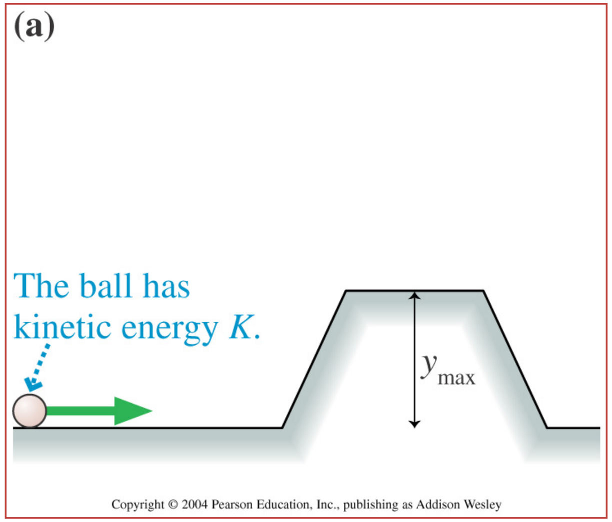
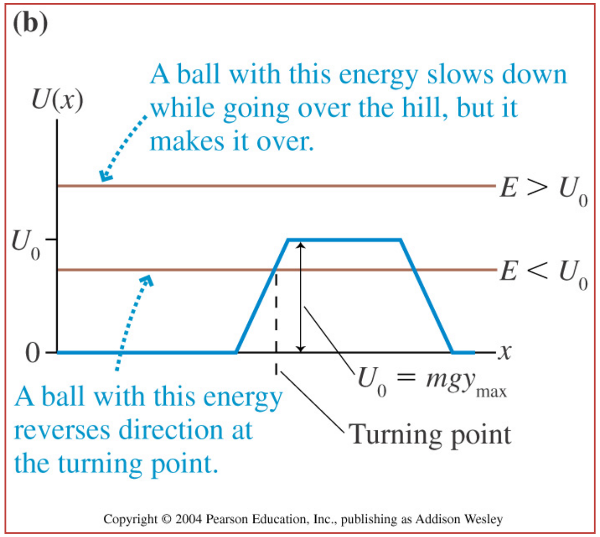
Quantum Mechanical Tunneling

The square barrier:

Behaviour of a classical ball rolling towards a hill (potential barrier):





If the ball has energy E less than the potential energy barrier (U=mgy), then it will not get over the hill.
The other side of the hill is a **classically forbidden** region.

Quantum Mechanical Tunneling

The square barrier:

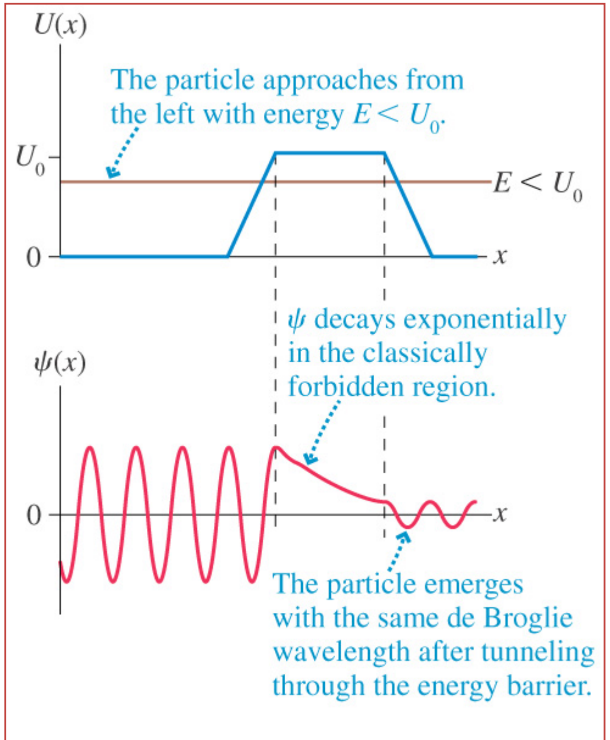
Behaviour of a quantum particle at a potential barrier

Solving the TISE for the square barrier problem yields a peculiar result:

If the quantum particle has energy E less than the potential energy barrier U, there is still a non-zero probability of finding the particle classically forbidden region !

This phenomenon is called **tunneling**.

To see how this works let us solve the TISE…



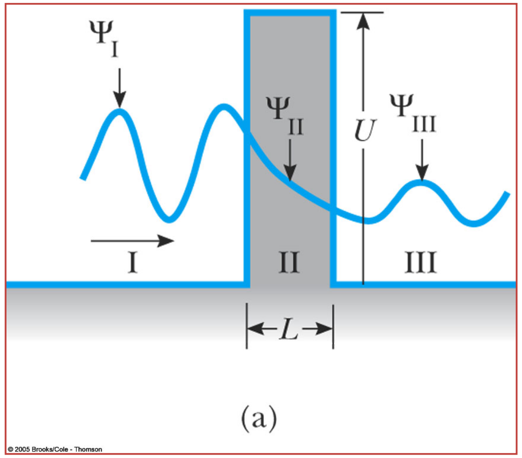
Quantum Mechanical Tunneling

The square barrier:

Behaviour of a quantum particle at a potential barrier

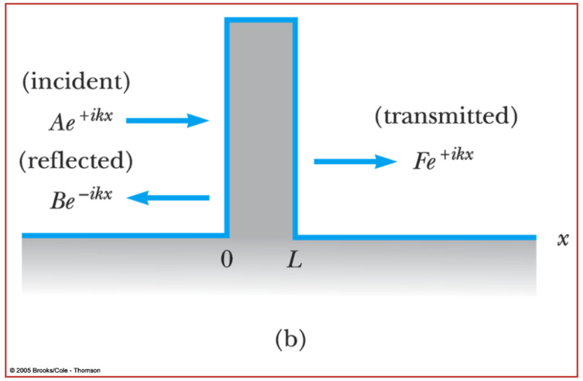
To the left of the barrier (region I), U=0
Solutions are free particle plane waves:

$$\phi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$



(a)

The first term is the incident wave moving to the **right**
The second term is the reflected wave moving to the **left**.



(b)

Reflection coefficient: $$R = \frac{|\phi_{reflected}|^2}{|\phi_{incident}|^2} = \frac{|B|^2}{|A|^2}$$

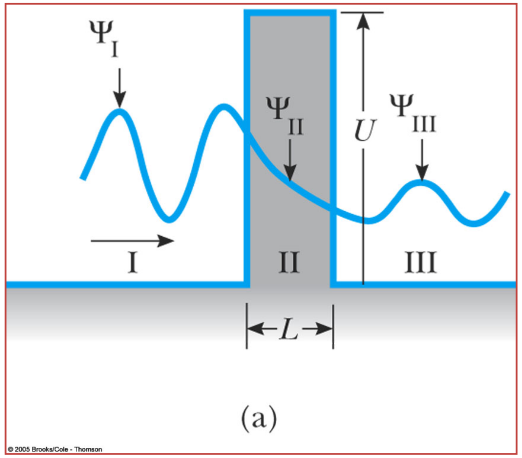
Quantum Mechanical Tunneling

The square barrier:

Behaviour of a quantum particle at a potential barrier

To the right of the barrier (region III), U=0. Solutions are free particle plane waves:

$$\phi(x) = Fe^{ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

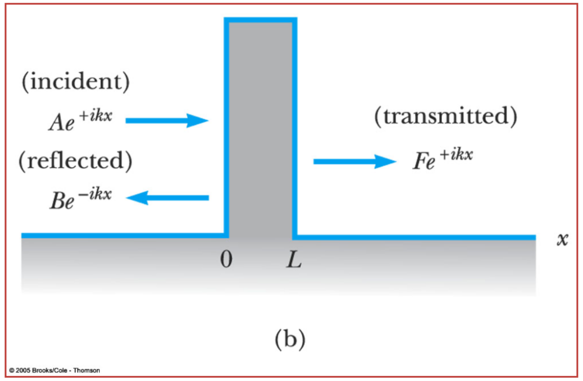


This is the transmitted wave moving to the **right**

Transmission coefficient:

$$T = \frac{|\phi_{transmitted}|^2}{|\phi_{incident}|^2} = \frac{|F|^2}{|A|^2}$$

$$T + R = 1$$



Quantum Mechanical Tunneling

The square barrier:

Behaviour of a quantum particle at a potential barrier

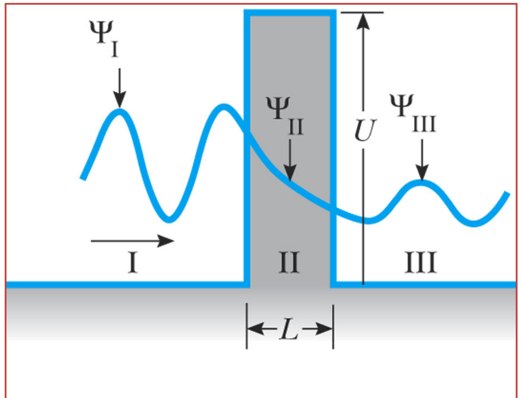
In the barrier region (region II), the TISE is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x)=(E-U)\phi(x)$$

