UNSW AUSTRALIA

Physics 3112: Experimental & Computational Physics

T1 2025

Never Stand Still | Science | School of Physics

Eigenvalue Problems

Quantum Mechanics: Time independent Schrodinger Equation

Particles as waves --> Wave equation

- Describes the microscopic world
- Properties of materials
- Electronics

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Kinetic Energy

Potential Energy

Total Energy

$V(r), \psi(r), \qquad r = x, y, z$

Time independent: Standing waves

Input: $V(r)$

Output/Unknowns:

$E, \psi(r)$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$$

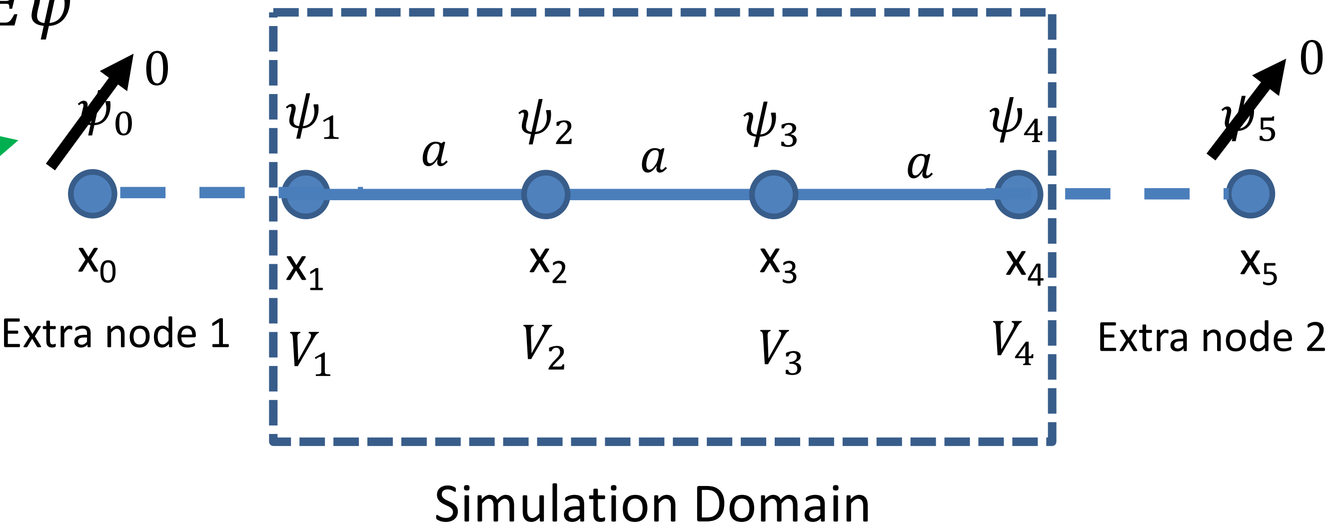
$H\psi = E\psi \longrightarrow$ Eigen value problem

$H \longrightarrow$ Hamiltonian $\quad E \longrightarrow$ Eigenvalues $\quad \psi(r) \longrightarrow$ Eigenvectors

Representing Hamiltonian (H): Finite Difference Method

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)\psi = E\psi$$

Dirichlet BC



$$t = \frac{\hbar^2}{2ma^2}$$

Matrix H

$$\begin{bmatrix} 2t+V_1 & -t & 0 & 0 \\ -t & 2t+V_2 & -t & 0 \\ 0 & -t & 2t+V_3 & -t \\ 0 & 0 & -t & 2t+V_4 \end{bmatrix}$$

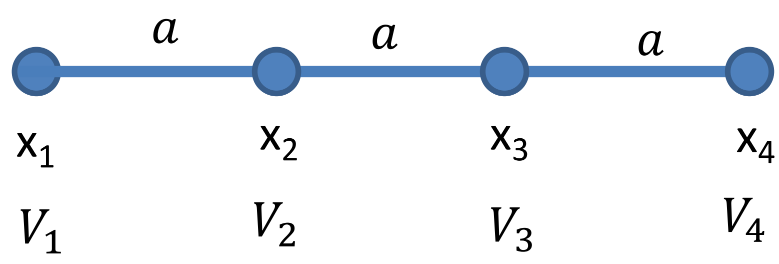
x_2 $\quad -t(\psi_3 - 2\psi_2 + \psi_1) + V_2\,\psi_2$

x_1 $\quad -t(\psi_2 - 2\psi_1 + \psi_0) + V_1\,\psi_1$

0

Defining the Potential Energy (V)

