Schrödinger Wave Equation

- Time-dependent SE

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

- Properties of solutions
  - Linear: if Ψ_1 and Ψ_2 are solutions, so is $\Psi = a\Psi_1 + b\Psi_2$, where a and b are constants
  - A very useful solution is $\Psi(x,t) = A\exp[i(kx-\omega t)]$
  - $P(x,t)dx = \Psi^*(x,t)\,\Psi(x,t)dx$
  - Normalization: $\int_{-\infty}^{\infty} P(x,t)dx = \int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx = 1$
  - Boundary conditions:
    - Ψ must be finite and single valued
    - Ψ and its derivatives must be continuous and
    - Ψ must approach 0 as x goes to infinity

Time-independent SE

- Separation of variables leads to the time-independent SE: $$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V\psi(x)=E\psi(x)$$
- So that $\Psi(x,t)=\psi(x)e^{-i\omega t}$
- Stationary States: P(x) independent of time ; $P(x)=\psi^*(x)\psi(x)=|\psi|^2$

3D SE

- Generalizing the time-dependent SE to 3D, we have

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

- The time-independent SE becomes

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

- We will return to this later for the hydrogen atom

Average Values = Expectation Values

- For discrete set:

$$\overline{x} = \frac{\sum_i N_i x_i}{\sum_i N_i}$$

- For continuous variable:

$$\overline{x} = \frac{\int_{-\infty}^{\infty} xP(x)dx}{\int_{-\infty}^{\infty} P(x)dx}$$

- In QM:

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

- For any g(x):

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

Operators – momentum & energy

- Motivation for attributing $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ and $\hat{E} = i\hbar \frac{\partial}{\partial t}$

- Operator expectation values:

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

- So,

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t) \frac{\partial \Psi(x,t)}{\partial x} dx \quad and$$

$$\langle E \rangle = i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t) \frac{\partial \Psi(x,t)}{\partial t} dx$$

- Examples

Infinite Square-Well Potential

- Schrödinger equation within well – find solutions and match to boundary conditions:

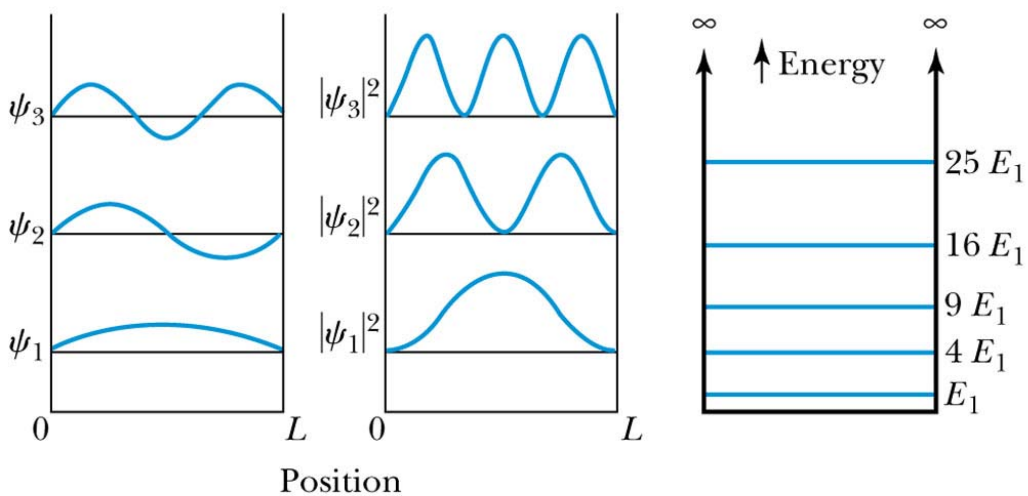
$$\psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$$

- Normalize wave functions to find A:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

