# Chapter 6

## The Schrödinger Equation

# The Schrödinger Equation

Wave equation of E&M wave $$\frac{\partial^2 \xi}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 \xi}{\partial t^2}$$

$$\xi(x,t) = \xi_0 \cos(kx - \omega t)$$

$$E = pc$$

Postulates: $$\frac{\partial}{\partial x} = ik \qquad \frac{\partial}{\partial t} = -i\omega$$

# The Schrödinger Equation

$$E = \frac{p^2}{2m} + V$$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V$$

$$\frac{\partial}{\partial x} = ik \qquad \frac{\partial}{\partial t} = -i\omega$$

$$\boxed{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)}$$

# The Schrödinger Equation

- Wave function is an imaginary function.
- Wave function of matter is not a measurable function/quantity.
- Instead, it is the probability interpretation of the particle.

$$P(x,t)dx = \Psi^*(x,t)\Psi(x,t)dx = |\Psi(x,t)|^2 dx$$

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx = 1$$

# Separation of Time and Space Variables

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right)\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

$$\Psi(x,t)=\psi(x)\phi(t)$$

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

$$i\hbar\frac{d\phi(t)}{dt}=E\phi(t)$$

$$\phi(t)=e^{-iEt/\hbar}$$

$$\int_{-\infty}^{\infty}\Psi^*(x,t)\Psi(x,t)dx=1 \quad \Rightarrow \quad \int_{-\infty}^{\infty}\psi^*(x,t)\psi(x)dx=1$$

# Conditions for Acceptable Wave Functions

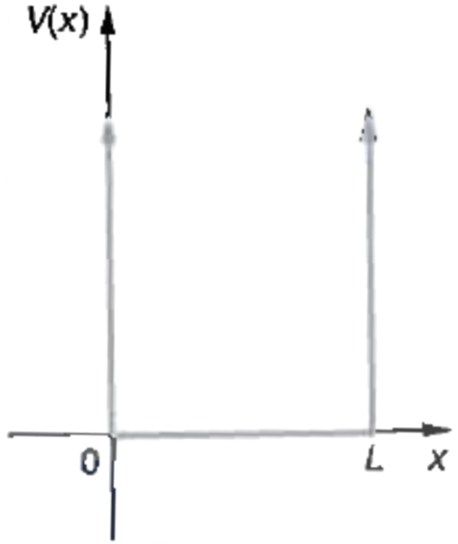
- $\psi(x)$ must exist and satisfy the Schrödinger equation.
- $\psi(x)$ and $d\psi/dx$ must be continuous.
- $\psi(x)$ and $d\psi/dx$ must be finite.
- $\psi(x)$ and $d\psi/dx$ must be single valued.
- $\psi(x) \rightarrow 0$ fast enough as $x \rightarrow \pm\infty$ so that the normalization integral remain bounded.

# Example

- Show that for a free particle of mass $m$ moving in one dimension, the function $\psi(x) = Asinkx + Bcoskx$ is a solution to the time-independent Schrödinger equation for any values of the constants A and B.

# The Infinite Square Well

$$V(x) = 0 \qquad 0 < x < L$$
$$V(x) = \infty \qquad x < 0 \;\; and \; x > L$$




Standing Wave method

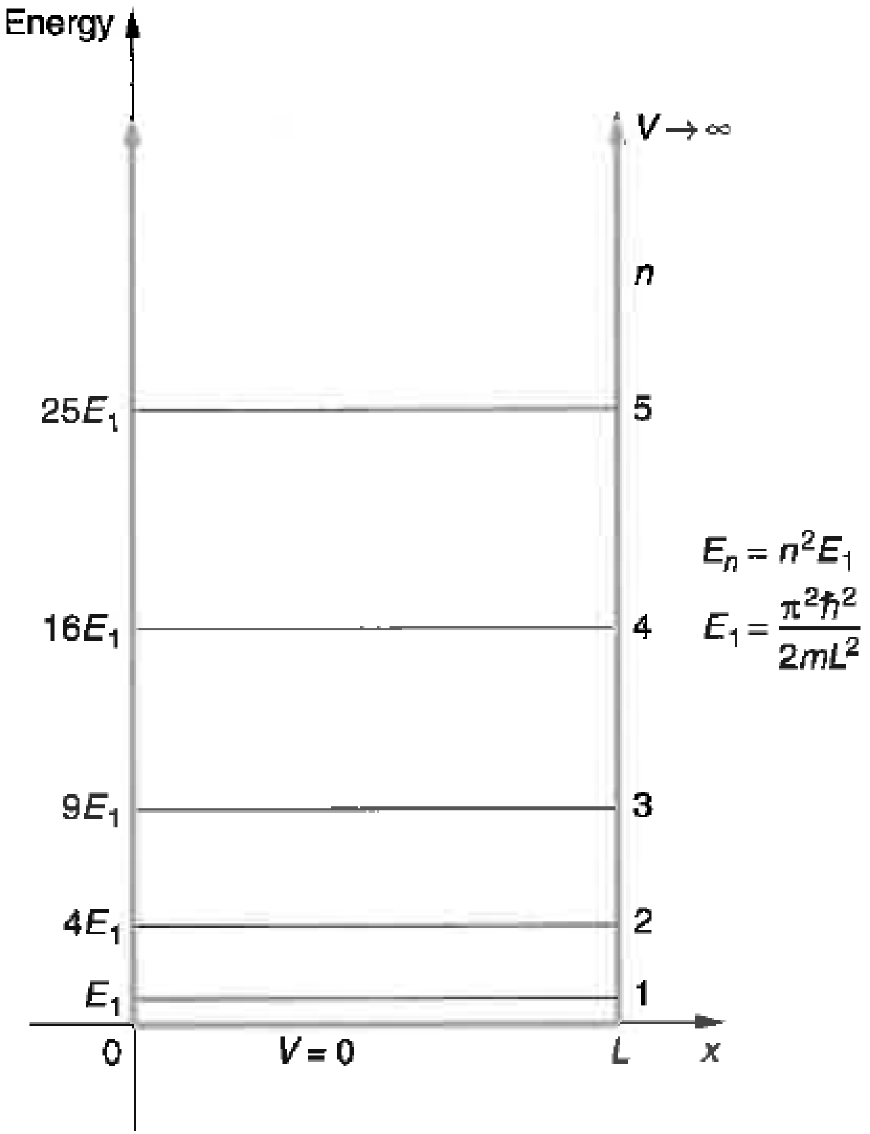
$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 E_1$$

