Speedy Quantum Mechanics

The Schrödinger Equation

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \Psi}{\partial t^2}$$

The Classical Wave Equation

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

The Time-Dependent Schrödinger Equation

$\Psi(x,\ t)$ represents the quantum wave function of a particle of mass *m*, moving in a straight line, with zero net force acting on it.

The Schrödinger Equation

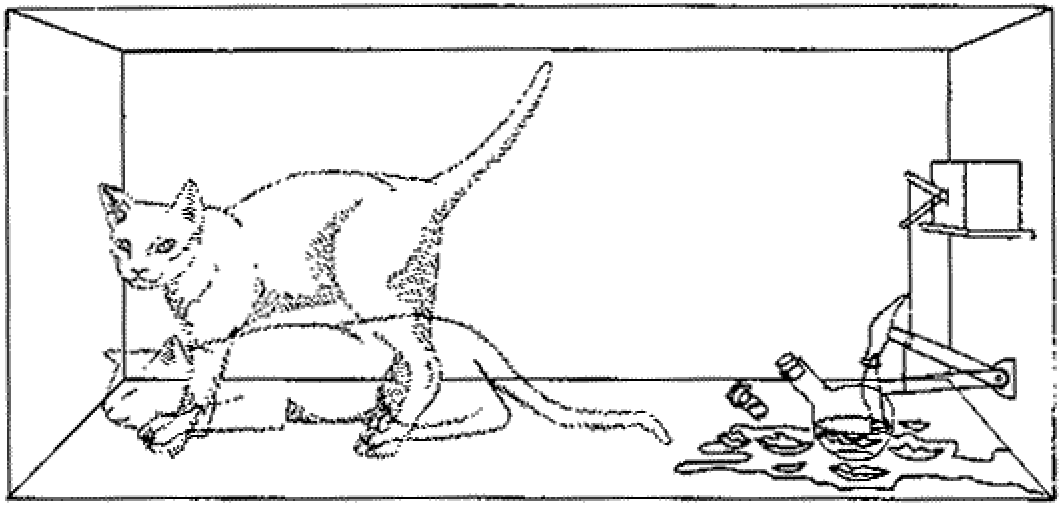
- This equation, like the classical wave equation, has solutions that look like we expect waves to behave, i.e., $\cos[2\pi(x/\lambda - t/T)]$, but for quantum waves, $\lambda = h/p$ is the de Broglie wavelength of the particle, and $f = E/h$ is the quantum wave frequency.
- Unlike a classical wave, this wave can be complex and it does not describe some measurable entity like string displacement.
- Instead, the square of Ψ is the physical, measurable property.
- $\Psi^*(x,t)\Psi(x,t) = |\Psi(x,t)|^2$ is called the probability amplitude and represents the probability that the particle will be found at point *x* at time *t*.

The Probabilistic Interpretation of the Wave Function

It is this last statement, the probabilistic interpretation of the wave function, that gives quantum theory all its weirdness. It means, among other things, that

- a single electron can pass through a double slit apparatus and exhibit 50% probability of passing through each of the holes. This means that the part of the probability wave that passed through one slit can interfere with the part that passed through the other slit, causing an interference pattern.
- a radioactive nucleus can, at one moment, have a 50% probability of being decayed and 50% probability of being intact.
- Schrödinger's cat can, at one moment, have a 50% probability of being dead and 50% probability of being alive (thus the visit to Professor Schrödinger from the Royal Society for the Prevention of Cruelty to Animals.)

Schrödinger's Cat



"And you're quite sure it's just a hypothetical cat?"