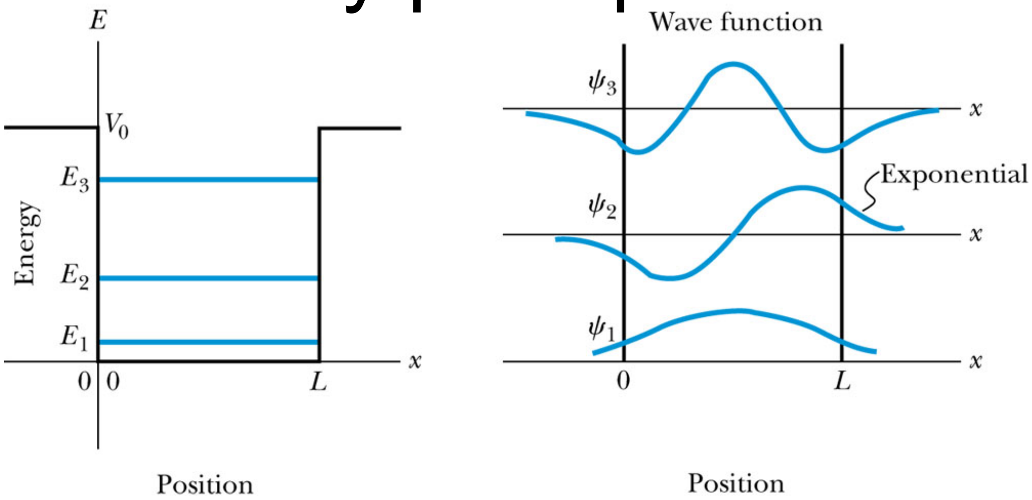
- Find possible energies:

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



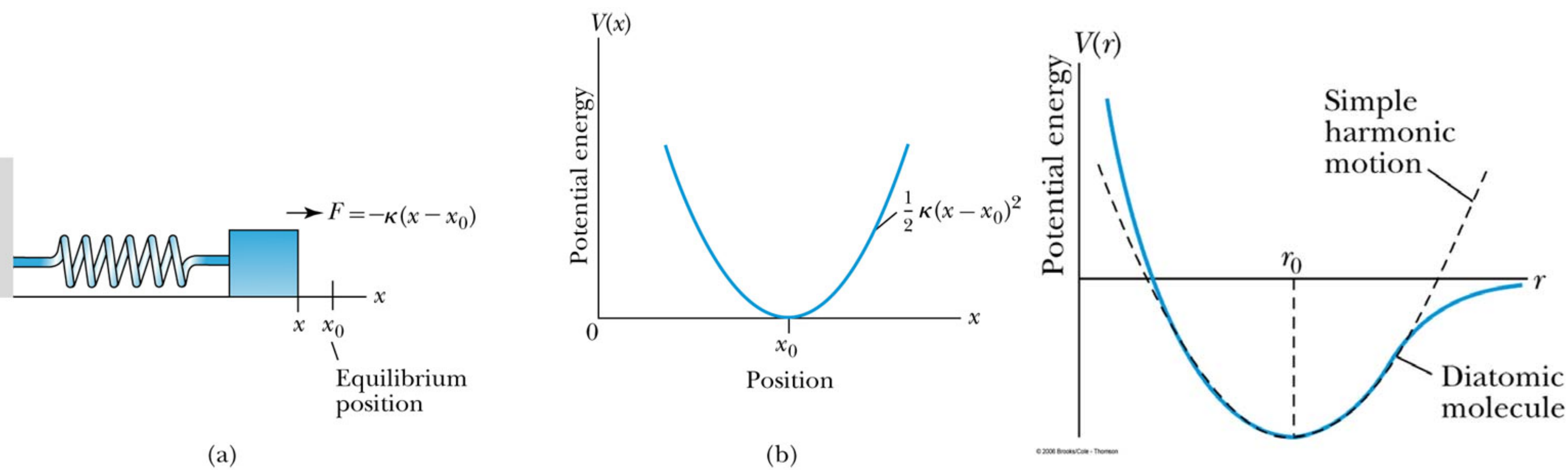
Finite Square Well

- Divide up space into 3 regions and solve SE in each
- Use matching Ψ and $\partial\Psi / \partial x$ at boundaries to solve for coefficients
- Tunneling/penetration depth ideas tied in with uncertainty principle



Simple Harmonic Oscillator in 1D

- Hooke's Law gives a quadratic potential energy
- Very important problem, since every V that has a minimum can be approximated by a quadratic V near the minimum