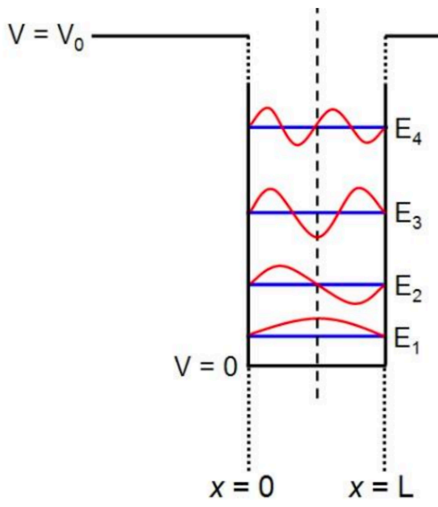
Input: A potential energy V of arbitrary shape

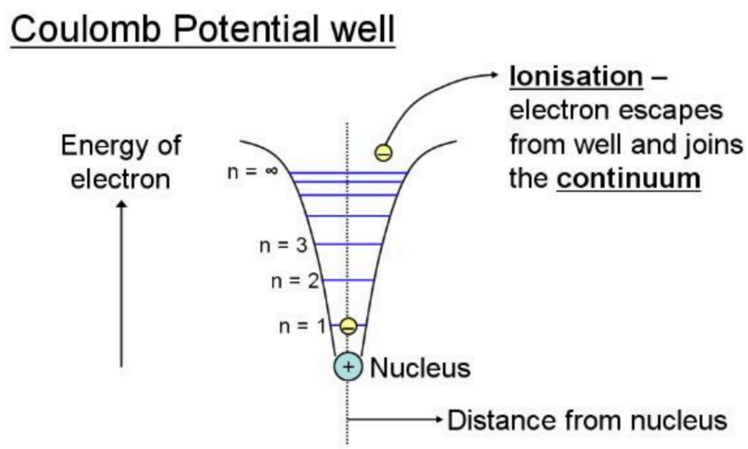


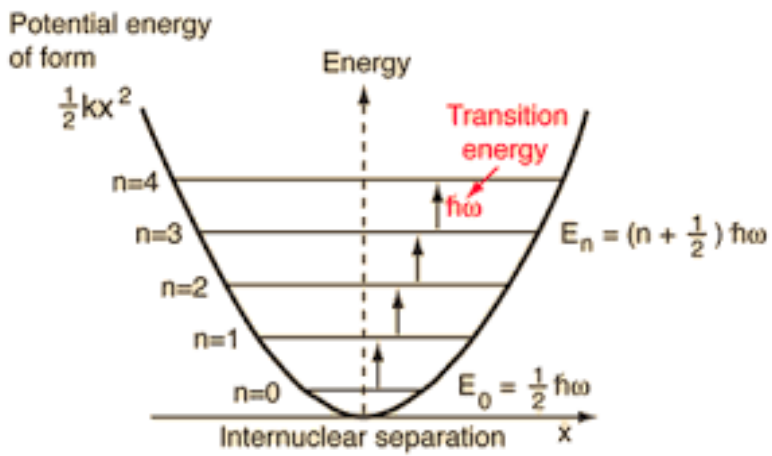
Particle in a box

Atoms

Quantum Harmonic Oscillator







https://cronodon.com/Atomic/Quantum_Measurement.html

http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc2.html

Solving the Hamiltonian (Python)

numpy.linalg.eig(*H*)

numpy.linalg.eigh(*H*)

Hermitian conjugate matrix

$$\begin{bmatrix} 2 & 1+3i \\ 1-3i & 5 \end{bmatrix}$$

Transpose and complex conjugate=original matrix

```
from numpy import linalg as LA

W, V = LA.eig(H)
```

W is an array of eigenvalues

V is a matrix of eigenvectors

V(:,j) represents the eigenvector of eigenvalue w(j)

A set of orthonormal eigenvectors: Wavefunctions

np.dot(V(:,j),V(:,j))=1

np.dot(V(:,j),V(:,k))=0

N x N Hamiltonian

Jth-wavefunction

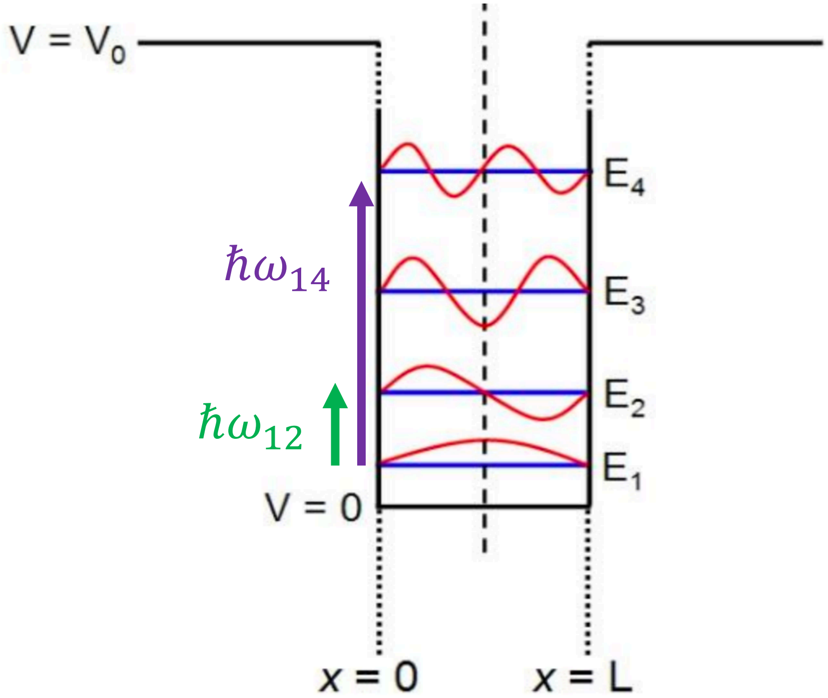
$$\begin{bmatrix} \psi_{1,j} \\ \psi_{2,j} \\ \vdots \\ \psi_{N,j} \end{bmatrix}$$

