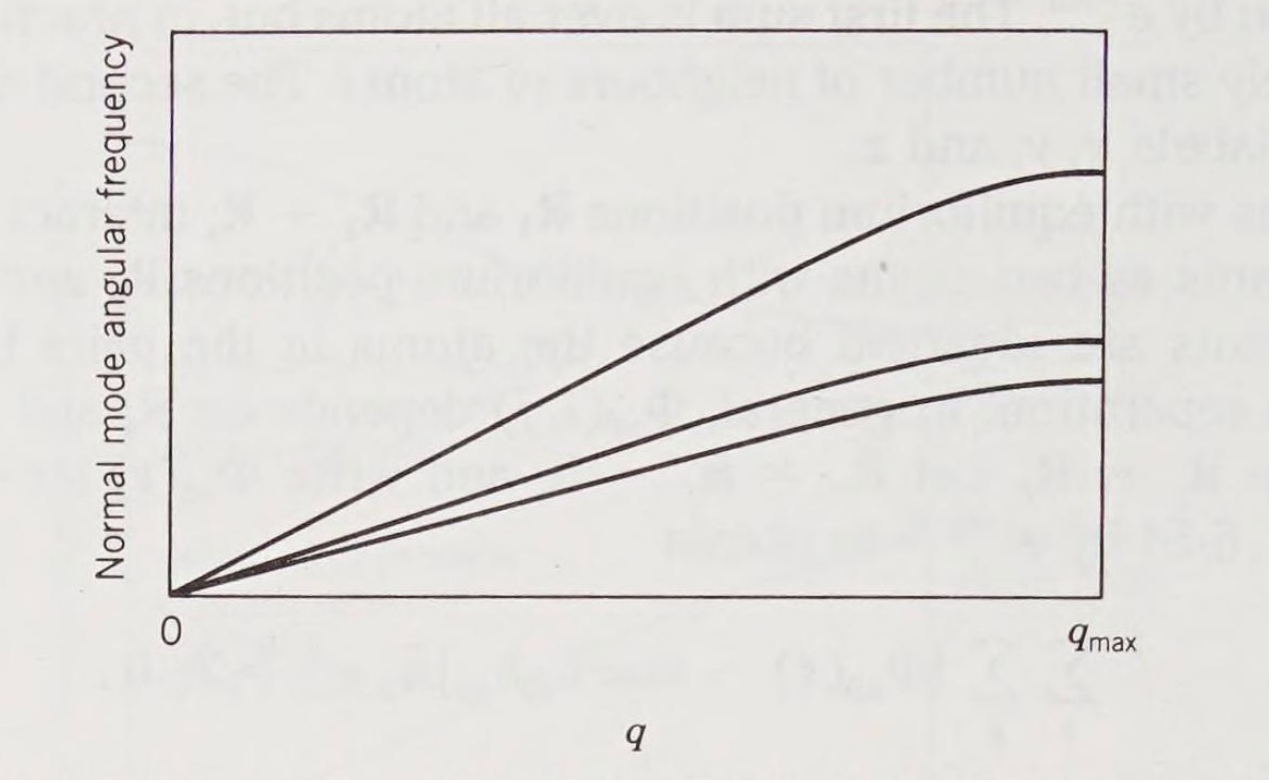




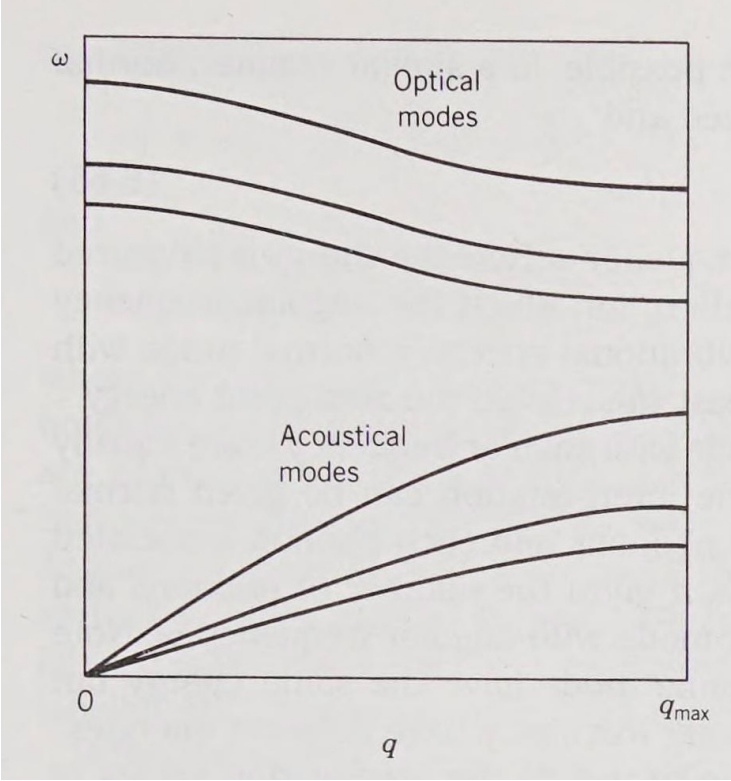
1d lattice with basis of two atoms: extended zone