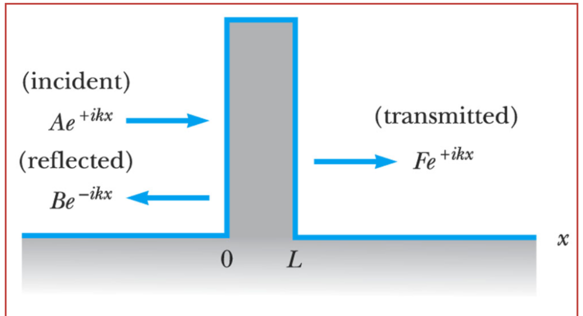
Solutions are

$$\boxed{\phi(x)=Ce^{-\alpha x}+De^{\alpha x}}$$

$$\boxed{\alpha=\frac{\sqrt{2m(U-E)}}{\hbar}}$$



(a)



(b)

Quantum Mechanical Tunneling

The square barrier:

Behaviour of a quantum particle at a potential barrier

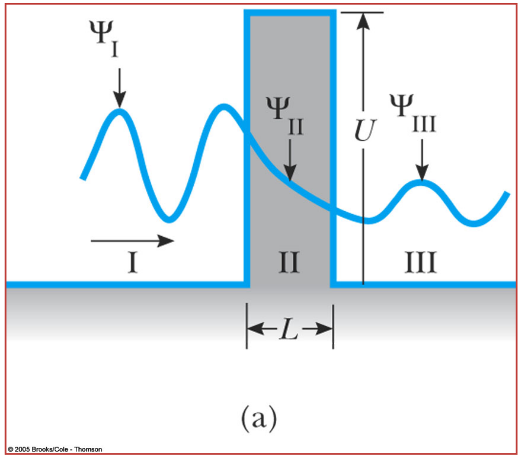
At x=0, region I wave function = region II wave function:

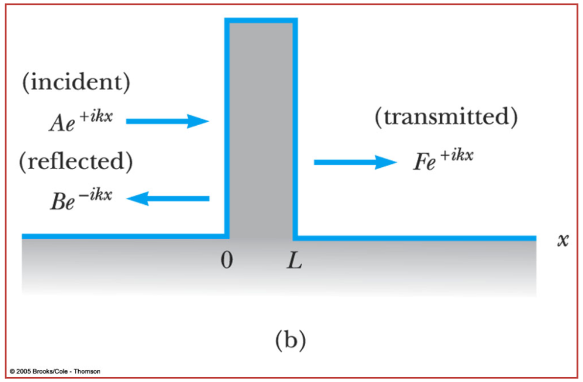
$$Ae^{ikx} + Be^{-ikx} = Ce^{-\alpha x} + De^{\alpha x}$$

$$A + B = C + D$$

At x=L, region II wave function = region III wave function:

$$Ce^{-\alpha L} + De^{\alpha L} = Fe^{ikL}$$





Quantum Mechanical Tunneling

The square barrier:

Behaviour of a quantum particle at a potential barrier

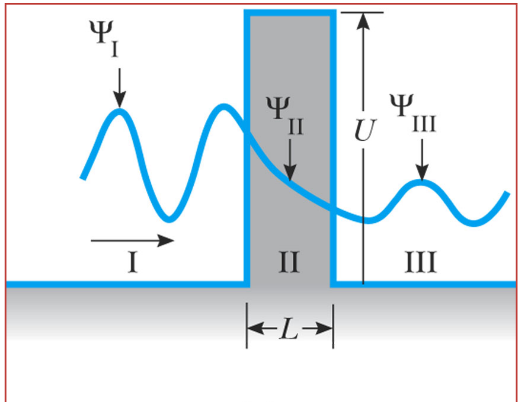
At x=0, dφ/dx in region I = dφ/dx in region II:

$$\boxed{ikAe^{ikx} - ikBe^{-ikx} = -\alpha Ce^{-\alpha x} + \alpha De^{\alpha x}}$$

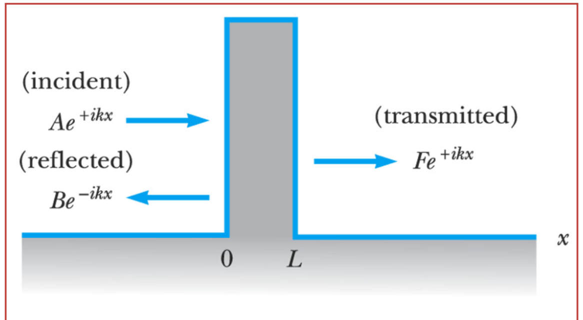
$$\boxed{ikA - ikB = -\alpha C + \alpha D}$$

At x=L, dφ/dx in region II = dφ/dx in region III :

$$\boxed{-\alpha Ce^{-\alpha L} + \alpha De^{\alpha L} = ikFe^{ikL}}$$



(a)



(b)

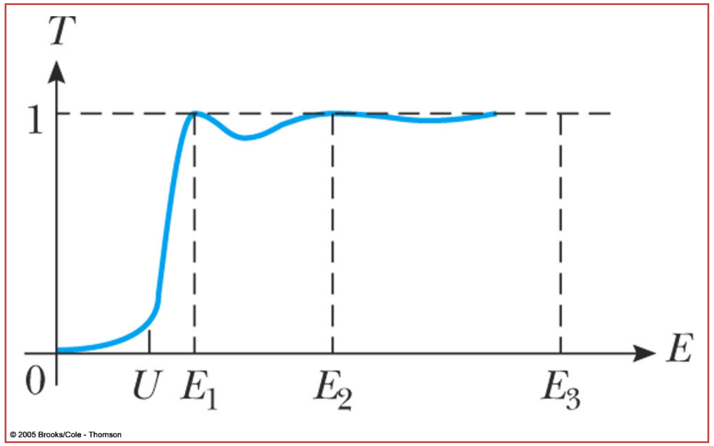
Quantum Mechanical Tunneling

The square barrier:

Behaviour of a quantum particle at a potential barrier

Solving the 4 equations, we get

$$T = \frac{1}{1+\frac{1}{4}\left[\frac{U^2}{E(U-E)}\right]\left[\frac{e^{\alpha L}+e^{-\alpha L}}{2}\right]^2}$$



For low energies and wide barriers,

$$T \approx e^{-\alpha L}$$

For some energies, T=1, so the wave function is fully transmitted **(transmission resonances).**

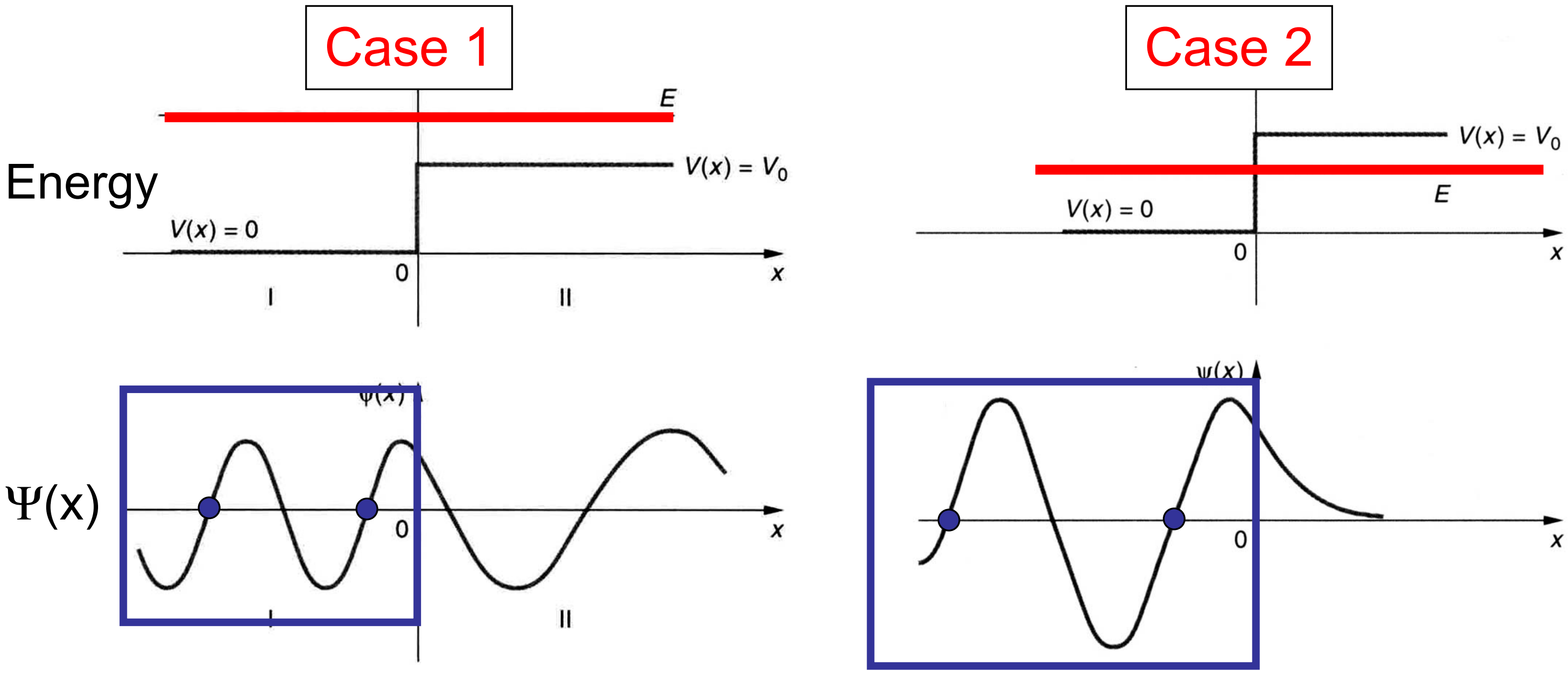
This occurs due to wave interference, so that the reflected wave function is completely suppressed.