Qualitative SE solutions to SHO

- SE for SHO $$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left(E - \frac{\kappa x^2}{2}\right)\psi$$
- Writing

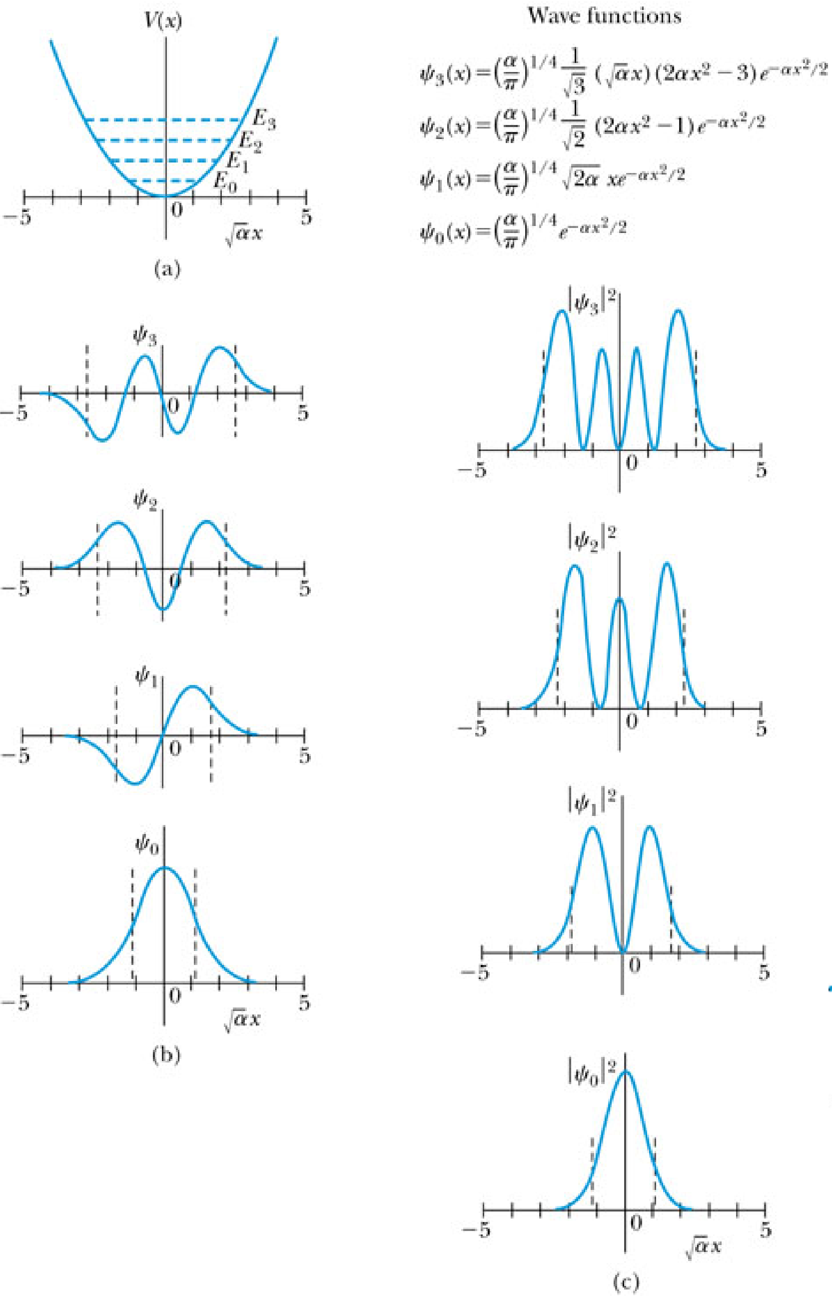
$$\alpha^2 = \frac{m\kappa}{\hbar^2} \quad and \quad \beta = \frac{2mE}{\hbar^2} \quad we\ have \quad \frac{d^2\psi}{dx^2} = (\alpha^2 x^2 - \beta)\psi$$

- Minimum energy E_o cannot = 0 – a calculation based on the uncertainty principle shows that $$E_o = \frac{\hbar}{2}\sqrt{\frac{\kappa}{m}} = \frac{\hbar\omega}{2}$$