Solving Schrödinger equation

$$\psi_n = \sqrt{\frac{2}{L}} sin \frac{n\pi x}{L}$$

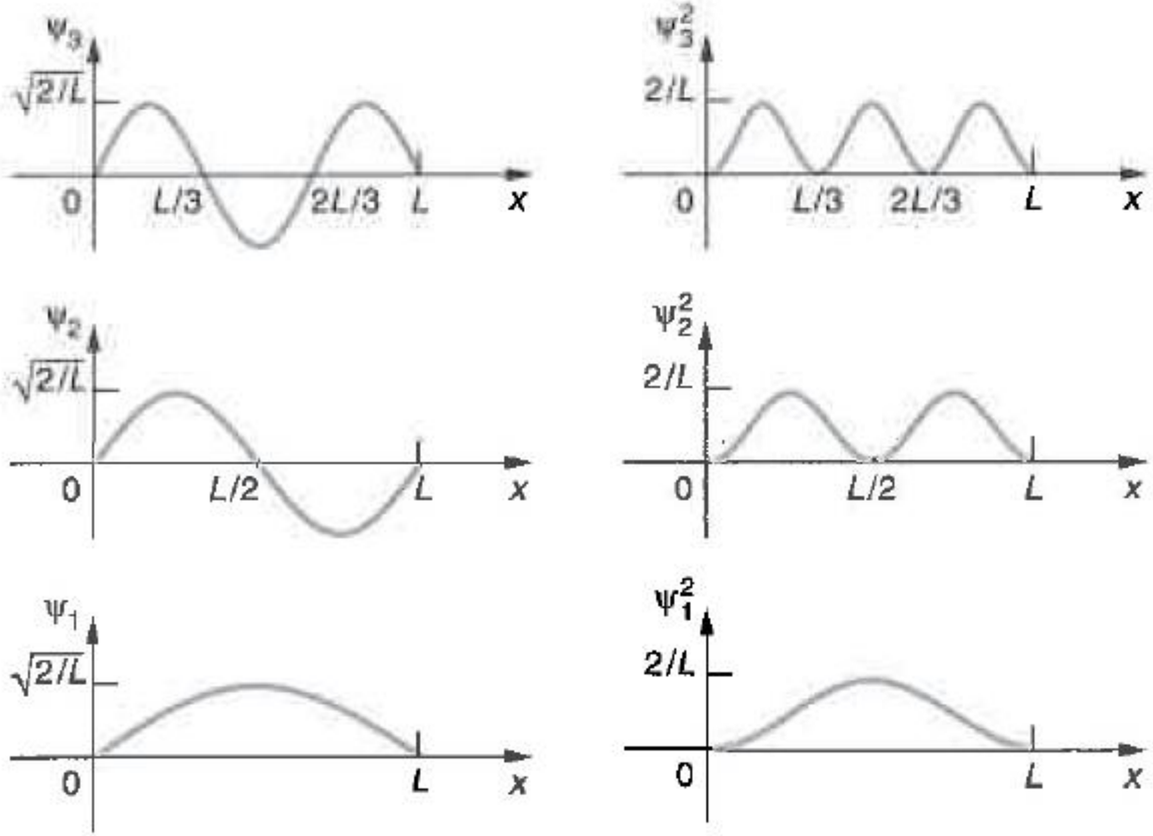
# The Infinite Square Well

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 E_1$$



# The Infinite Square Well

$$\psi_n = \sqrt{\frac{2}{L}} sin \frac{n\pi x}{L}$$



# The Infinite Square Well – the Complete Wave Function

$$\Psi(x,t) = \psi(x)\phi(t)$$

$$\psi_n = \sqrt{\frac{2}{L}} sin\frac{n\pi x}{L}$$

$$\phi(t) = e^{-iEt/\hbar}$$

$$\phi_n(t) = e^{-iE_n t/\hbar}$$

$$\Psi(x,t) = \frac{1}{2i}\sqrt{\frac{2}{L}}\left[e^{i(k_n x - \omega_n t)} - e^{-i(k_n x + \omega_n t)}\right]$$

# Example

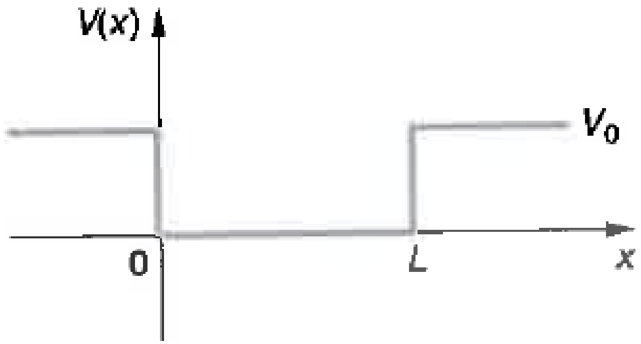
- An electron moving in a thin metal wire is a reasonable approximation of a particle in a one-dimensional infinite well. The potential inside the wire is constant on average but rise sharply at each end. Suppose the electron is in a wire 1.0 cm long. (a) Compute the ground-state energy for the electron. (b) If the electron's energy is equal to the average kinetic energy of the molecules in a gas at T = 300 K, about 0.03 eV, what is the electron's quantum number *n*?