Quantum Mechanical Tunneling

The step barrier:

To the left of the barrier (region I), U=0.
Solutions are free particle plane waves:

$$\phi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$



Quantum Mechanical Tunneling

The step barrier:

Inside Step:
U = V_o

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) = (E - V_0)\phi(x)$$

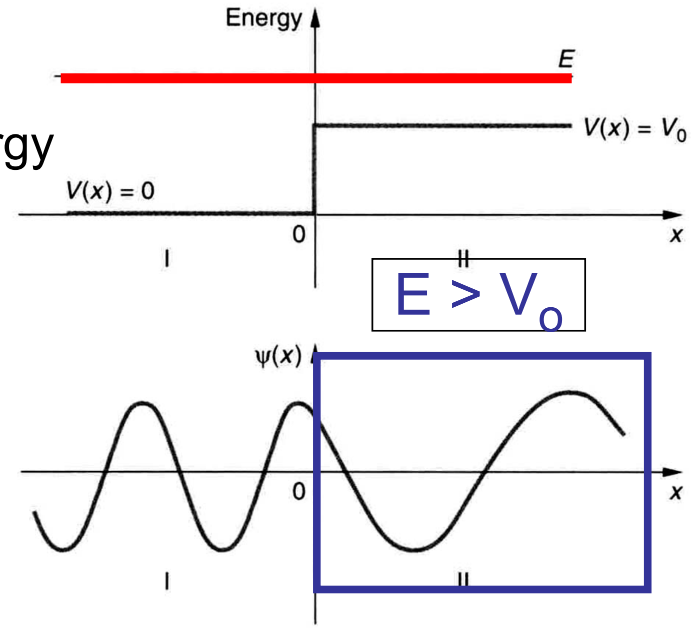
$$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

Case 1

Ψ(x) is oscillatory for $E > V_o$

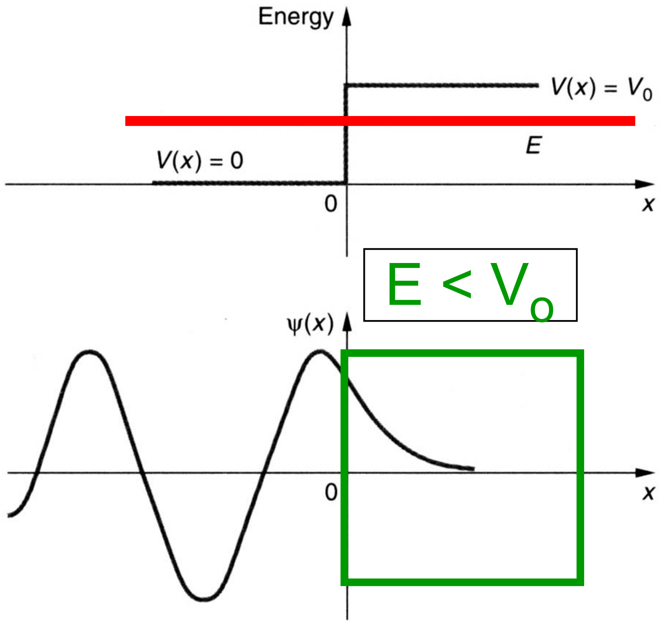
Energy

Ψ(x)



Case 2

Ψ(x) is decaying for $E < V_o$



Quantum Mechanical Tunneling

The step barrier:

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

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

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

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

R(reflection) + T(transmission) = 1

Reflection occurs at a barrier ($R \neq 0$), regardless if it is step-down or step-up.

R depends on the wave vector difference (k_1 - k_2) (or energy difference), but not on which is larger.

Classically, $R = 0$ for energy E larger than potential barrier (V_o).

Quantum Mechanical Tunneling

The step barrier:

A free particle of mass m, wave number k_1 , and energy E = $2V_o$ is traveling to the right. At x = 0, the potential jumps from zero to $-V_o$ and remains at this value for positive x. Find the wavenumber k_2 in the region $x > 0$ in terms of k_1 and V_o. Find the reflection and transmission coefficients R and T.

$$k_1 = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2m(2V_o)}}{\hbar} = \frac{\sqrt{4mV_o}}{\hbar} \quad and$$

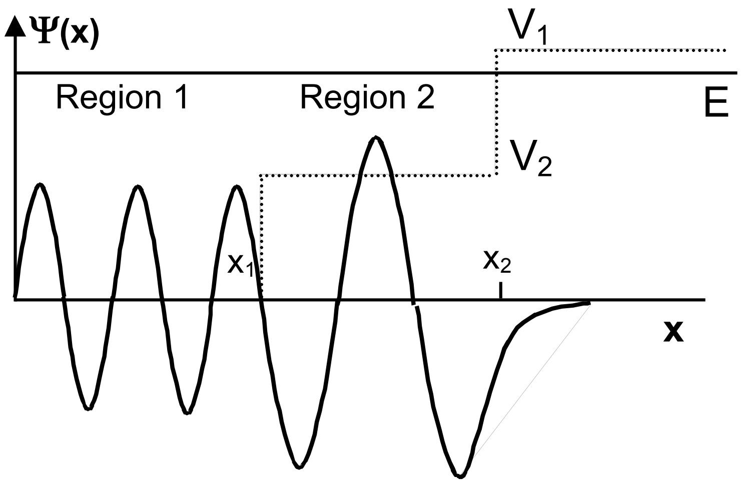
$$\boxed{k_2} = \frac{\sqrt{2m|V-E|}}{\hbar} = \frac{\sqrt{2m|-V_o-2V_o|}}{\hbar} = \frac{\sqrt{2m(3V_o)}}{\hbar} = \boxed{\frac{\sqrt{6mV_o}}{\hbar} \quad or \quad \sqrt{\frac{3}{2}}\,k_1}$$

$$\boxed{R} = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 = \left(\frac{k_1-\sqrt{\frac{3}{2}}k_1}{k_1+\sqrt{\frac{3}{2}}k_1}\right)^2 = \left(\frac{-0.225}{2.225}\right)^2 = \boxed{0.0102} \quad (1\%\ \ \text{reflected})$$

$$T = 1-R = 1-0.0102 = 0.99 \quad (99\%\ \ \text{transmitted})$$

Quantum Mechanical Tunneling

Sketch the **wave function** $\psi(x)$ corresponding to a particle with energy E in the potential well shown below. Explain how and why the wavelengths and amplitudes of $\psi(x)$ are **different** in regions 1 and 2.



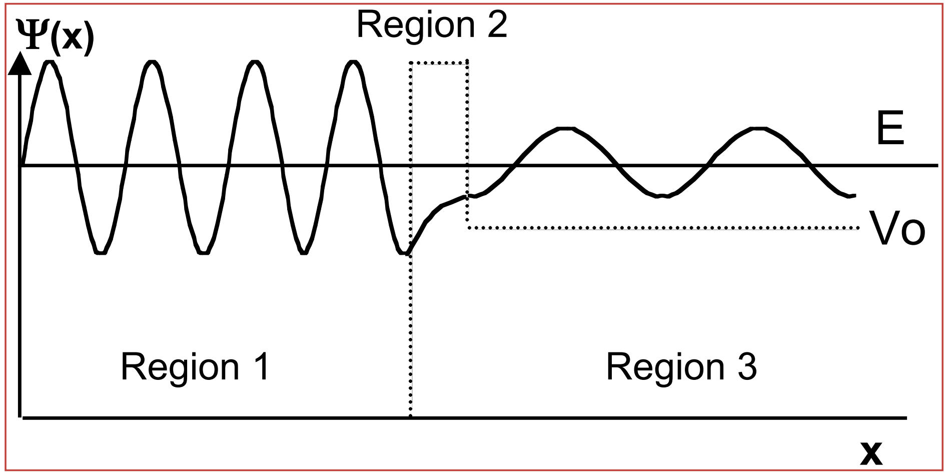
$\psi(x)$ **oscillates inside** the potential well because $E > V(x)$, and **decays exponentially outside** the well because $E < V(x)$.