probability

$$\begin{bmatrix} |\psi_{1,j}|^2 \\ |\psi_{2,j}|^2 \\ \vdots \\ |\psi_{N,j}|^2 \end{bmatrix}$$

Using the Wavefunction

Particle in a box



Transitions between different levels induced by a photon

$$E_j - E_i = \hbar\omega_{ij} = hf_{ij}$$

Various properties can be obtained from wavefunctions.

Expectation values: $\langle \psi_i | A | \psi_j \rangle$

Integral form: $\int_{-\infty}^{+\infty} \psi_i^*(x) A \psi_j(x) dx$

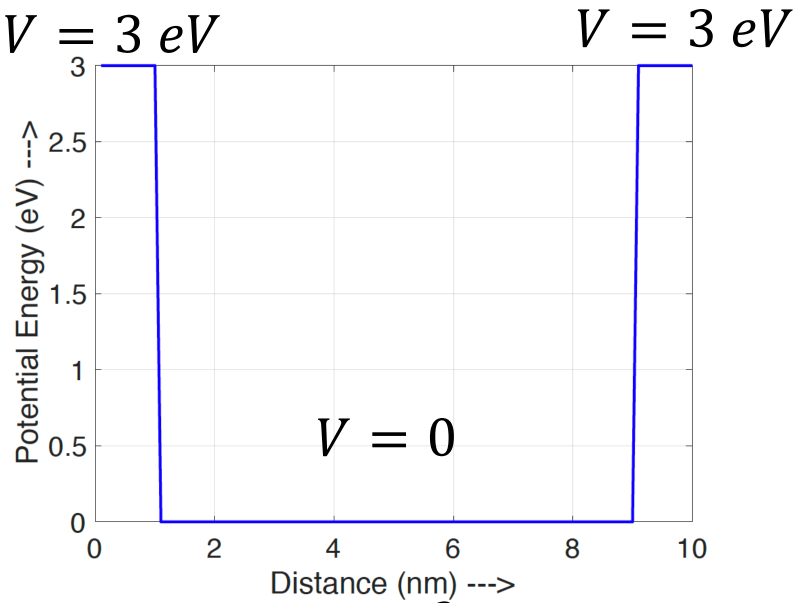
Discretized form: $\sum_{k=1}^{N} \psi_i^*(x_k) A \psi_j(x_k) \Delta x$

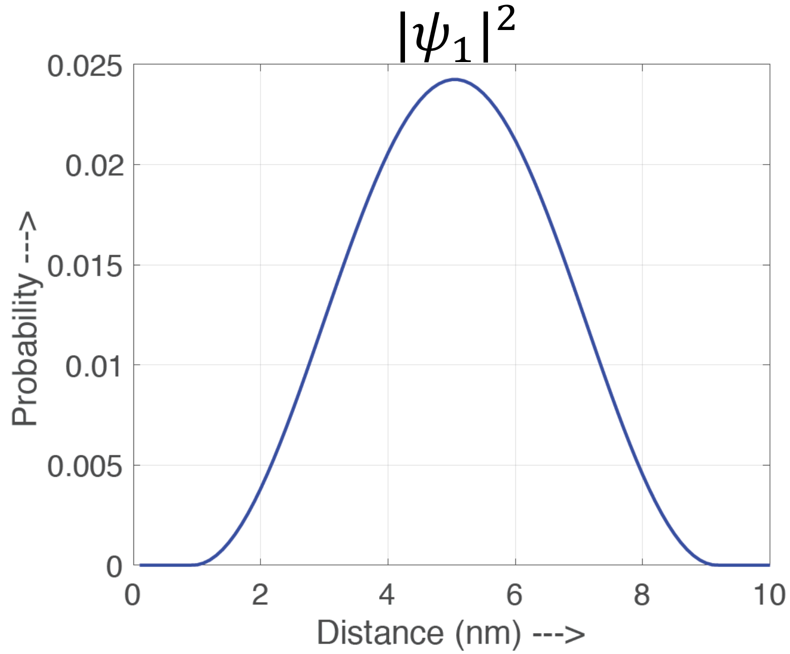
Example: Optical Dipole $\langle \psi_i | x | \psi_j \rangle$