- Solutions are $\psi_n = H_n(x)e^{-\alpha x^2/2}$

with $E_n = (n + \frac{1}{2})\hbar\sqrt{\kappa / m} = (n + \frac{1}{2})\hbar\omega$

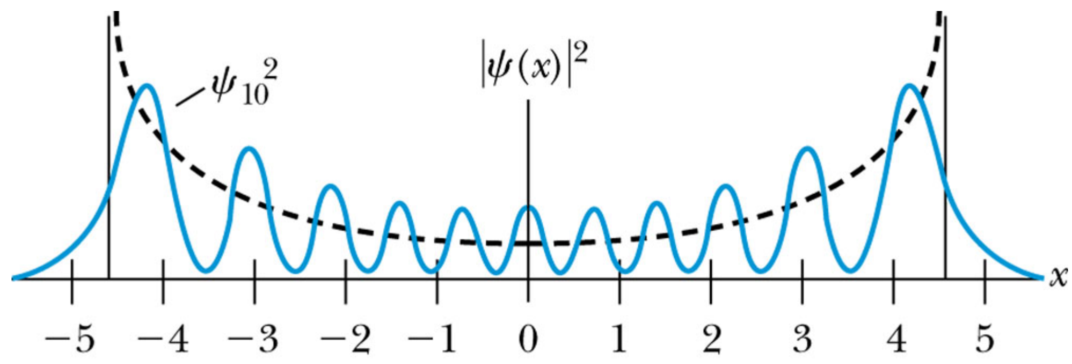
SHO Solutions



First 4 energy levels (left) and wave functions (right)

Wave functions are plotted (left) and probability distributions (right)

Below is probability distribution for n = 10 and the classical results (dotted line)



Barriers and Tunneling

Classically, when a particle of energy E meets a barrier of height V_o, if $E>V_o$ the particle would pass right by, reducing its v when in the region of V_o (since $K = E - V_o = \frac{1}{2} mv^2$). If the particle has energy less than V_o it will always be reflected from the barrier wall because it cannot enter the barrier.

In QM, things will be different because the particle has wave-like properties. In regions I and III outside the barrier, the wave numbers are

$$k_I = k_{III} = \frac{\sqrt{2mE}}{\hbar} \quad since\ \mathrm{V{=}0}$$

while in the barrier region

$$k_{II} = \frac{\sqrt{2m(E-V_o)}}{\hbar}$$

Analogy with optics: when light in air enters a piece of glass (with a different index of refraction) its wavelength changes and at the air-glass interface some light is reflected and some is transmitted – the same will happen here in QM with our particle (remember $k = 2\pi/\lambda$)

Solve SE in each of the 3 regions and match the BC at the barrier walls – first for $E > V_o$

Barriers & Tunneling (for E>V_o) - 2

- Probability of particle being reflected = R

$$R = \frac{\left|\Psi_1(reflected)\right|^2}{\left|\Psi_1(incident)\right|^2} = \frac{B^* B}{A^* A}$$

- Probability of particle being transmitted = T

$$T = \frac{\left|\Psi_{III}(transmitted)\right|^2}{\left|\Psi_1(incident)\right|^2} = \frac{F^* F}{A^* A} = 1 - R$$

- Result for T is $T = \left[1 + \frac{V_o^2 \sin^2(k_{II} L)}{4E(E - V_o)}\right]^{-1}$
- Can have T = 1- when? When $k_{II}L = n\pi$ - reflections at x = 0 and x = L cancel out by interference