The **frequency** of $\psi(x)$ is **higher in Region 1** vs. Region 2 because the kinetic energy is higher [$E_k = E - V(x)$].

The **amplitude** of $\psi(x)$ is **lower in Region 1** because its higher E_k gives a higher velocity, and the particle therefore spends less time in that region.

Quantum Mechanical Tunneling

Sketch the wave function ψ(x) corresponding to a particle with energy E in the potential shown below. Explain how and why the wavelengths and amplitudes of ψ(x) are different in regions 1 and 3.



ψ(x) **oscillates** in **regions 1 and 3** because E > V(x), and **decays exponentially** in **region 2** because E < V(x).

Frequency of ψ(x) is **higher in Region 1** vs. 3 because kinetic energy is higher there.

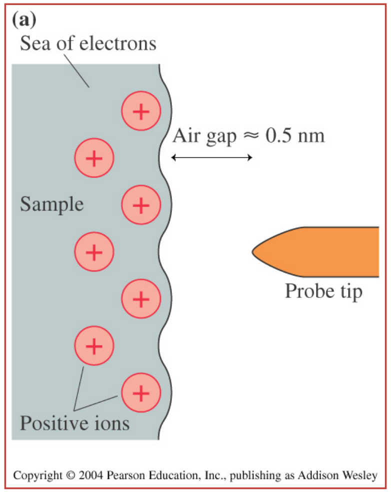
Amplitude of ψ(x) in Regions 1 and 3 depends on the initial location of the wave packet. If we assume a bound particle in Region 1, then the amplitude is higher there and decays into Region 3 (case shown above).

Quantum Mechanical Tunneling

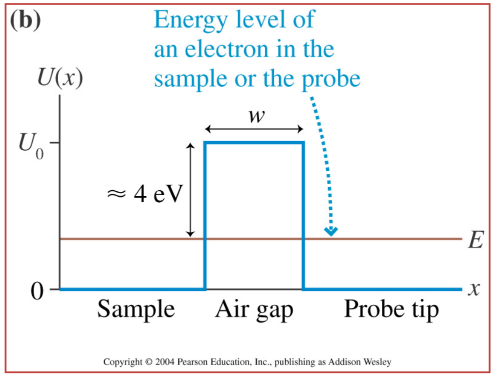
IMP

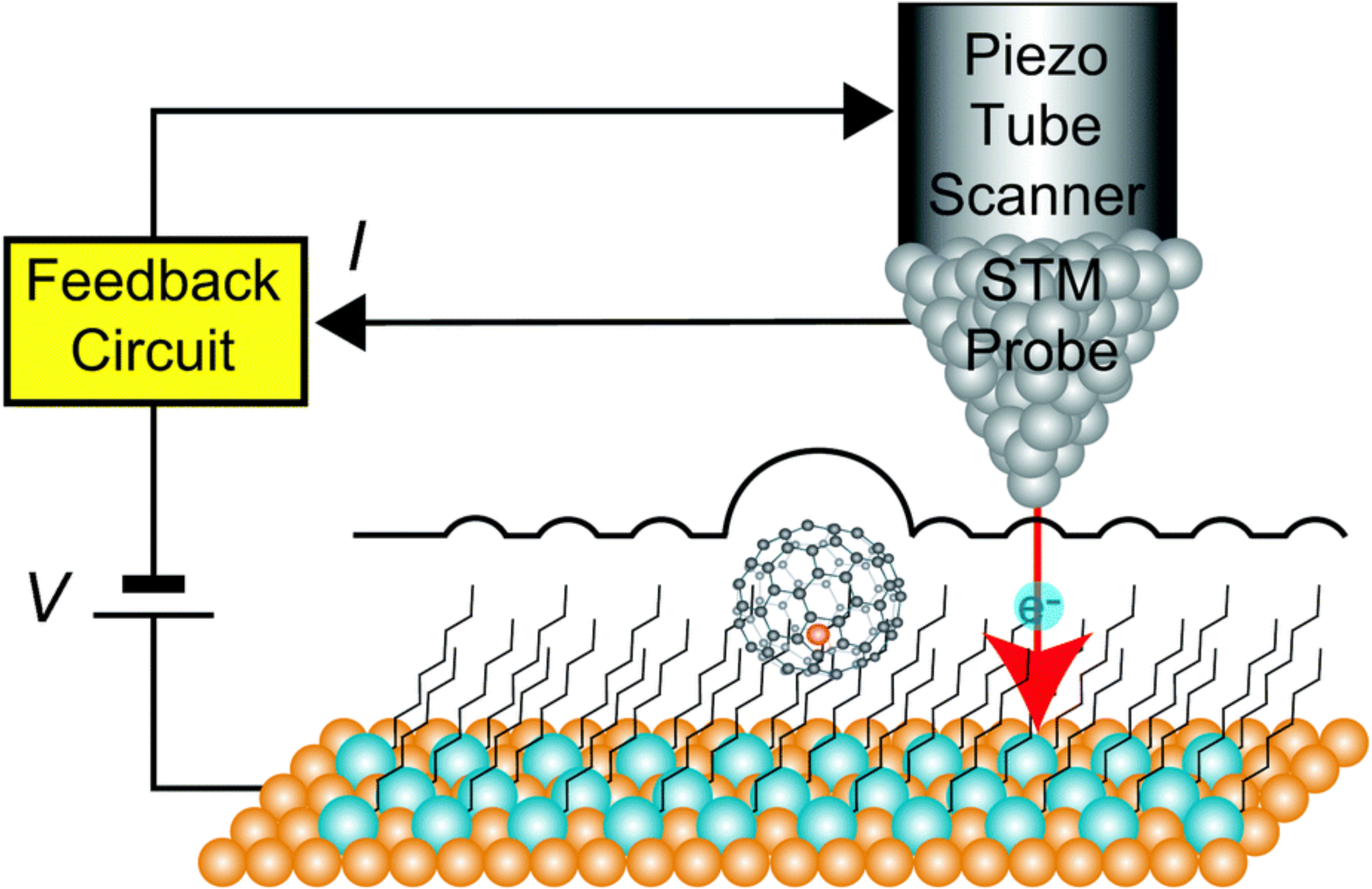
The scanning tunneling microscope:

Scanning-tunneling microscopes allow us to see objects at the atomic level.



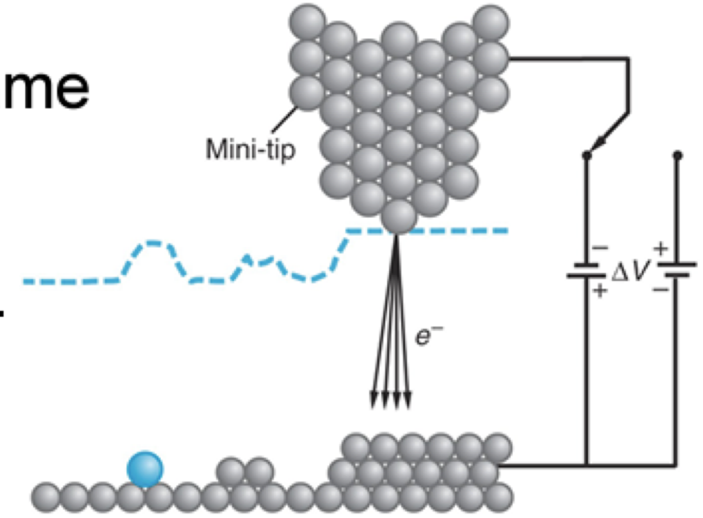
- A small air gap between the probe and the sample acts as a potential barrier.
- Energy of an electron is less than the energy of a free electron by an amount equal to the work function.
- Electrons can tunnel through the barrier to create a current in the probe.
- The current is highly sensitive to the thickness of the air gap.
- As the probe is scanned across the sample, the surface structure is mapped by the change in the tunneling current.