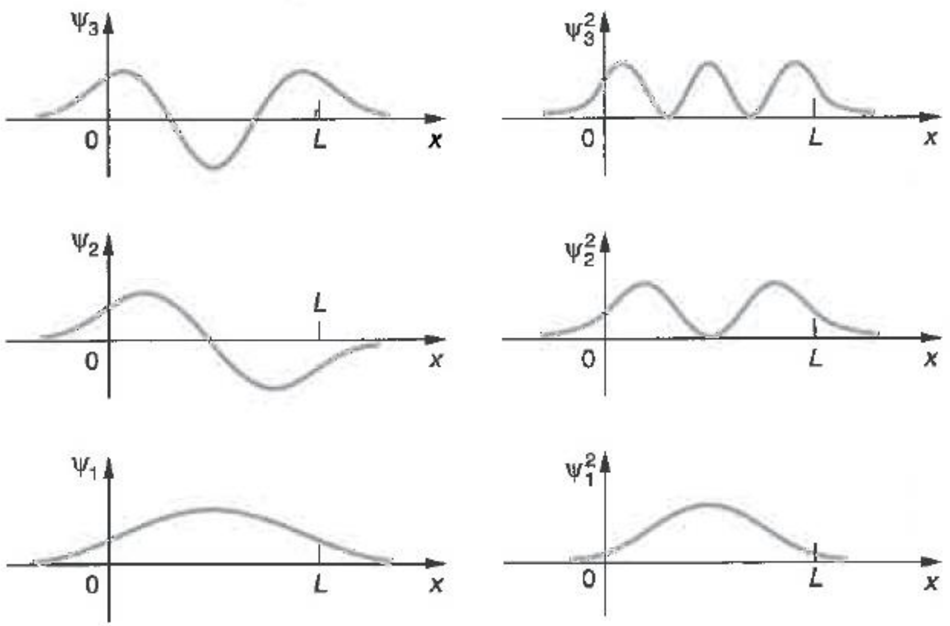
# Example

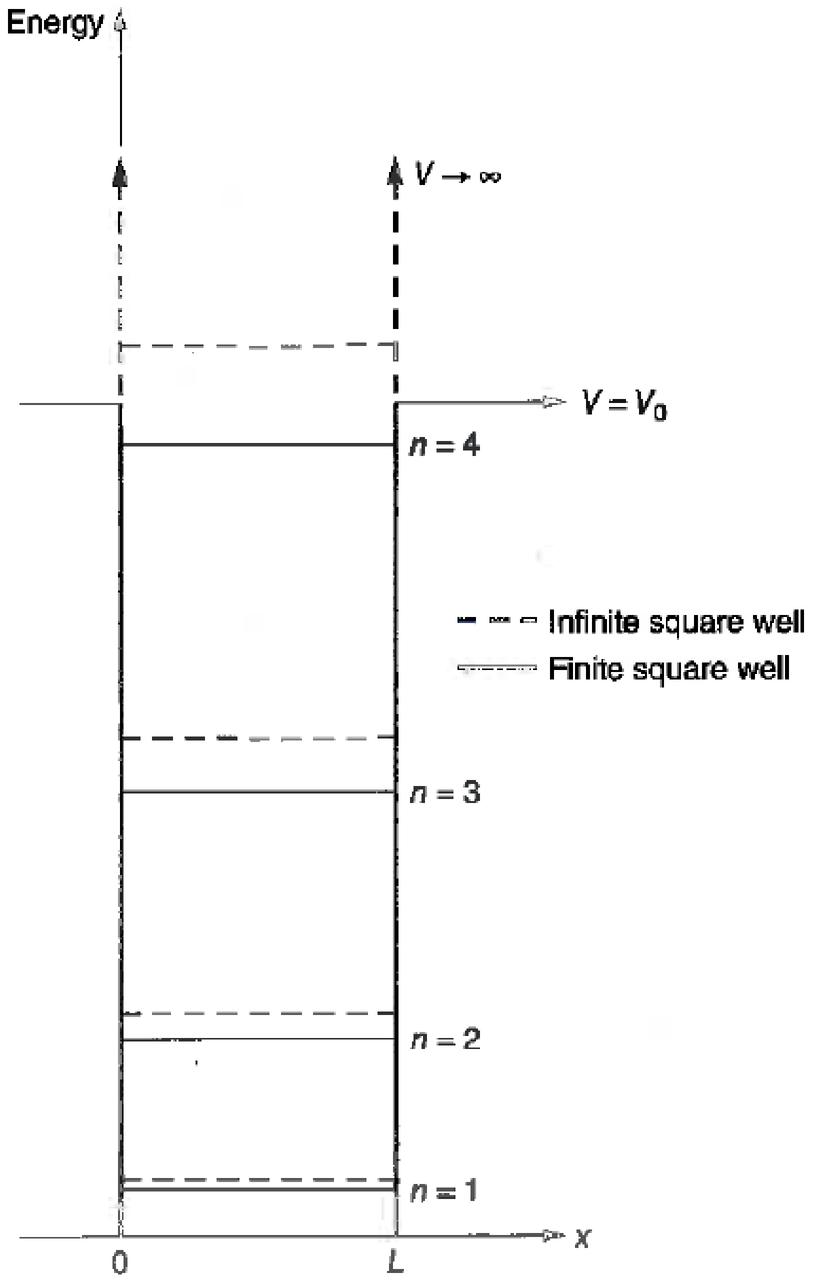
- Suppose that the electron in the above example could be “seen” while in its ground state. (a) What would be the probability of finding it somewhere in the region $0 < x < L/4$? (b) What would be the probability of finding it in a very narrow region $\Delta x = 0.01\ L$ wide centered at $x = 5L/8$?