Barriers & Tunneling (for E<V_o) - 3

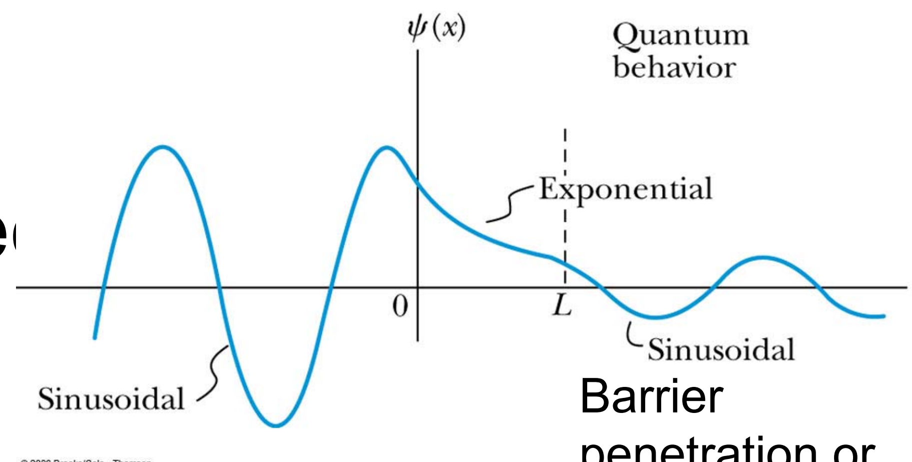
- Re-solve SE and match BC – inside barrier in region II let $k_{II} = \frac{\sqrt{2m(V_o - E)}}{\hbar} > 0$

- Then, similarly, we find that there is a probability for tunneling through the barrier

$$T = \left[1 + \frac{V_o^2 \sinh^2(k_{II} L)}{4E(V_o - E)}\right]^{-1}$$

- For large k_{II}L this be

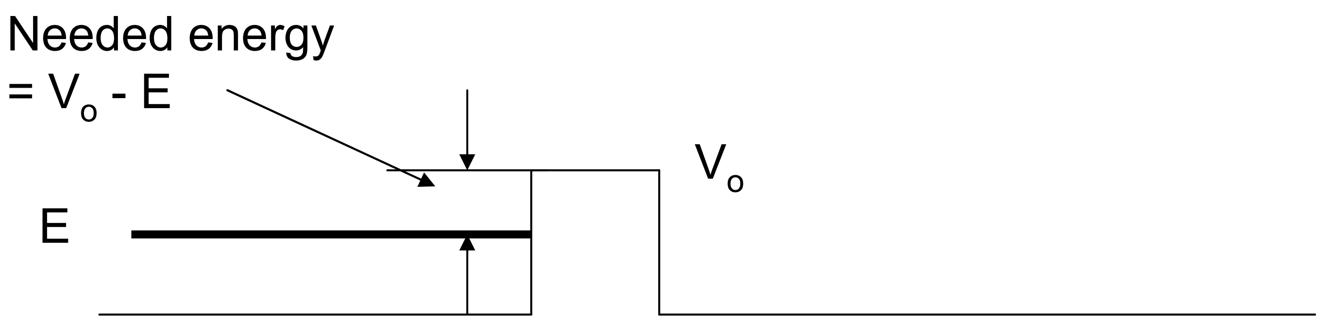
$$T = 16\frac{E}{V_o}\left(1 - \frac{E}{V_o}\right)e^{-2k_{II}L}$$



Barrier penetration or tunneling

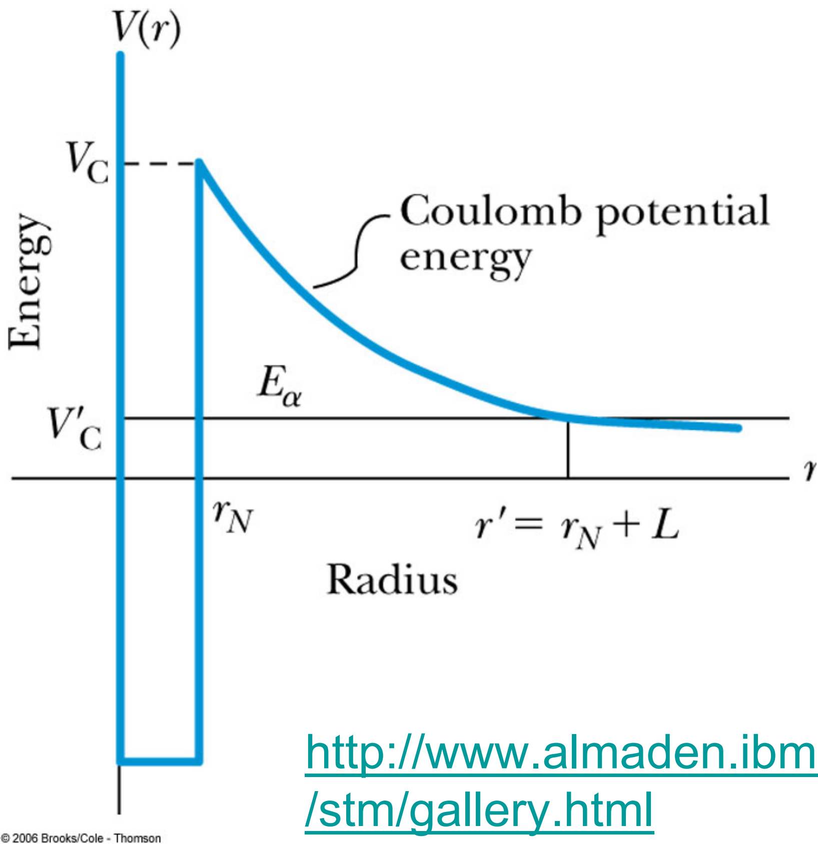
Uncertainty Principle explanation of Tunneling