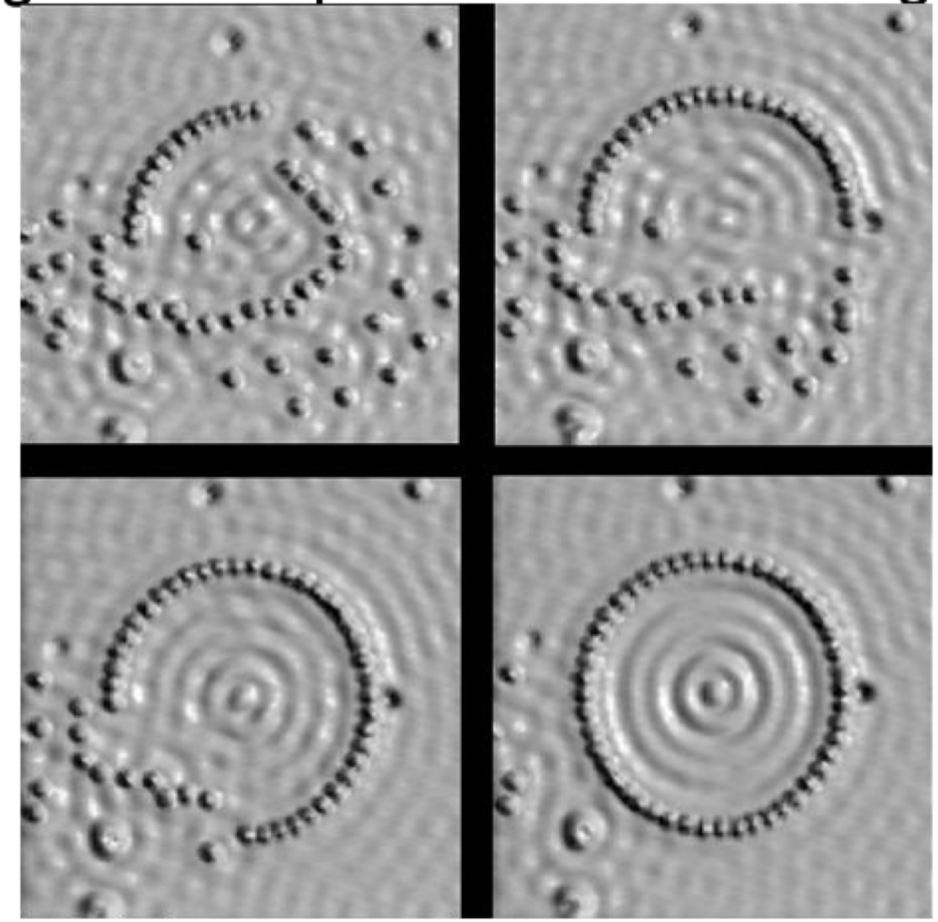



Piezo
Tube
Scanner
STM
Probe
Feedback
Circuit
I
V
e⁻

STM details

Actual STM uses feedback to keep the current (and therefore the distance) the same by moving the tip up or down and keeping track of how far it needed to move. This gives a map of the surface being scanned.





STM's can also be used to slide atoms around as shown.

How sensitive is the STM?

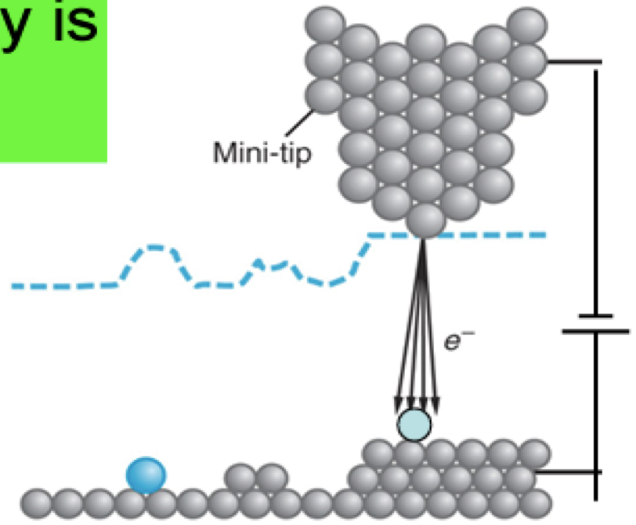
Remember tunneling probability is $P \approx e^{-2\alpha L}$ with $\alpha = \frac{\sqrt{2m(V-E)}}{\hbar}$

For work function of 4 eV $\alpha = \frac{\sqrt{2m(V-E)}}{\hbar} \approx 10\ \mathrm{nm}^{-1}$

Note this corresponds to a penetration depth of $\lambda = 1/\alpha = 0.1\ \mathrm{nm}$

If probe is 0.3 nm away ($L=0.3$ nm), probability is

$$e^{-2\alpha L} = e^{-2(10\ \mathrm{nm}^{-1})(0.3\ \mathrm{nm})} = e^{-6} = 0.0025$$

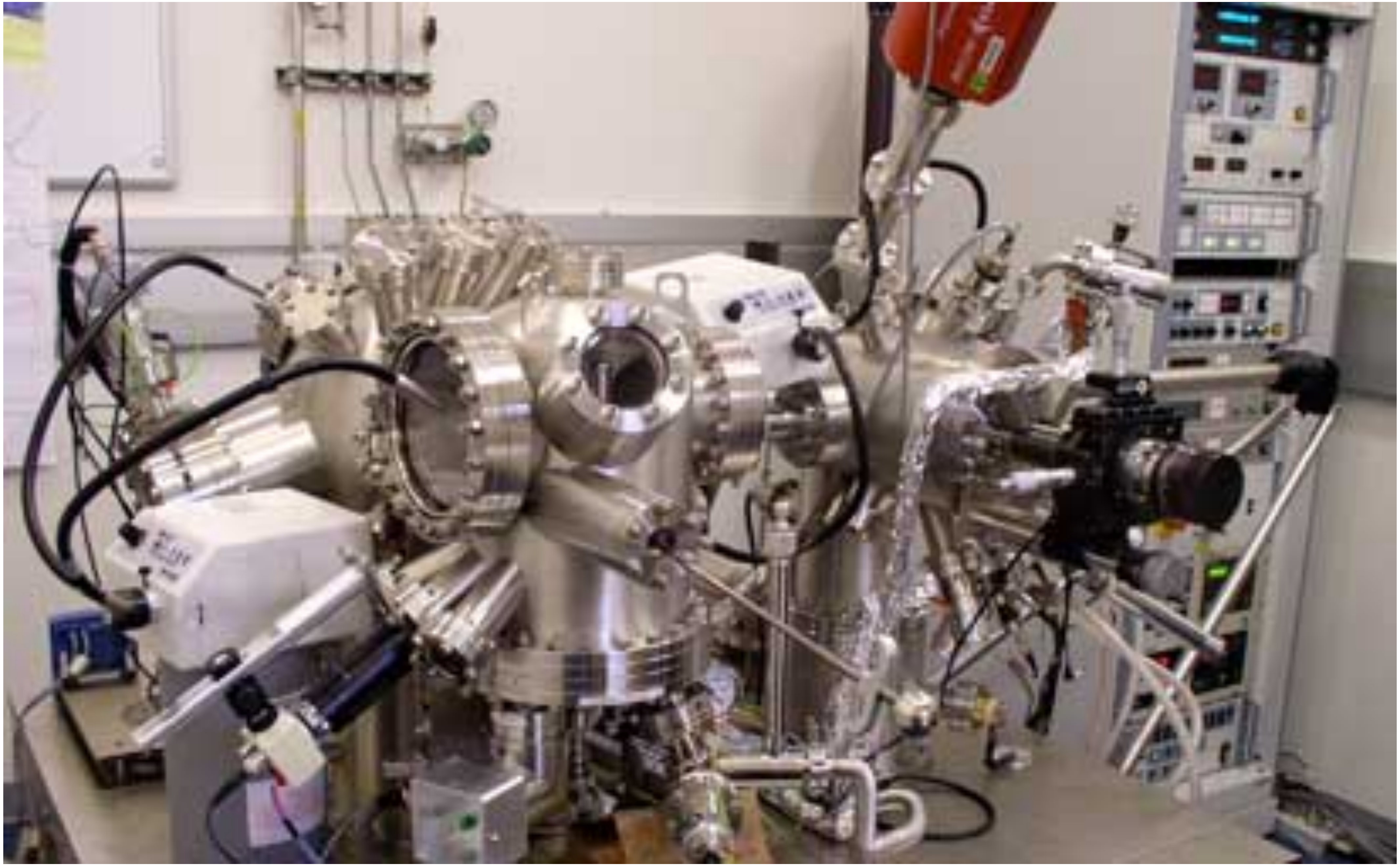


An extra atom on top decreases the distance by 0.1 nm so L = 0.2 nm giving a tunneling probability of

$$e^{-2\alpha L} = e^{-2(10\ \mathrm{nm}^{-1})(0.2\ \mathrm{nm})} = e^{-4} = 0.018$$

Current is proportional to the probability of an electron tunneling.

One atom increases current by 0.018/0.0025 = 7 times!