# The Finite Square Well

$$V(x) = 0 \qquad 0 < x < L$$
$$V(x) = V_0 \qquad x < 0 \ and \ x > L$$



# Expectation Values

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} \psi^*(x,t) f(x) \psi(x) dx$$

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi^*(x,t) x \psi(x) dx$$

$$\langle x^2\rangle = \int_{-\infty}^{\infty} \psi^*(x,t) x^2 \psi(x) dx$$

How about <p>?

# Expectation Values and Operators

$$\frac{\partial}{\partial x} = ik \qquad\qquad p = \hbar k = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi(x)dx = \int_{-\infty}^{\infty} \frac{\hbar}{i}\psi^*(x,t)\frac{\partial\psi(x)}{\partial x}dx$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi(x)dx = -\int_{-\infty}^{\infty} \hbar^2\psi^*(x,t)\frac{\partial^2\psi(x)}{\partial x^2}dx$$

# Example

- Find $\langle p \rangle$ and $\langle p^2 \rangle$ for the ground-state wave function of the infinite square well.

# Operators in Quantum Mechanics

Position operator $$x_{op}\psi(x) = x\psi(x)$$

Momentum operator $$p_{op}\psi(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x)$$

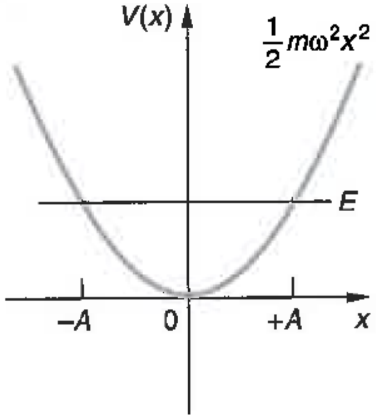
Hamiltonian (energy operator) in time-independent

$$H_{op}\psi(x) = \left(\frac{p_{op}^2}{2m} + V(x)\right)\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

Hamiltonian (energy operator) in time-dependent

$$H_{op}\phi(t) = i\hbar\frac{\partial}{\partial t}\phi(t) = E\phi(t)$$

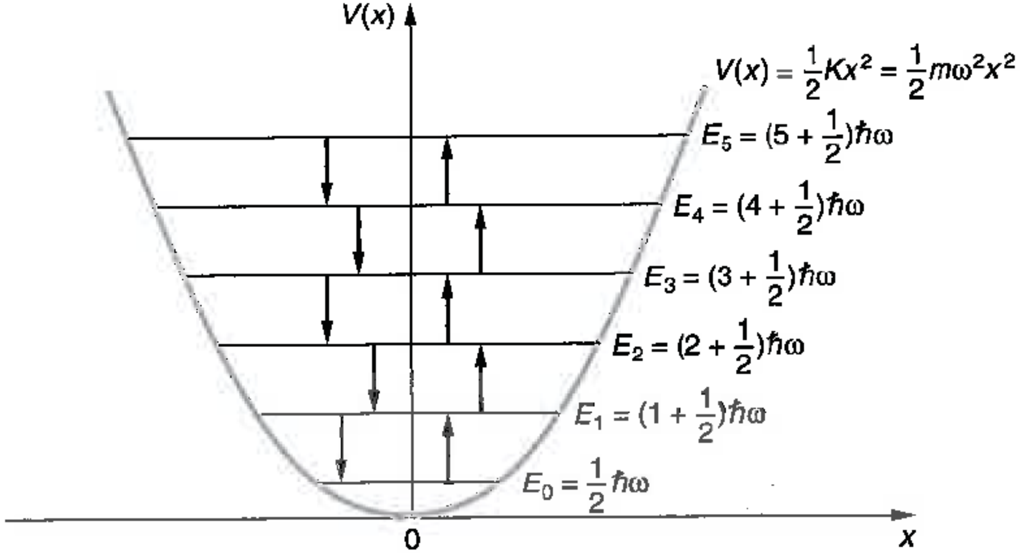
# Simple Harmonic Oscillator




$$V(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2x^2$$

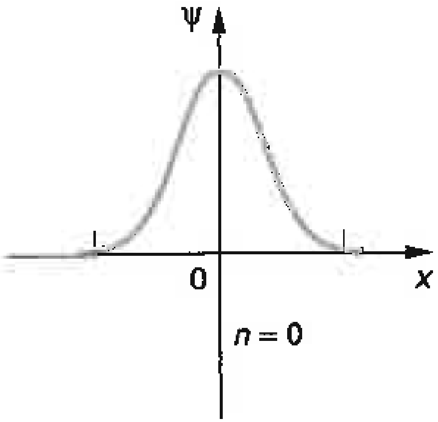
$$H_{op}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x)$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$



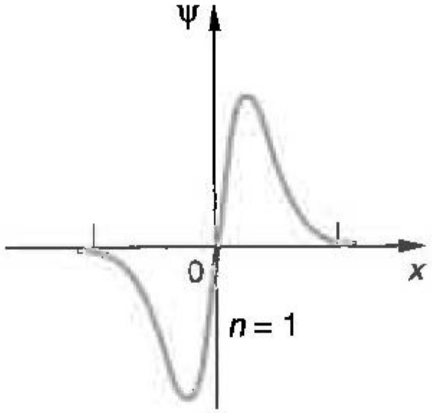
# Simple Harmonic Oscillator

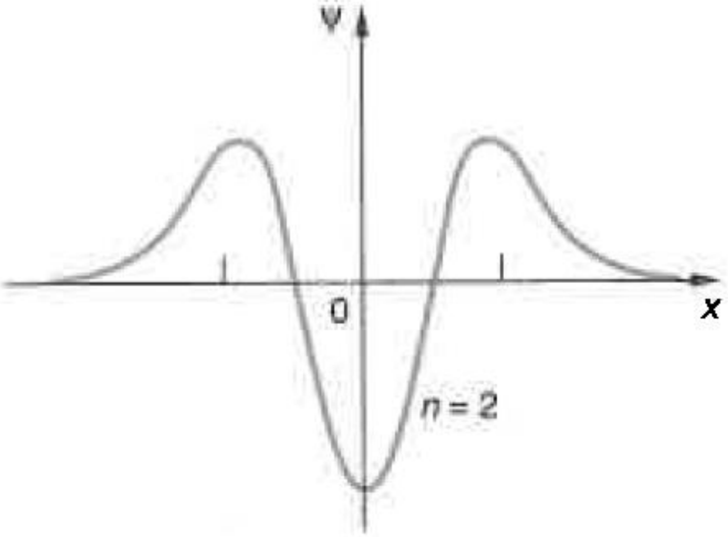
$$\psi_0(x) = A_0 e^{-m\omega x^2/2\hbar}$$