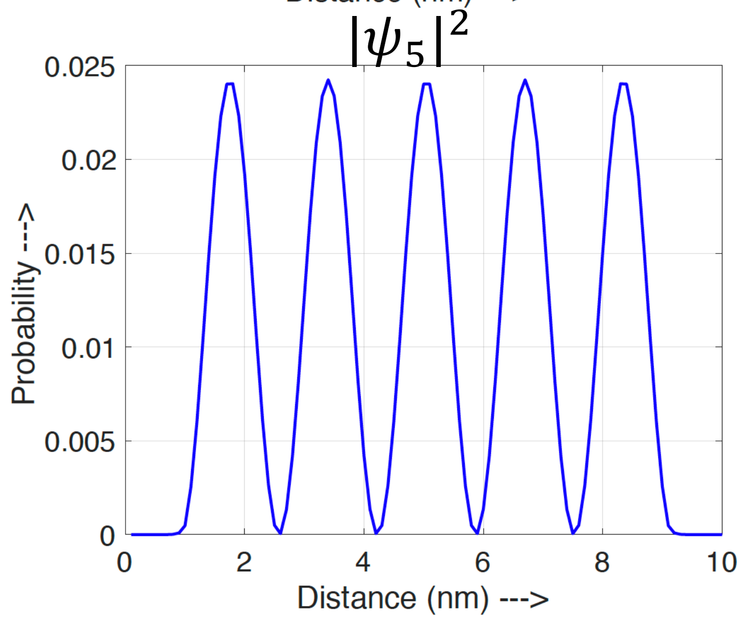
Gives a transition probability by a photon --> a selection rule.

$$\sum_{k=1}^{N} \psi_i^*(x_k) x_k \psi_j(x_k) \Delta x$$

Example - Particle in a box: A case of atoms







E_1=0.0055 eV E_5=0.1380 eV

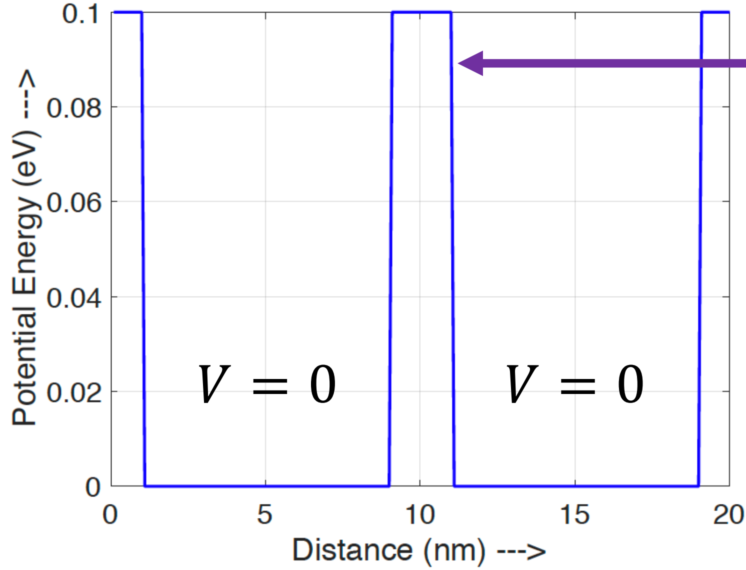
$$E_5 - E_1 = hf_{15} = 132.5\ meV$$

$$f_{15} = 32\ THz$$

Reality: 3D Coulomb potential from nuclear charge (3D confinement by 1/r)

Particle in coupled boxes: Molecules (Small tunneling)

$V = 0.1\ eV$ $\quad 0.1\ eV$ $\quad 0.1\ eV$



Large barrier (no/small tunneling)