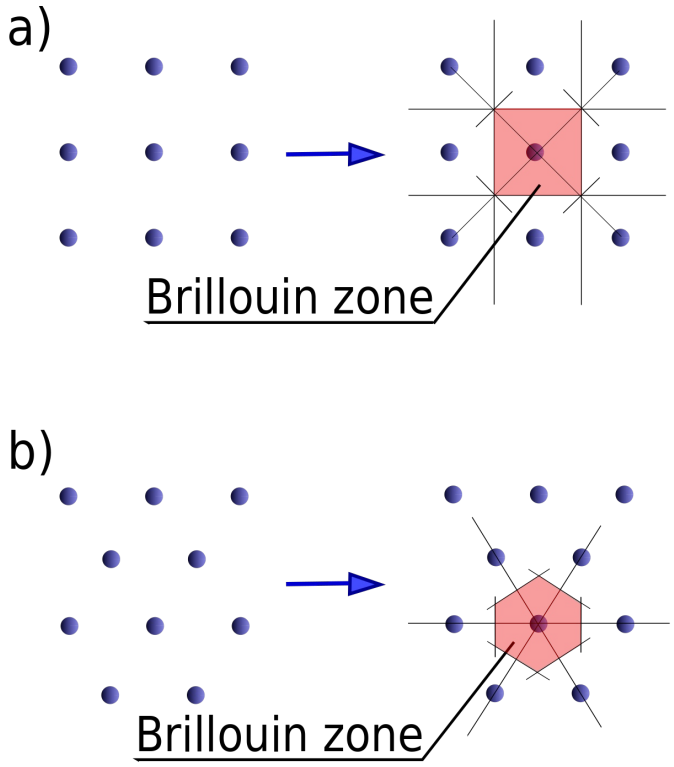
3d lattice



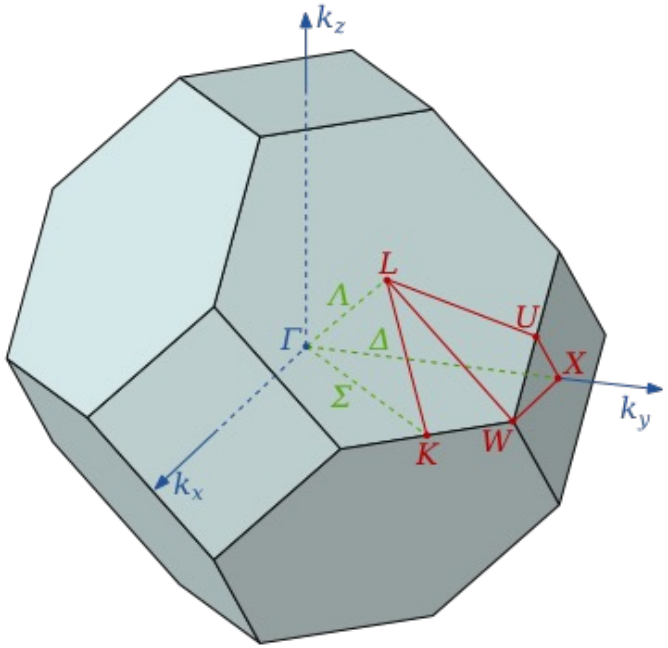
3d lattice with basis of two atoms

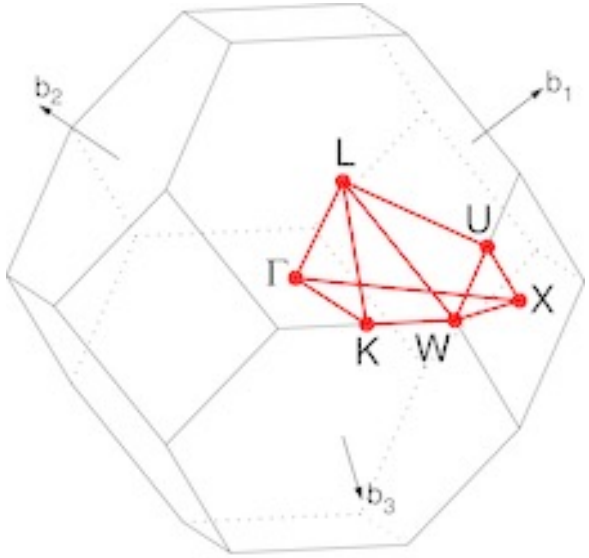


Brioullin zone



Brioullin zone