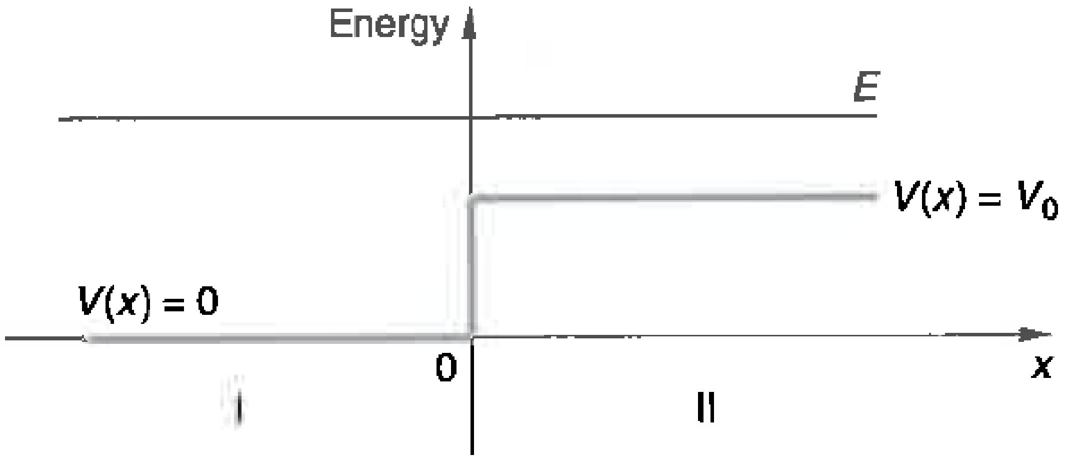

$$\psi_2(x) = A_2\left(1 - \frac{2m\omega x^2}{\hbar}\right)e^{-m\omega x^2/2\hbar}$$

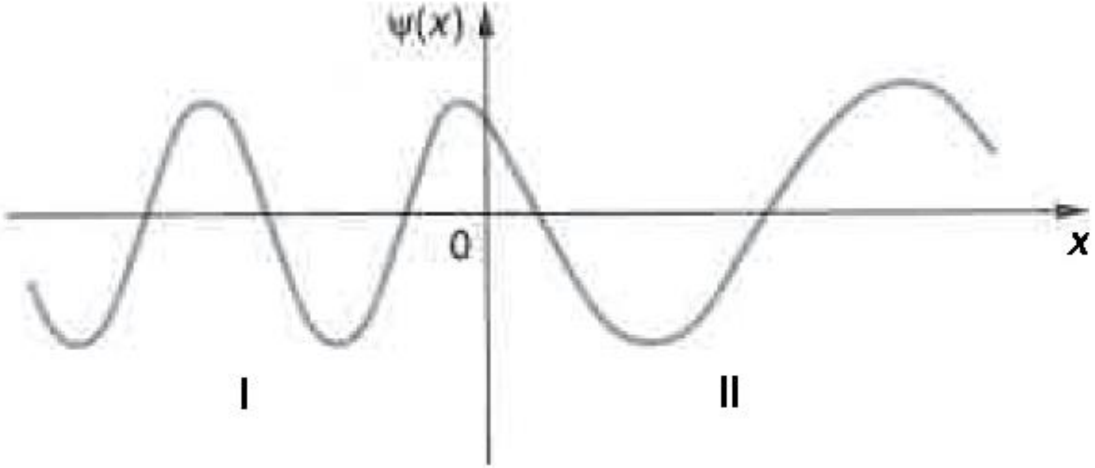
$$\psi_1(x) = A_1\sqrt{\frac{m\omega}{\hbar}}\,x e^{-m\omega x^2/2\hbar}$$