E_1=0.0044 eV $\qquad$ E_5=0.0045 eV

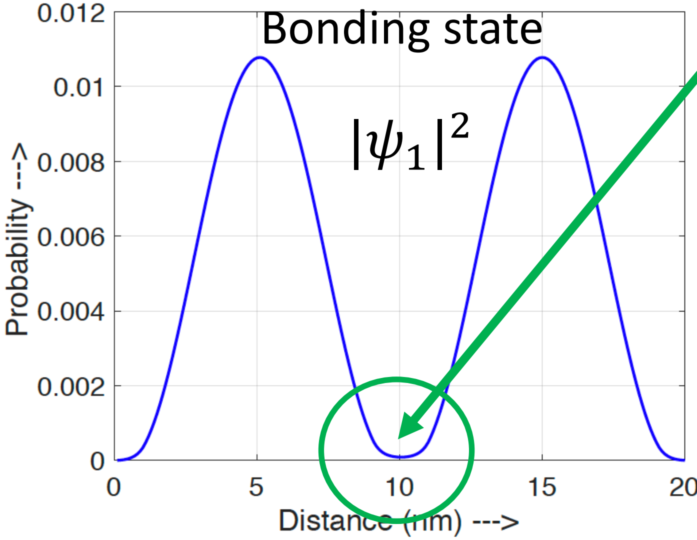
$$E_2 - E_1 = 0.1\ meV$$

~ 0 probability in between

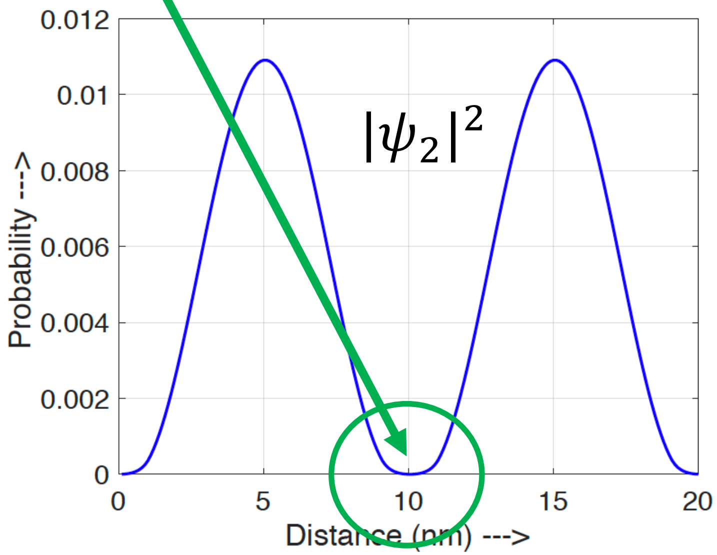
Monatomic or inert molecules.

Electrons bound to atoms, but not shared with other atoms.

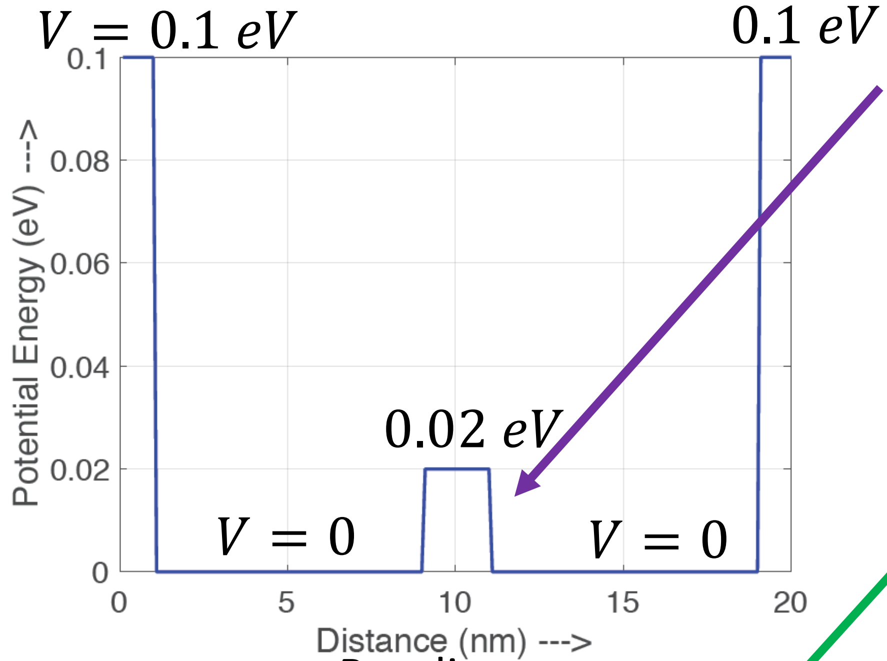
Bonding state



Anti-bonding state



Particle in coupled boxes: Molecules (Large tunneling)