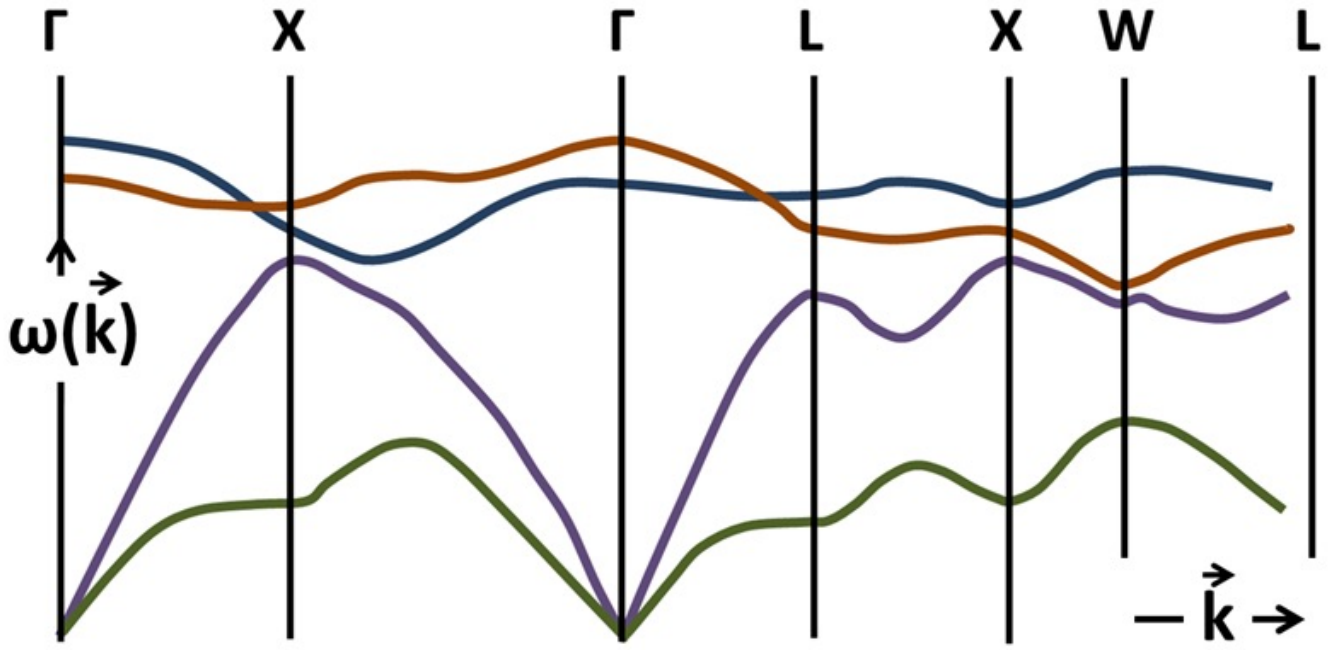




FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

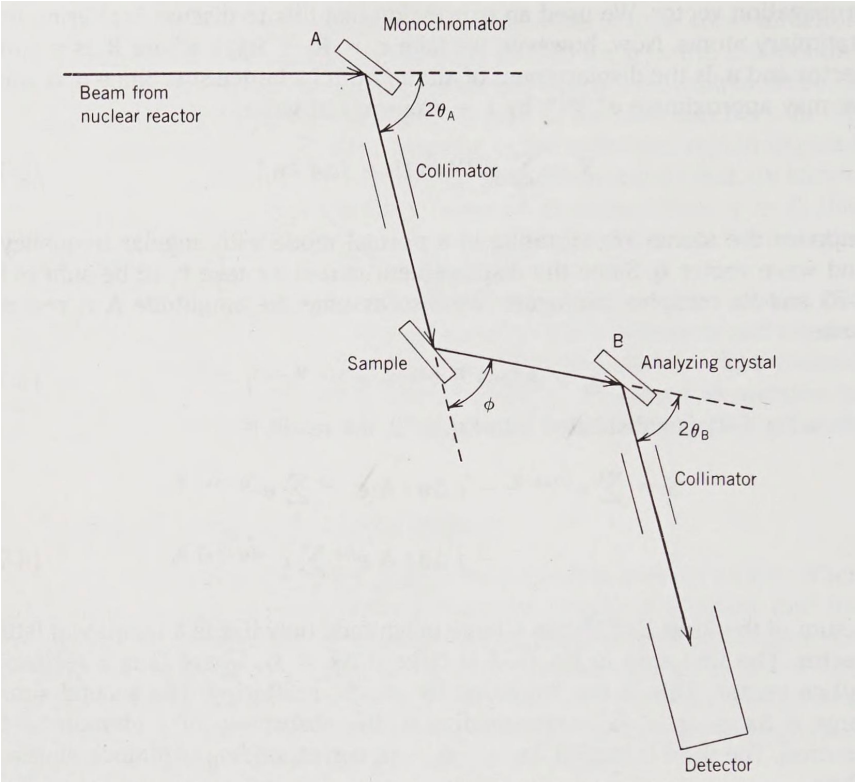
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