# Reflection and Transmission



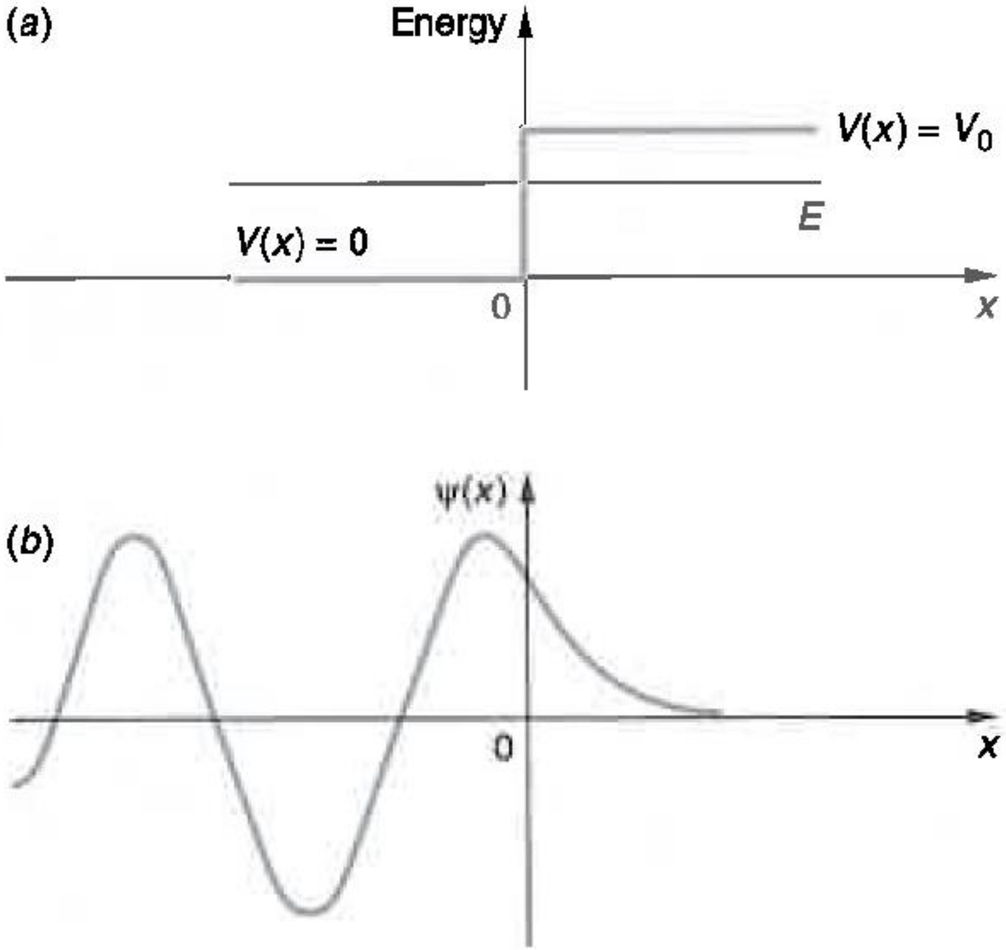

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

$$R + T = 1$$

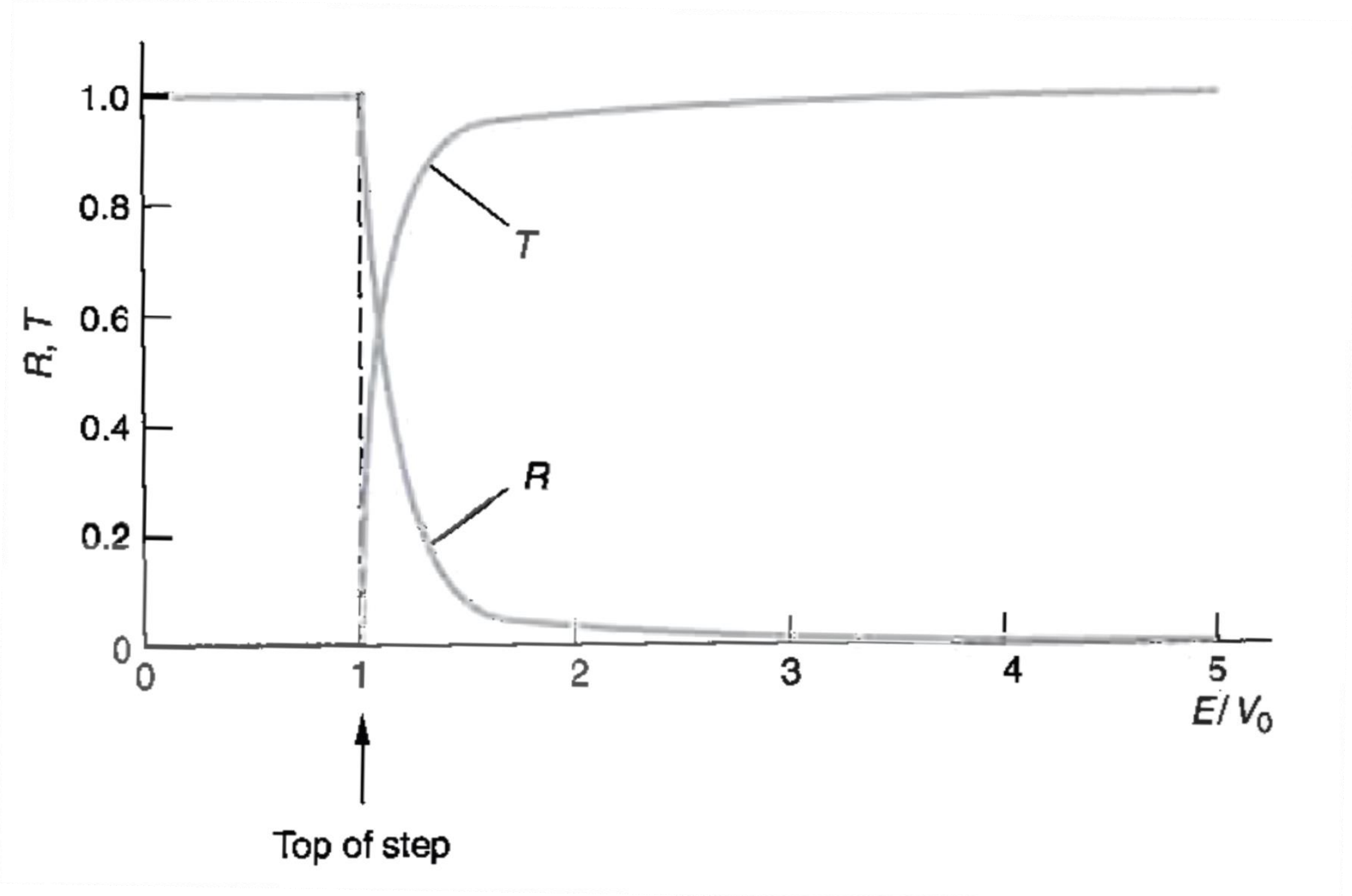
# Reflection and Transmission




$$R = 1$$