Quantum Mechanical Tunneling

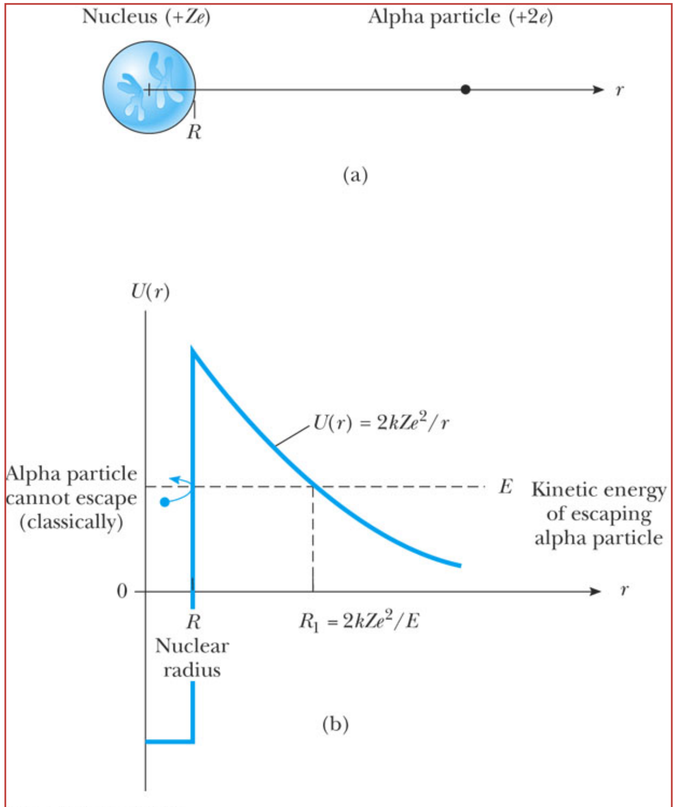
Decay of radioactive elements:

Emission of α particles (helium nucleii) in the decay of radioactive elements is an example of tunneling

- α particles are confined in the nucleus modeled as a square well
- α particles can eventually tunnel through the Coulomb potential barrier.
- Tunneling rate is very sensitive to small changes in energy, accounting for the wide range of decay times:

$$T = e^{8\sqrt{\frac{ZR}{r_0}} - 4\pi Z\sqrt{\frac{E_0}{E}}},$$

$$r_0 \approx 7.25\, fm,\ E_0 = 0.0993 MeV$$



Quantum Mechanical Tunneling

Decay of radioactive elements:

Emission of α particles (helium nucleii) in the decay of radioactive elements is an example of tunneling

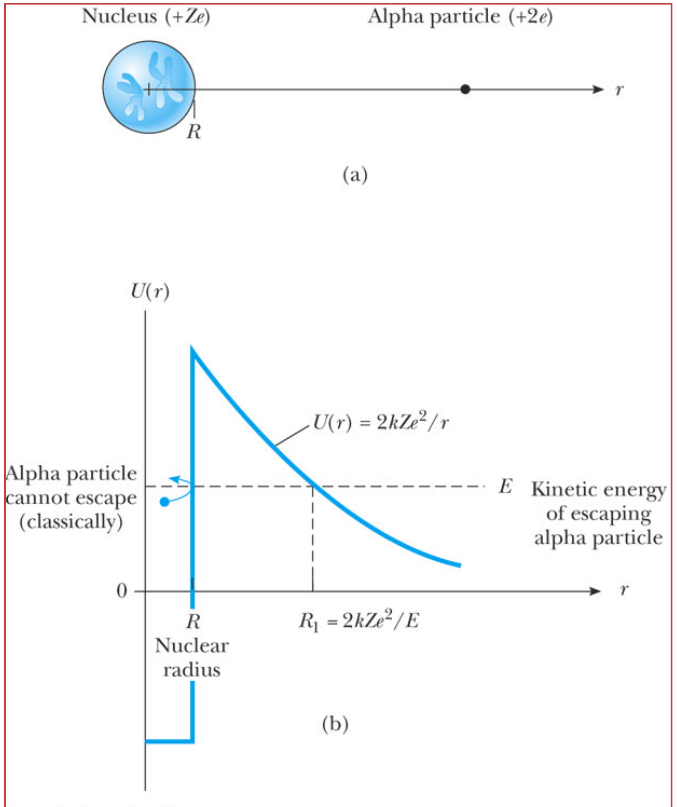
- Transmission probability:

$$T = e^{8\sqrt{\frac{ZR}{r_0}} - 4\pi Z\sqrt{\frac{E_0}{E}}},$$
$$r_0 \approx 7.25\, fm,\ E_0 = 0.0993 MeV$$

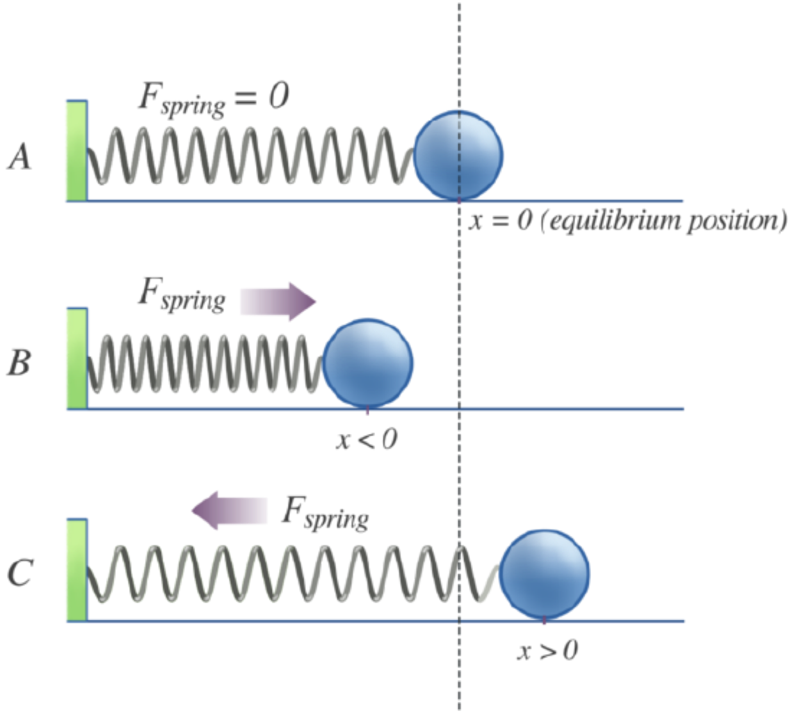
- Transmission rate λ = frequency of collisions with the barrier x T

$$\lambda = fT \approx 10^{21} e^{8\sqrt{\frac{ZR}{r_0}} - 4\pi Z\sqrt{\frac{E_0}{E}}},$$

- Half life: $$t_{1/2} = \frac{0.693}{\lambda}$$



Harmonic Oscillator



The Classic Harmonic Oscillator

A simple harmonic oscillator is a particle or system that undergoes harmonic motion about an equilibrium position, such as an object with mass vibrating on a spring. In this section, we consider oscillations in one-dimension only. Suppose a mass moves back-and-forth along the x-direction about the equilibrium position, $x = 0$. In classical mechanics, the particle moves in response to a linear restoring force given by $F_x = -kx$, where x is the displacement of the particle from its equilibrium position. The motion takes place between two turning points, $x \pm A$, where **A** denotes the amplitude of the motion. The position of the object varies periodically in time with angular frequency $\omega = \sqrt{k/m}$, which depends on the mass **m** of the oscillator and on the force constant k of the net force, and can be written as

$$x(t) = A\cos(\omega t + \phi). \tag{7.6.1}$$

The total energy E of an oscillator is the sum of its kinetic energy $K = mu^2/2$ and the elastic potential energy of the force $U(x) = kx^2/2$,

$$E = \frac{1}{2}mu^2 + \frac{1}{2}kx^2. \tag{7.6.2}$$

At turning points $x = \pm A$, the speed of the oscillator is zero; therefore, at these points, the energy of oscillation is solely in the form of potential energy $E = kA^2/2$. The plot of the potential energy $U(x)$ of the oscillator versus its position x is a parabola (Figure $7.6.1$). The potential-energy function is a quadratic function of x, measured with respect to the equilibrium position. On the same graph, we also plot the total energy E of the oscillator, as a horizontal line that intercepts the parabola at $x = \pm A$. Then the kinetic energy K is represented as the vertical distance between the line of total energy and the potential energy parabola.