3d lattice with basis of two atoms

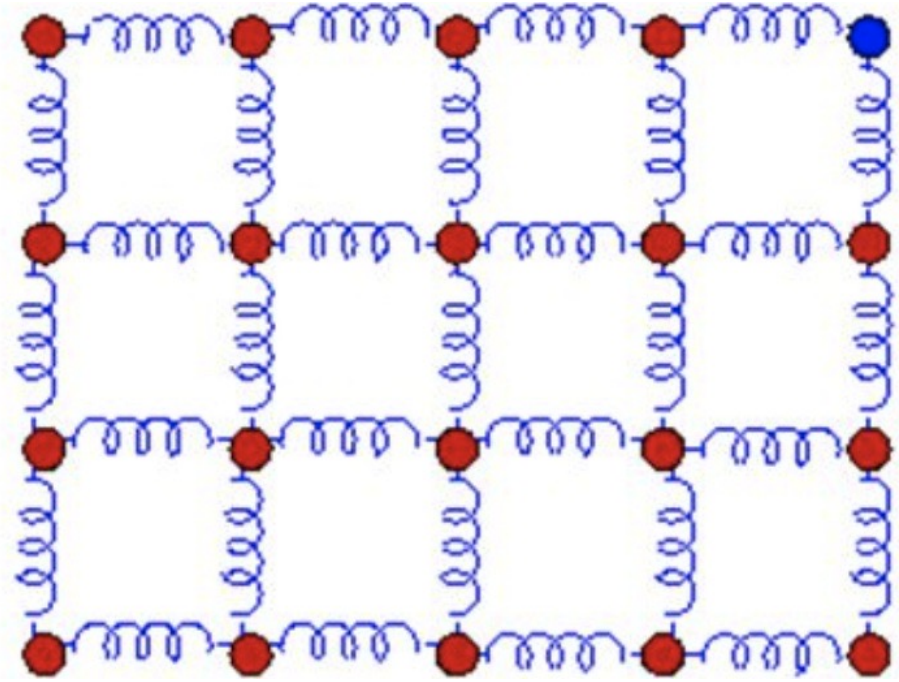


Crystal momentum

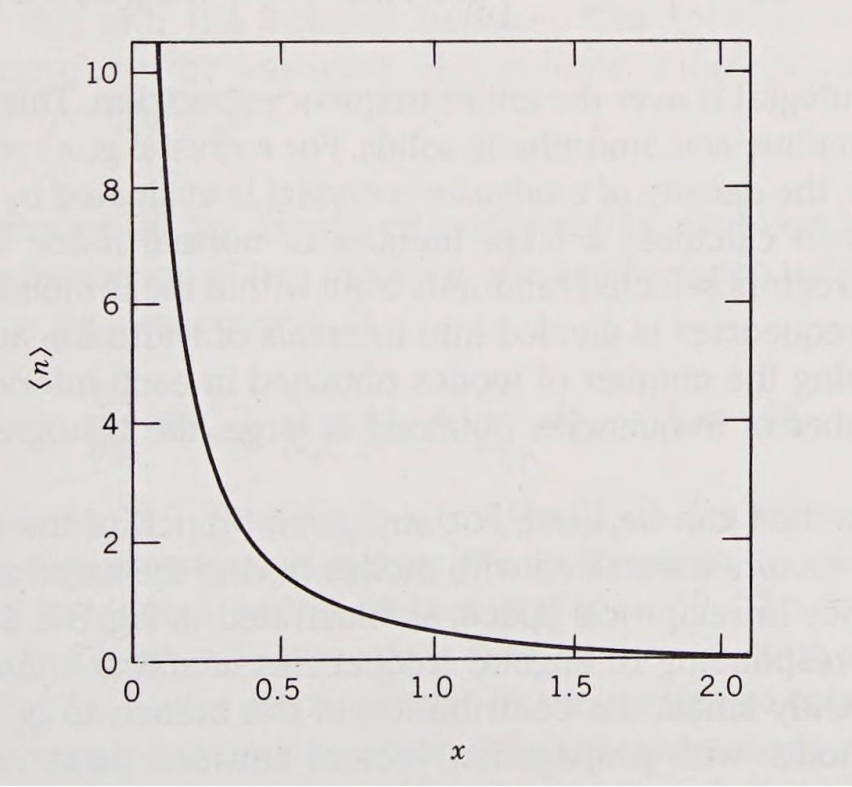
Triple axis neutron spectrometer



7. Termodinâmica de fonões



Number of phonons as a funtion of $x = \beta\hbar\omega$



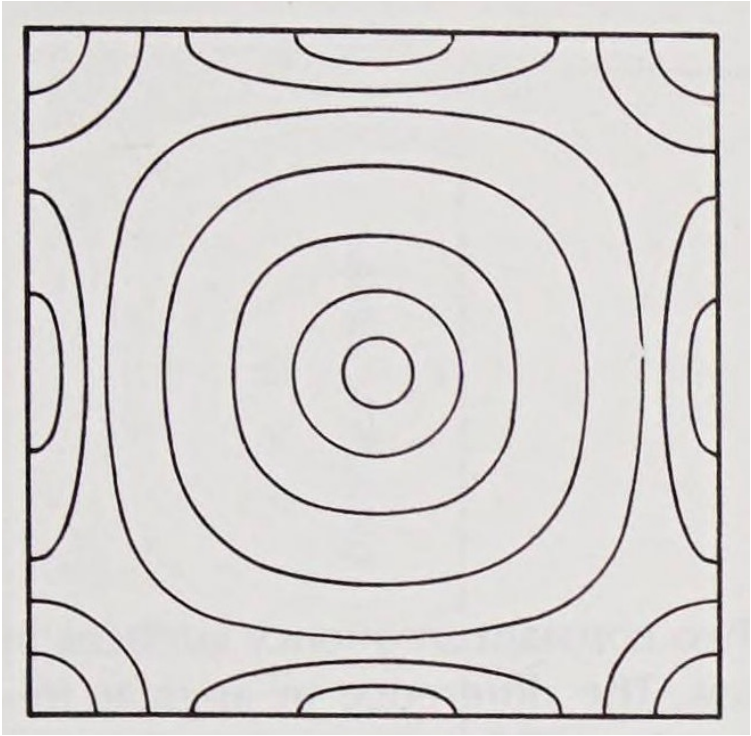
$$\langle n \rangle \longrightarrow e^{-\beta\hbar\omega}$$