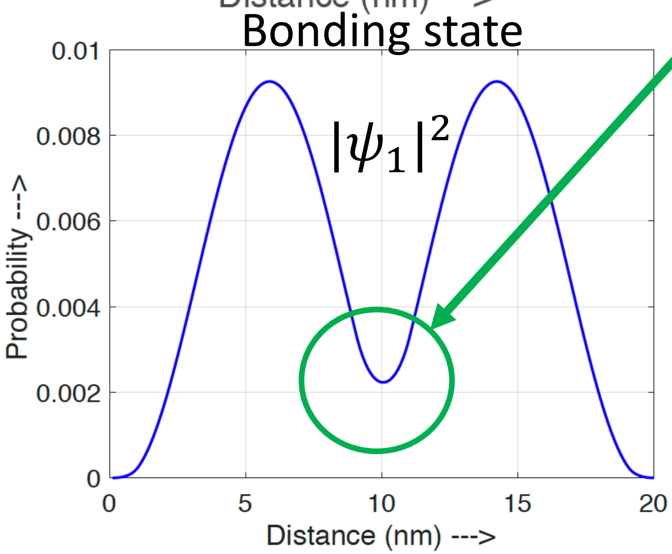


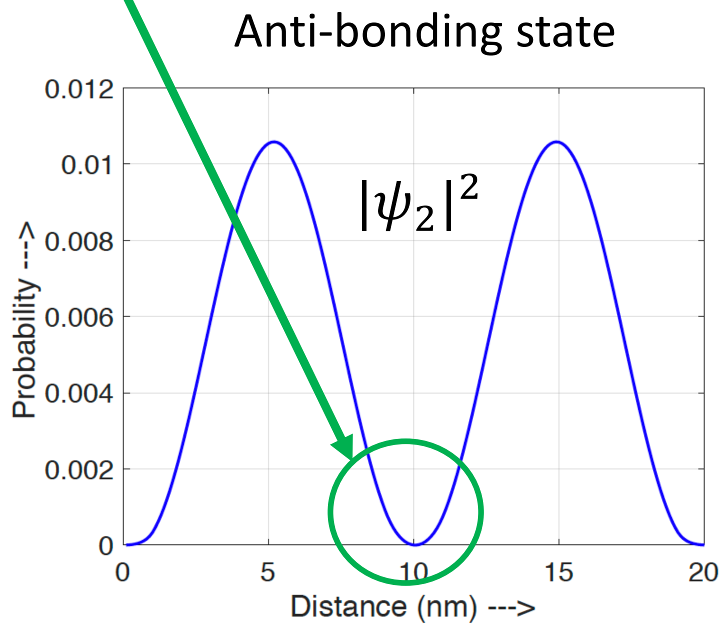
Small barrier (Large tunneling)

E_1=0.0032 eV E_5=0.0042 eV

$$E_2 - E_1 = 1\ meV$$ Larger Splitting

~ B-state has probability, AB state does not

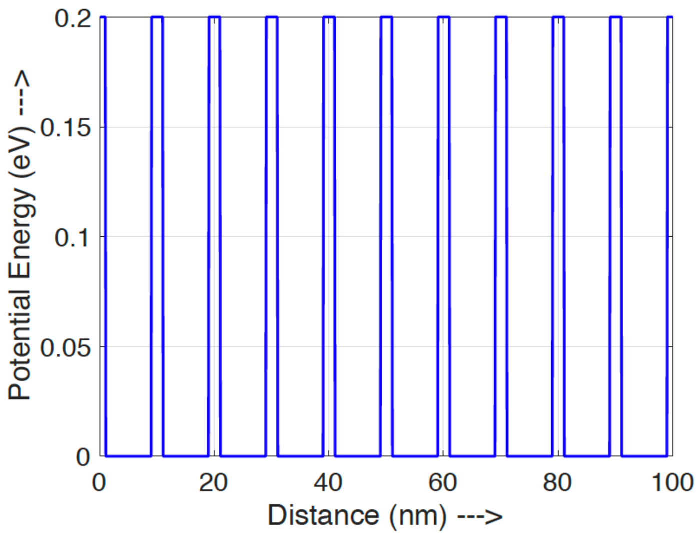


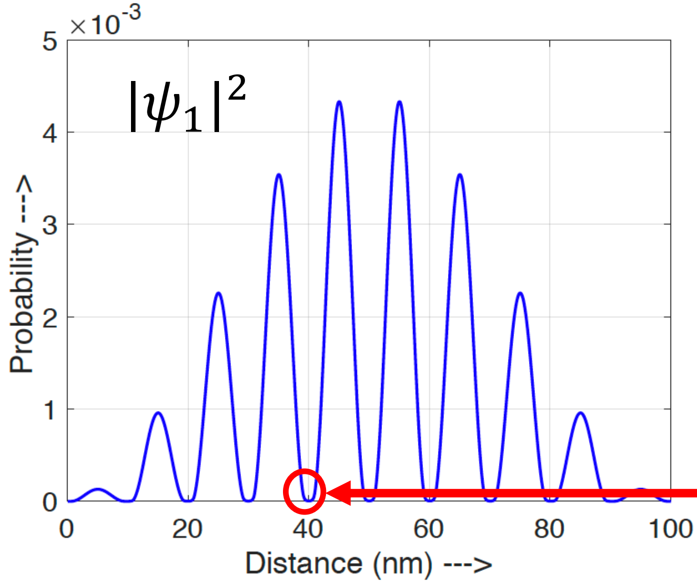


Covalent Bonding: Electrons shared between atoms.