- To penetrate a barrier of width L with wave-vector k (so $\Psi \sim e^{-2kx}$), we have $\Delta x \sim k^{-1}$, but $\Delta x \, \Delta p \geq \hbar$, so $\Delta p \geq (\hbar/\Delta x) = \hbar k$
- Then, $K_{min} = (\Delta p)^2/2m = \hbar^2 k^2/2m = V_o - E$



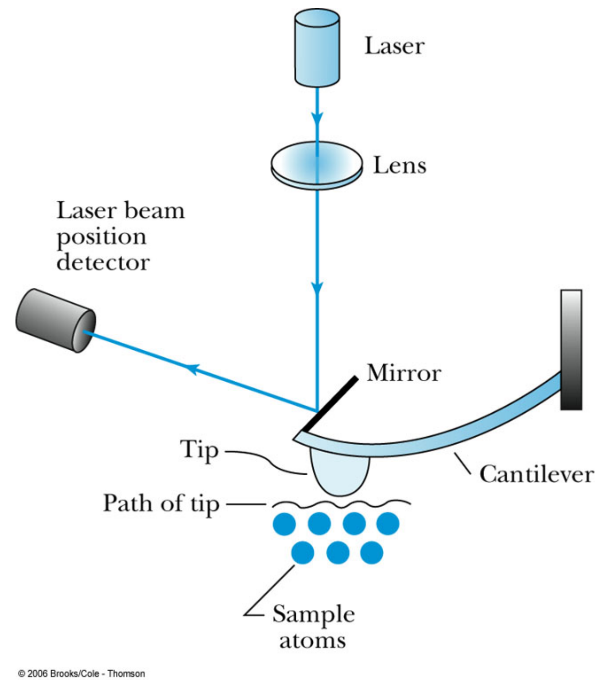
Tunneling Applications

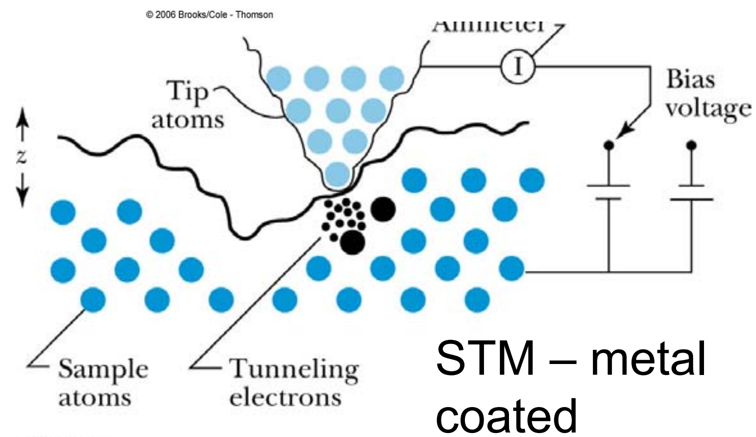
- First is electrician wiring- Al wires have oxide coating – twisting wires works via tunneling
- α decay from nucleus
- Scanning probe microscopy



http://www.almaden.ibm.com/vis/stm/gallery.html

AFM





STM – metal coated