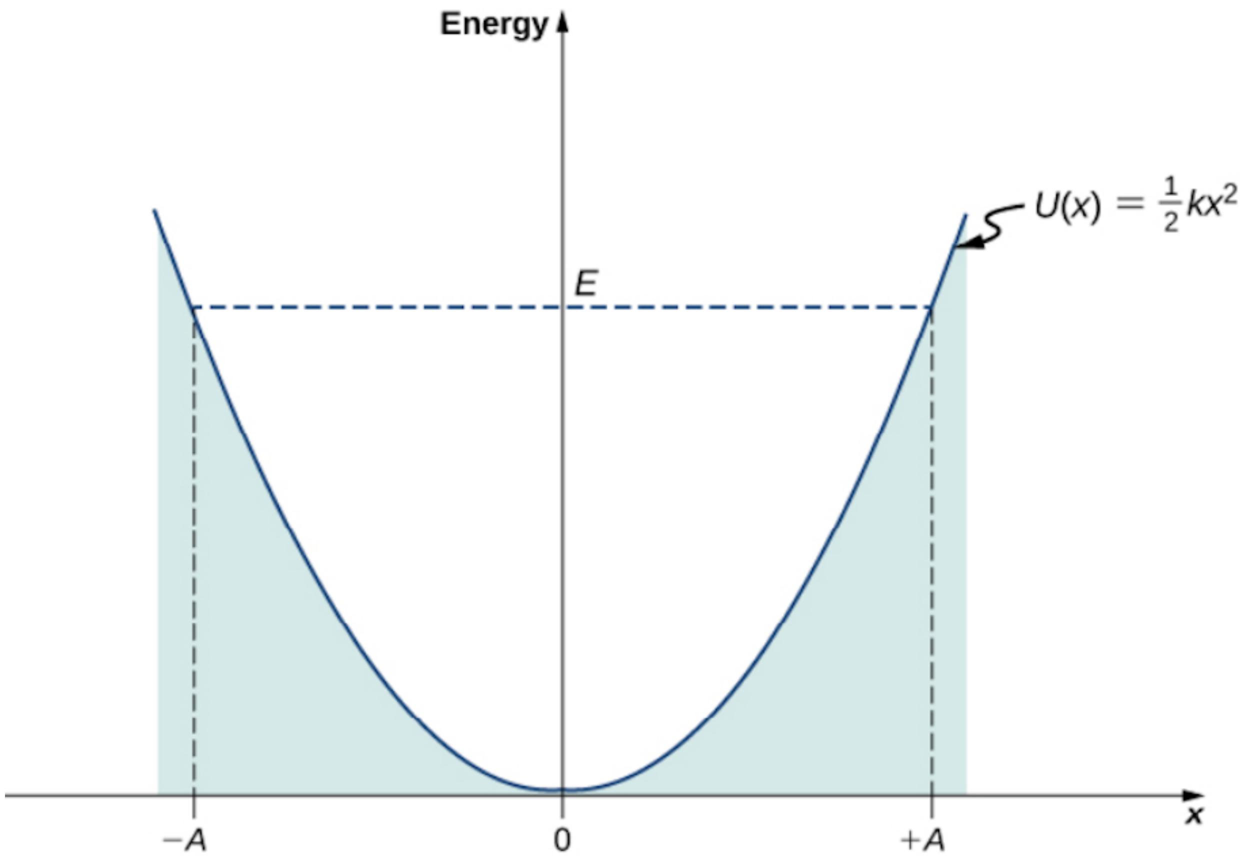


Figure 7.6.1

- In this plot, the motion of a classical oscillator is confined to the region where its kinetic energy is nonnegative, which is what the energy relation Equation
- Physically, it means that a classical oscillator can never be found beyond its turning points, and its energy depends only on how far the turning points are from its equilibrium position. The energy of a classical oscillator changes in a continuous way.

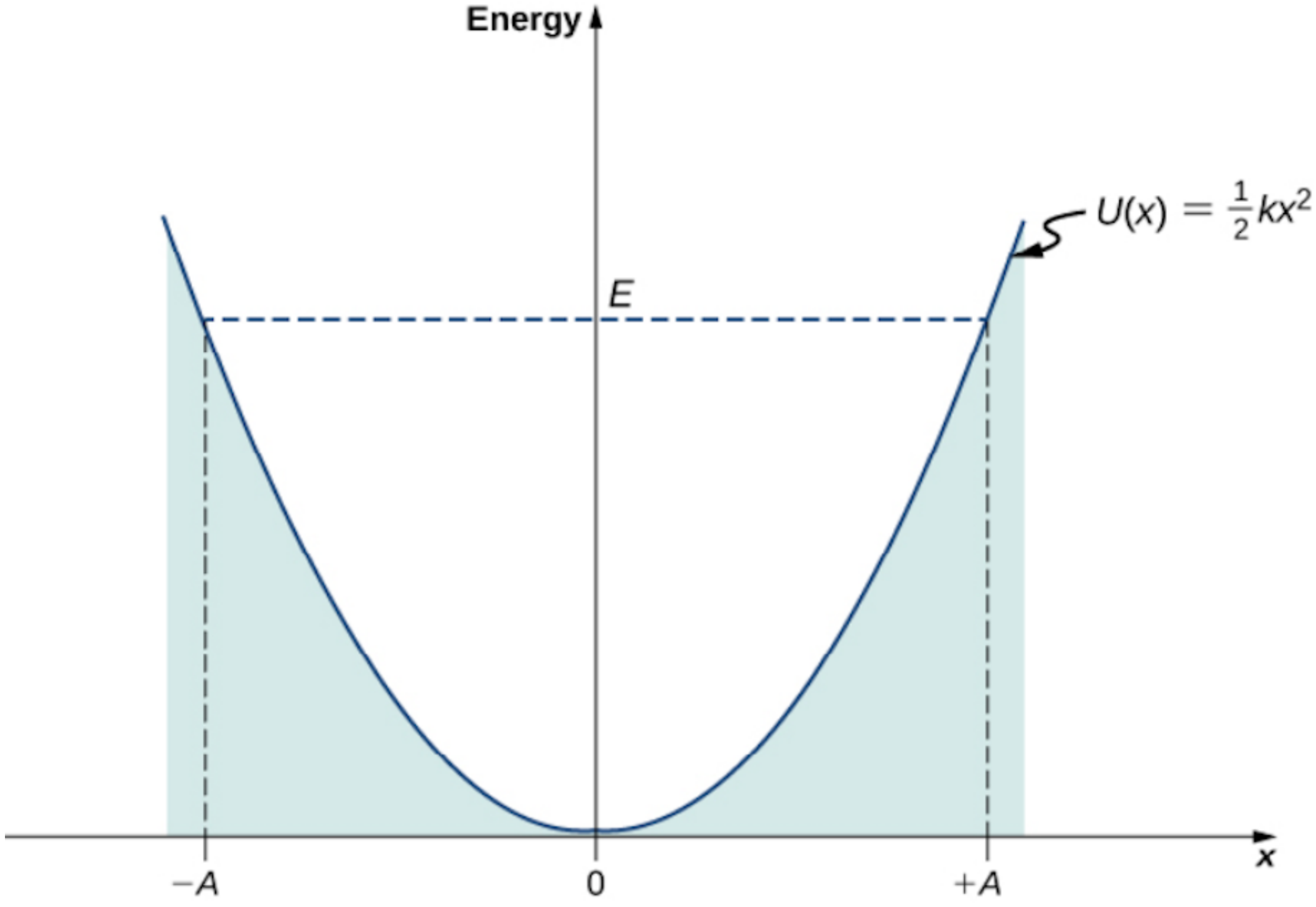


Figure 7.6.1

- The lowest energy that a classical oscillator may have is zero, which corresponds to a situation where an object is at rest at its equilibrium position. The zero-energy state of a classical oscillator simply means no oscillations and no motion at all (a classical particle sitting at the bottom of the potential well in Figure

When an object oscillates, no matter how big or small its energy may be, it spends the longest time near the turning points, because this is where it slows down and reverses its direction of motion. Therefore, the probability of finding a classical oscillator between the turning points is highest near the turning points and lowest at the equilibrium position.

The Quantum Harmonic Oscillator

One problem with this classical formulation is that it is not general. We cannot use it, for example, to describe vibrations of diatomic molecules, where quantum effects are important. A first step toward a quantum formulation is to use the classical expression $k = m\omega^2$ to limit mention of a "spring" constant between the atoms. In this way the potential energy function can be written in a more general form,

$$U(x) = \frac{1}{2} m\omega^2 x^2. \tag{7.6.3}$$

Combining this expression with the time-independent Schrödinger equation gives

$$-\frac{\hbar}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi(x) = E\psi(x). \tag{7.6.4}$$

To solve Equation 7.6.4, that is, to find the allowed energies E and their corresponding wavefunctions $\psi(x)$ - we require the wavefunctions to be symmetric about $x = 0$ (the bottom of the potential well) and to be normalizable. These conditions ensure that the probability density $|\psi(x)|^2$ must be finite when integrated over the entire range of **x** from $-\infty$ to $+\infty$. How to solve Equation 7.6.4 is the subject of a more advanced course in quantum mechanics; here, we simply cite the results. The allowed energies are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{7.6.5}$$