$$T = 0$$

# Reflection and Transmission



# Potential Barrier

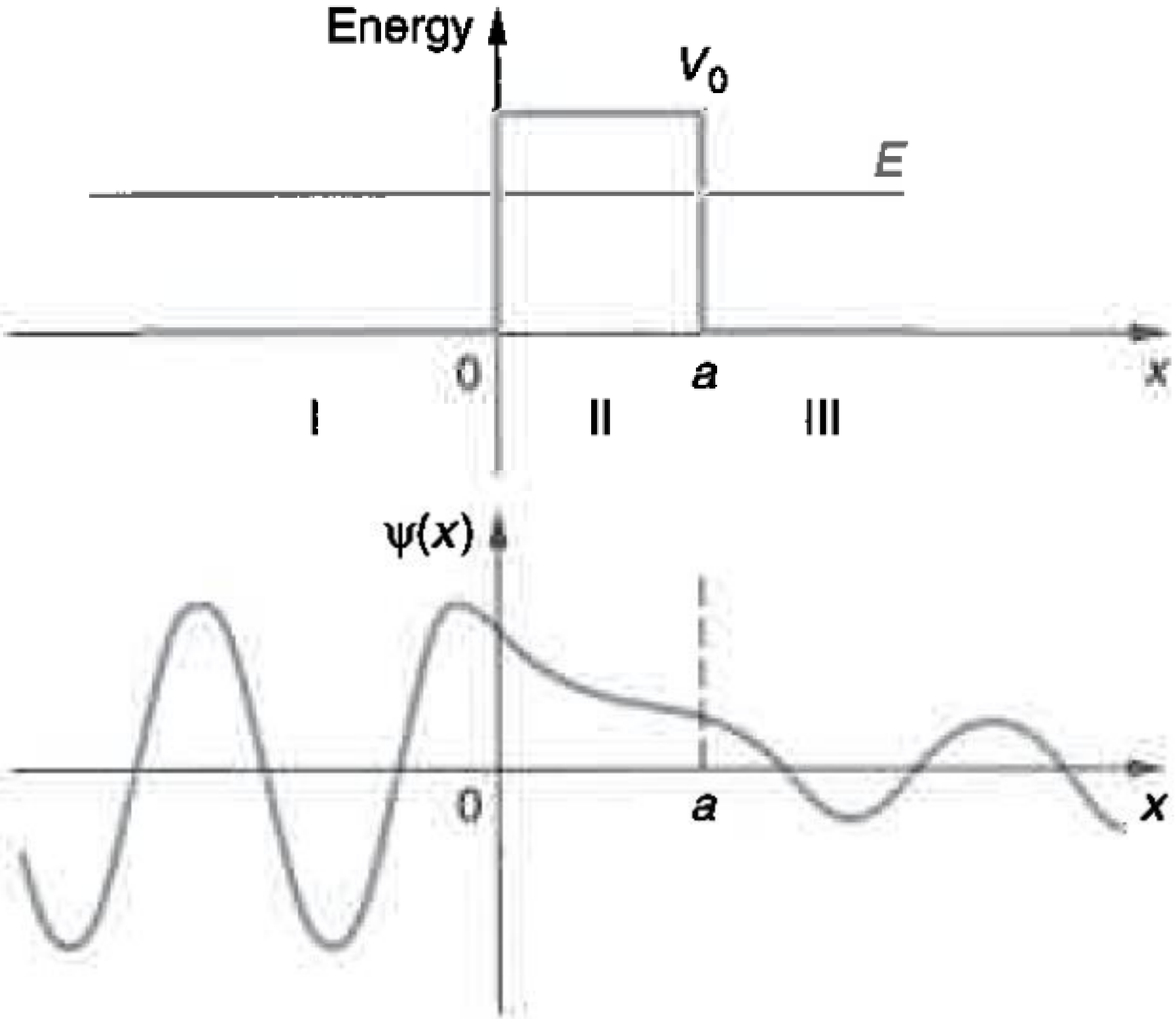
$$V(x) = \begin{cases} V_0 & \text{for } 0 < x < a \\ 0 & \text{for } 0 > x \text{ and } x > a \end{cases}$$