$$\langle E \rangle \longrightarrow \hbar\omega e^{-\beta\hbar\omega} + \tfrac{1}{2}\hbar\omega\,,$$

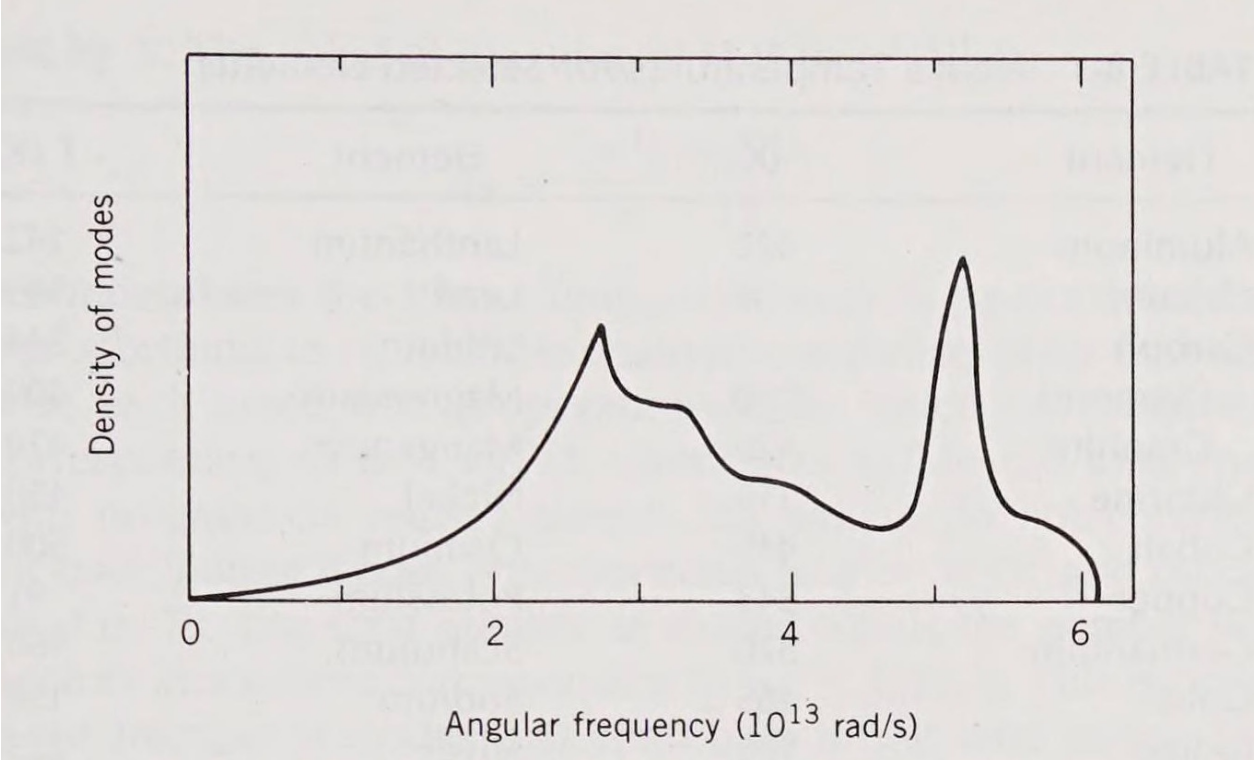
$$\langle n \rangle \longrightarrow \frac{1}{\beta\hbar\omega} = \frac{k_B T}{\hbar\omega}$$