(Molecular states H_2)

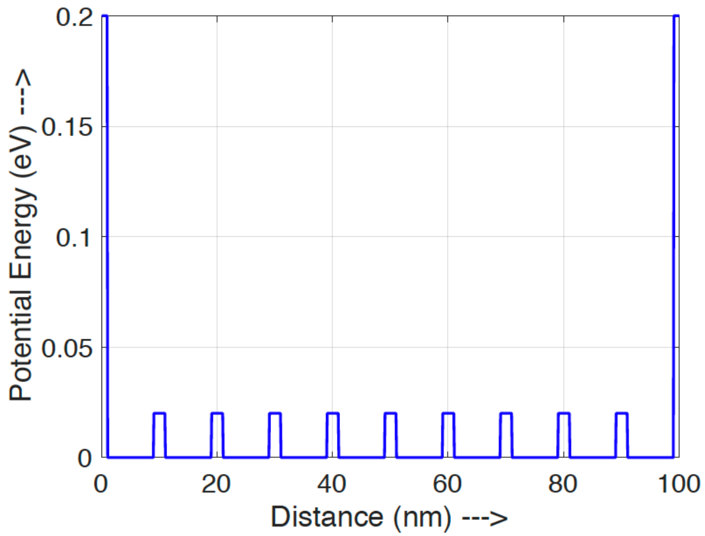
Many Boxes – Model of Solids (Large vs Small Barriers)

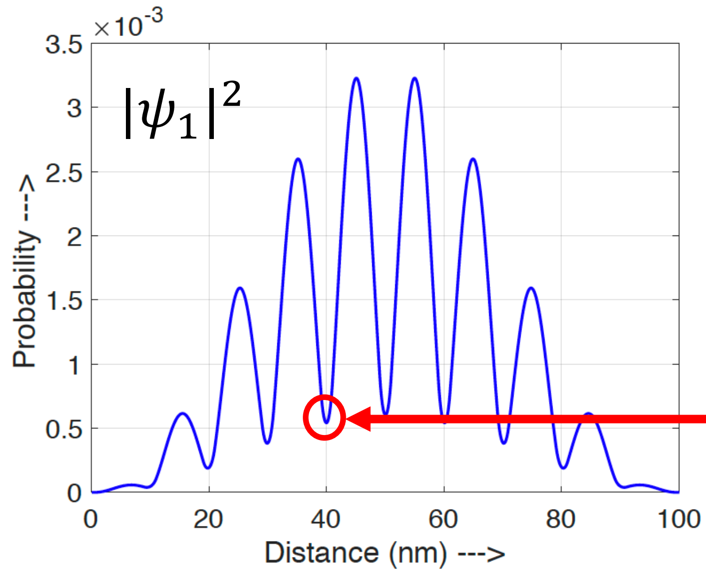




Insulators (electrons localized)

No tunneling





Metals (electrons delocalized)

Large tunneling

Schrodinger Equation in a Solid Material

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Effective Mass Schrodinger Equation

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi + V\psi = (E_c - E)\psi$$

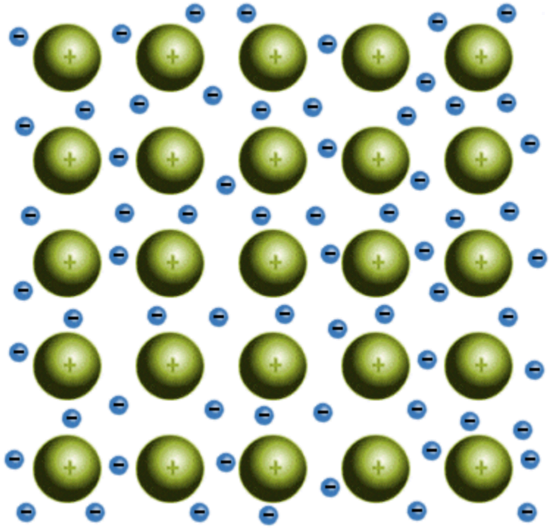
Effective mass

Band edge (conduction)

E_C and m* vary from material to material

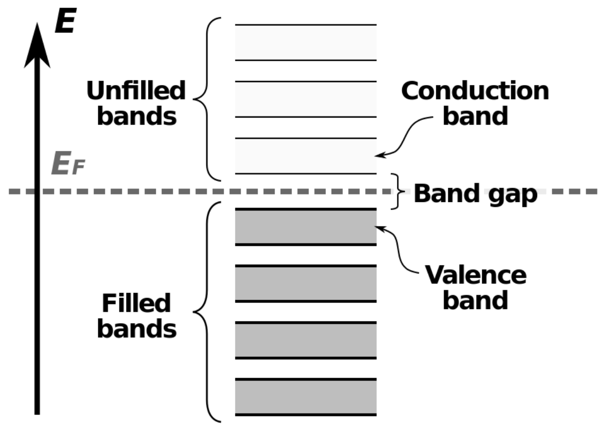
More than 1 material: Generalize

$$-\frac{\hbar^2}{2}\nabla\frac{1}{m^*(r)}\nabla\psi + V\psi = (E_c(r) - E)\psi$$