$$T \approx 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2\alpha a}$$

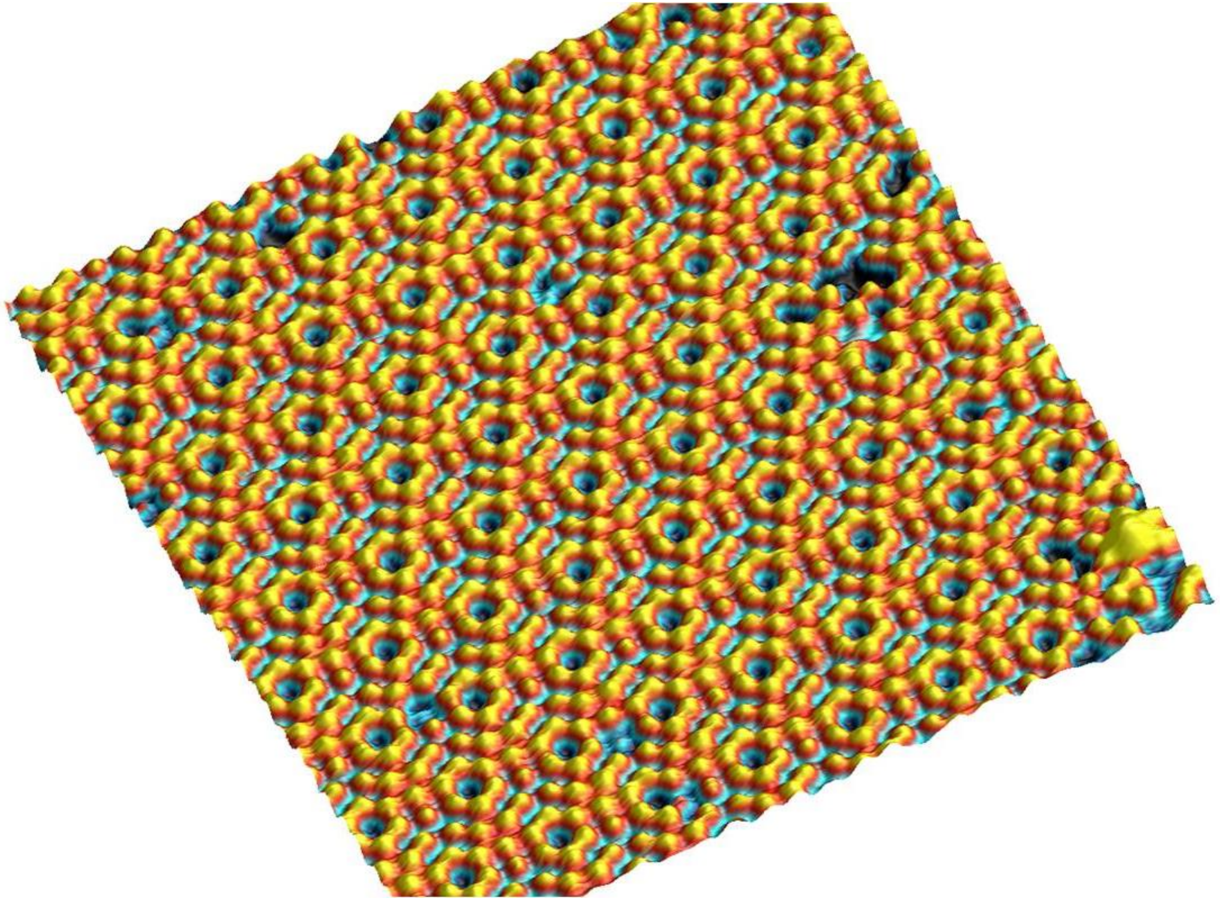
$$\psi_{\mathrm{I}}(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad x < 0$$

$$\psi_{\mathrm{II}}(x) = Ce^{-\alpha x} + De^{\alpha x} \qquad 0 < x < a$$

$$\psi_{\mathrm{III}}(x) = Fe^{ik_1x} + Ge^{-ik_1x} \qquad x > a$$



# Scanning Tunneling Microscopy



Si (111) 7x7 reconstruction

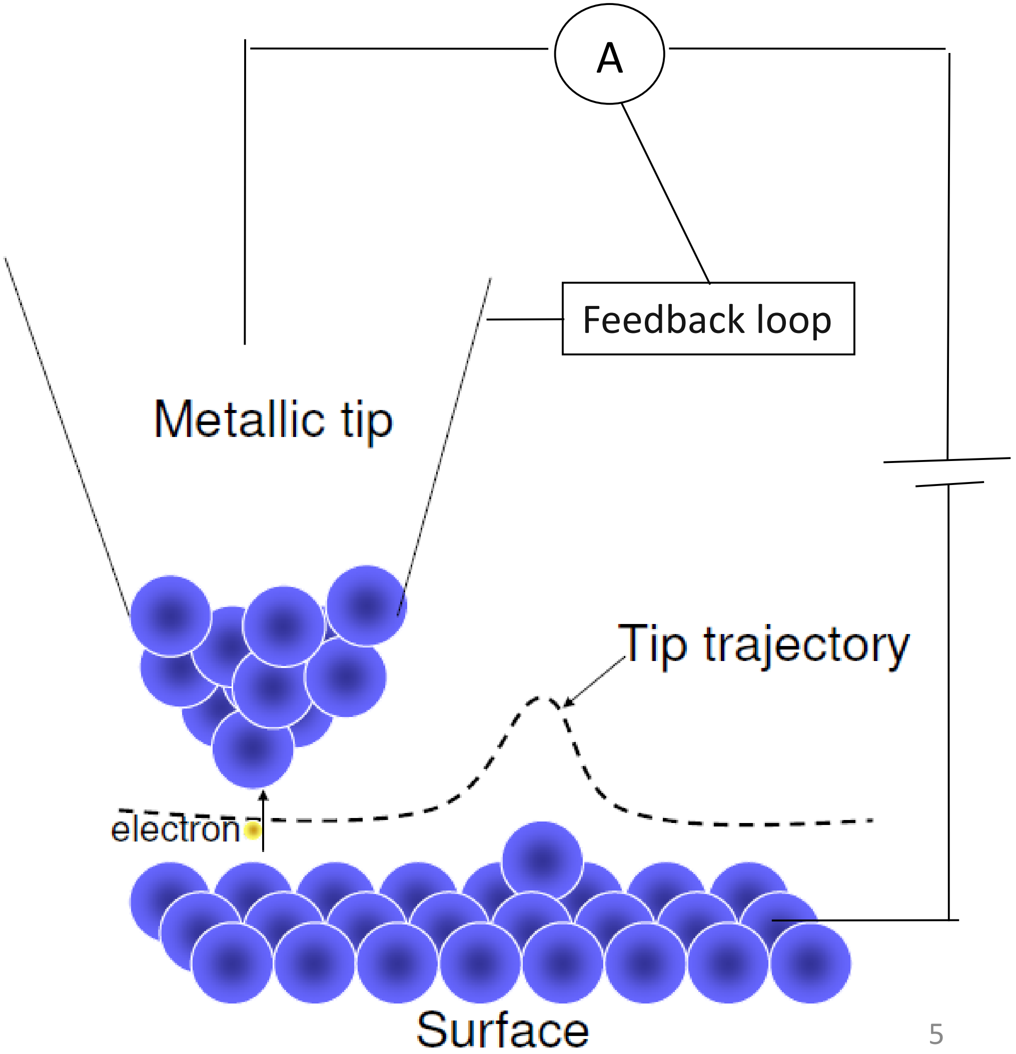





Image Credit: Andrew Yost

# Scanning Tunneling Microscopy