Constant frequency surface

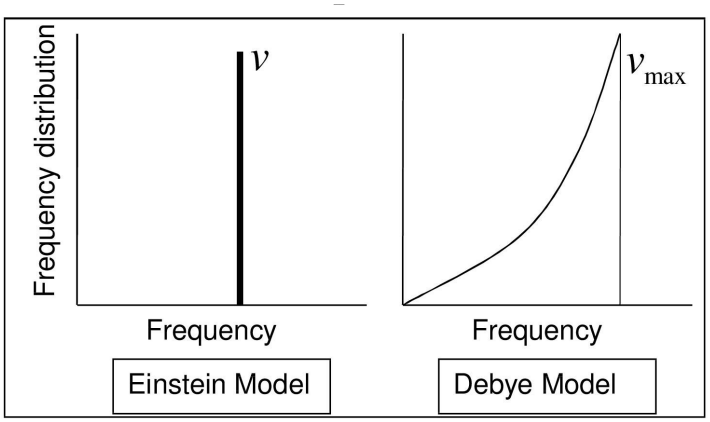
FIGURE 8-2 A schematic representation of constant frequency surfaces in reciprocal space. A Brillouin zone is shown and each contour is defined by propagation vectors such that $\omega(\mathbf{q}) = \text{constant}$. Different surfaces are associated with different values of ω.