http://www.technologyuk.net/science/matter/metallic-solids.shtml

Mass of electrons modified m*



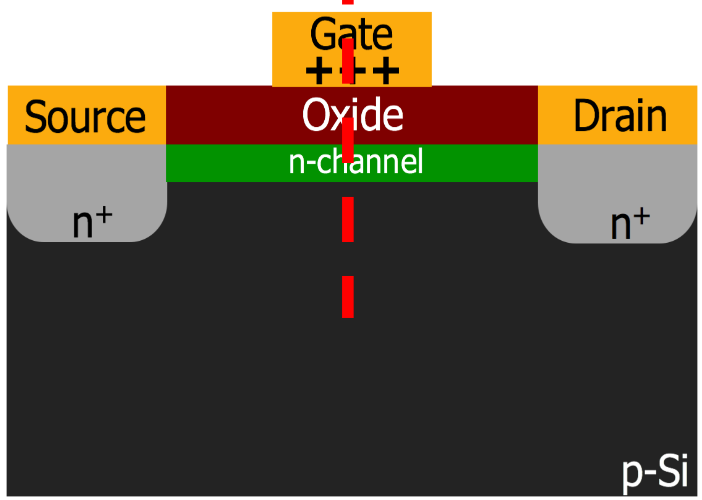
Semiconductor band structure
https://en.wikipedia.org/wiki/Valence_and_conduction_bands

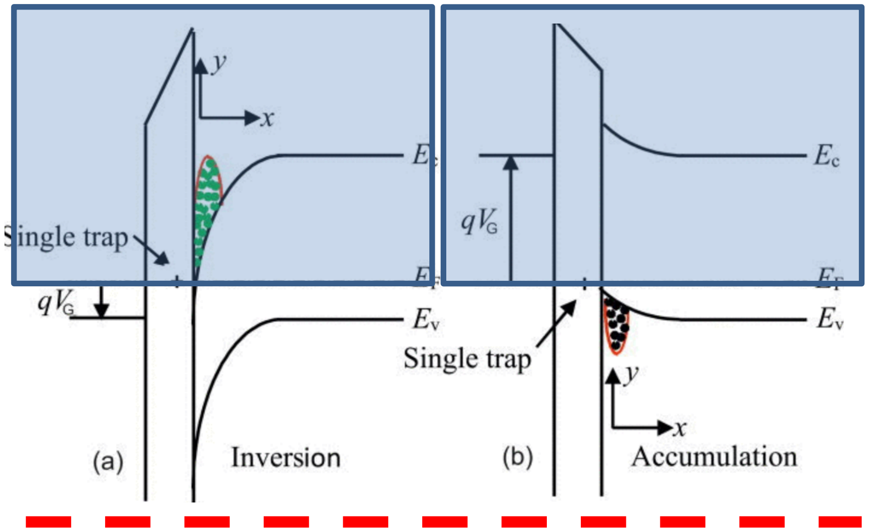
Energy appears in bands

conduction and valence bands

Modern Electronics & The Schrodinger Equation

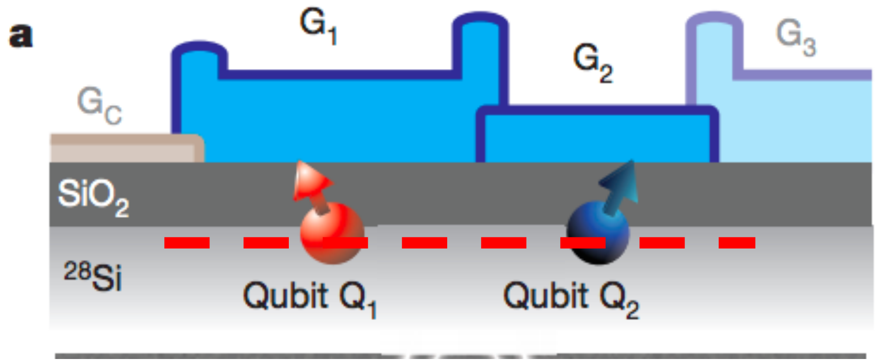
MOS Transistor (Integrated Circuits)



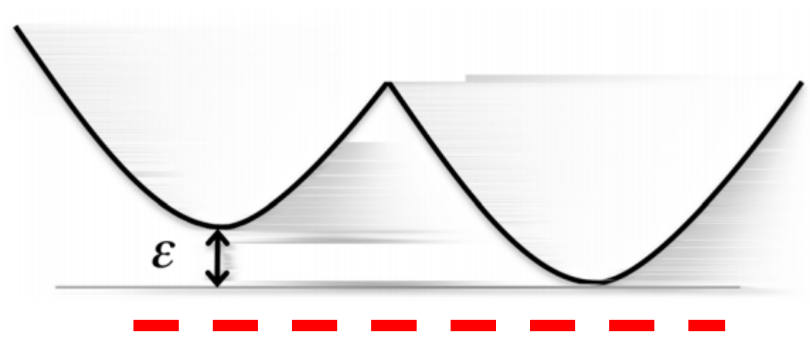


https://electronics.stackexchange.com/questions/380077/mos-capacitor-band-edges

Quantum Dot Qubits: Quantum Computing



Veldhorst/Dzurak Nature (2015).
https://www.nature.com/articles/nature15263



Model: Double parabola shifted in energy.