$$= \frac{2n+1}{2}\hbar\omega \tag{7.6.6}$$

with $n = 0, 1, 2, 3, \ldots$

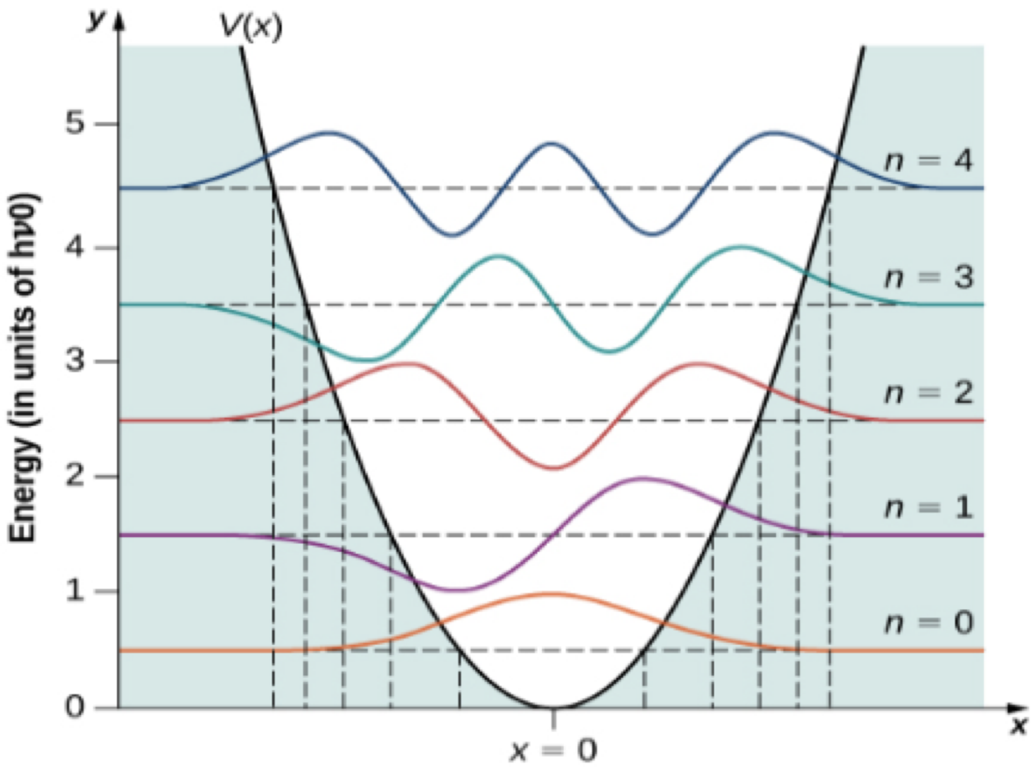
The wavefunctions that correspond to these energies (the stationary states or states of definite energy) are

$$\psi_n(x) = N_n e^{-\beta^2 x^2/2} H_n(\beta x),\ n = 0, 1, 2, 3, \ldots \tag{7.6.7}$$

where $\beta = \sqrt{m\omega/\hbar}$, N_n is the normalization constant, and $H_n(y)$ is a polynomial of degree n called a **Hermite polynomial**. The first four Hermite polynomials are

- $H_0(y) = 1$
- $H_1(y) = 2y$
- $H_2(y) = 4y^2 - 2$
- $H_3(y) = 8y^3 - 12y$.

A few sample wavefunctions are given in Figure 7.6.2. As the value of the principal number increases, the solutions alternate between even functions and odd functions about $x = 0$.



Several interesting features appear in this solution. Unlike a classical oscillator, the measured energies of a quantum oscillator can have only energy values given by Equation 7.6.6. Moreover, unlike the case for a quantum particle in a box, the allowable energy levels are evenly spaced,

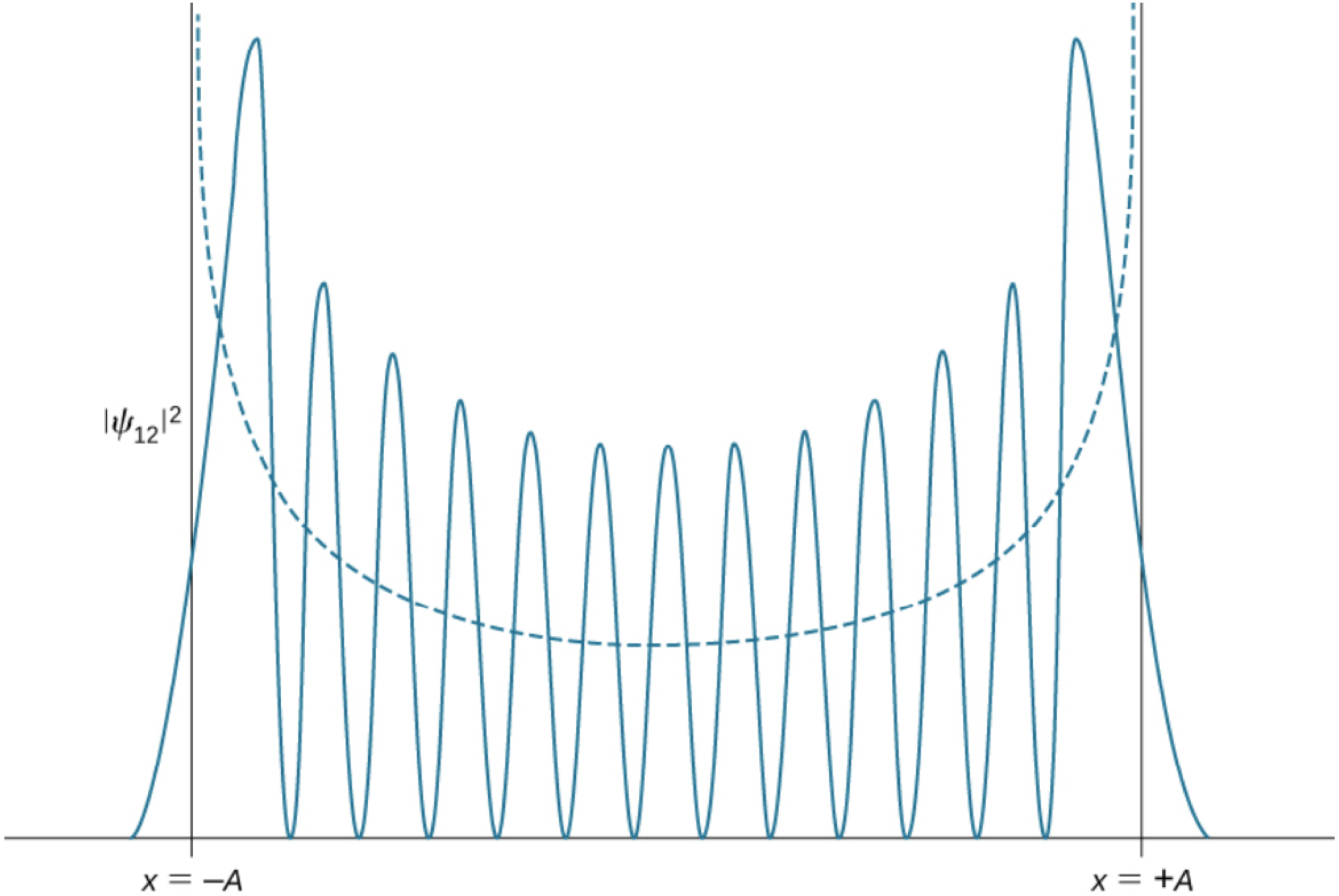
$$\begin{aligned} \Delta E &= E_{n+1} - E_n && (7.6.8) \\ &= \frac{2(n+1)+1}{2}\hbar\omega - \frac{2n+1}{2}\hbar\omega && (7.6.9) \\ &= \hbar\omega = hf. && (7.6.10) \end{aligned}$$

- When a particle bound to such a system makes a transition from a higher-energy state to a lower-energy state, the smallest- energy quantum carried by the emitted photon is necessarily hf .
- Similarly, when the particle makes a transition from a lower-energy state to a higher-energy state, the smallest-energy quantum that can be absorbed by the particle is hf.
- A quantum oscillator can absorb or emit energy only in multiples of this smallest-energy quantum. This is consistent with Planck’s hypothesis for the energy exchanges between radiation and the cavity walls in the blackbody radiation problem.

The quantum oscillator differs from the classic oscillator in three ways:

- First, the ground state of a quantum oscillator is $E_0 = \hbar\omega/2$, not zero. In the classical view, the lowest energy is zero. The nonexistence of a zero-energy state is common for all quantum-mechanical systems because of omnipresent fluctuations that are a consequence of the Heisenberg uncertainty principle. If a quantum particle sat motionless at the bottom of the potential well, its momentum as well as its position would have to be simultaneously exact, which would violate the Heisenberg uncertainty principle. Therefore, the lowest-energy state must be characterized by uncertainties in momentum and in position, so the ground state of a quantum particle must lie above the bottom of the potential well.
- Second, a particle in a quantum harmonic oscillator potential can be found with nonzero probability outside the interval $-A \leq x \leq +A$. In a classic formulation of the problem, the particle would not have any energy to be in this region. The probability of finding a ground-state quantum particle in the classically forbidden region is about 16%.
- Third, the probability density distributions $|\psi_n(x)|^2$ for a quantum oscillator in the ground low-energy state, $\psi_0(x)$, is largest at the middle of the well $(x = 0)$. For the particle to be found with greatest probability at the center of the well, we expect that the particle spends the most time there as it oscillates. This is opposite to the behavior of a classical oscillator, in which the particle spends most of its time moving with relative small speeds near the turning points.

The classical probability density distribution corresponding to the quantum energy of the $n = 12$ state is a reasonably good approximation of the quantum probability distribution for a quantum oscillator in this excited state. This agreement becomes increasingly better for highly excited states.



The probability density distribution for finding the quantum harmonic oscillator in its $n = 12$ quantum state. The dashed curve shows the probability density distribution of a classical oscillator with the same energy.