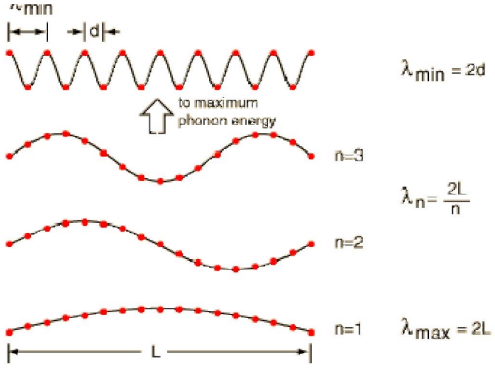


Density of modes

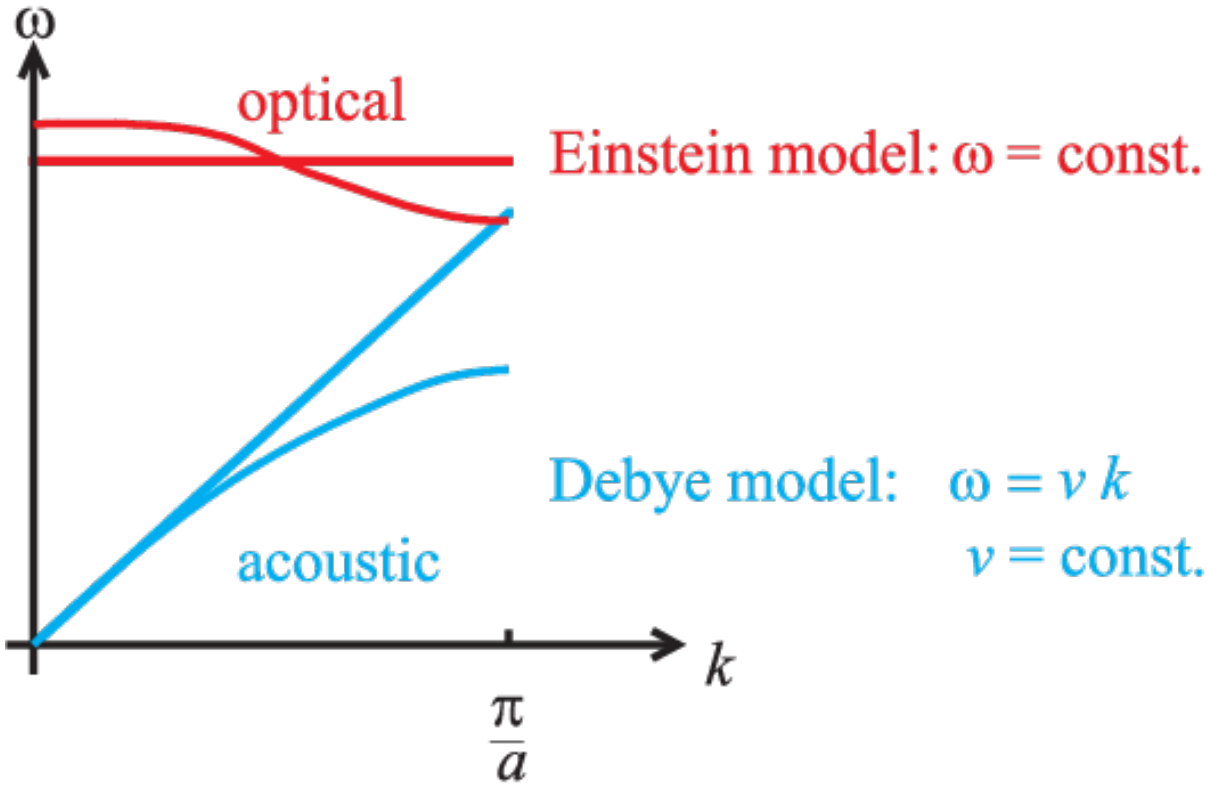


Models of Einstein and Debye

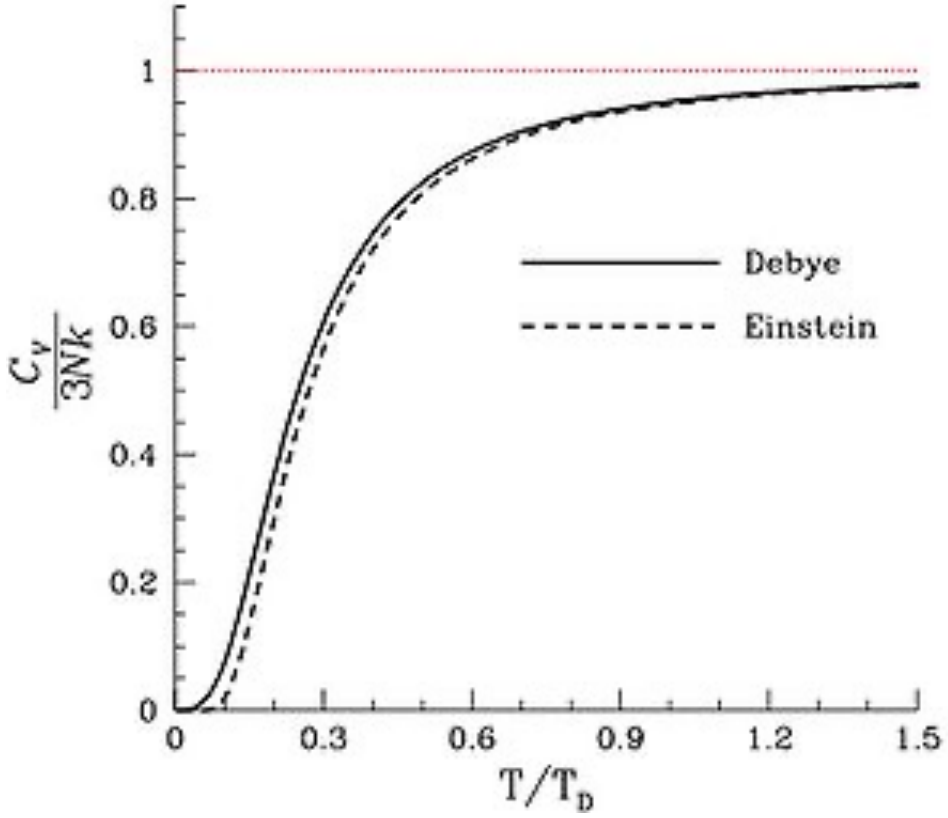




Models of Einstein and Debye



Models of Einstein and Debye



Model of Debye for various metals