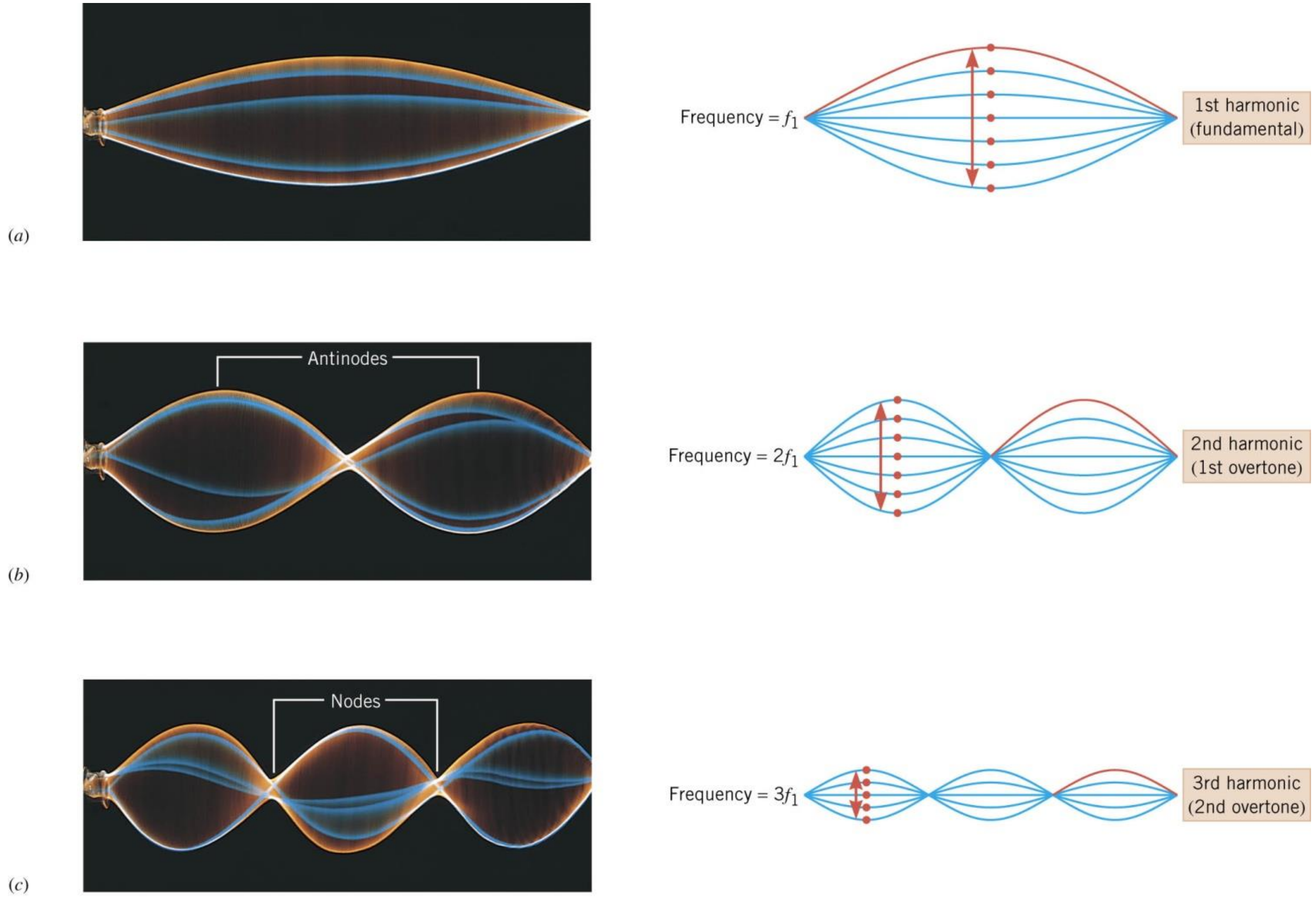
“Collapsing the Wave Function”

Ultimately, however, electrons, nuclei, and cats are particles, and when we look at them, they are either here or there, alive or dead. The key phrase here is “when we look.”

Matter, progressing through time unobserved, behaves in a probabilistic fashion, exhibiting quantum indeterminacy about where it is, how fast it is moving, even if it continues to exist. When we look, however, it is always seen to behave in the way we expect matter to behave, with a definitive location, speed, and mortality.

The act of looking, or more generally the act of measurement, projects quantum entities onto a screen of classical expectation. This, the effect of measurement upon the results of a measurement, is the form the Heisenberg Uncertainty Principle takes in Schrödinger’s version of quantum theory.

Classical Standing Waves



$$\lambda = \frac{2a}{n}, n = 1, 2, 3, \ldots$$

Standing Waves in Quantum Mechanics. Stationary States

$$\Psi(x,t) = \psi(x)(a\,cos\omega t + b\,sin\omega t)$$

- *classical wave function*
- *real number*
- *coefficients a and b are always real*

$$\Psi(x,t) = \psi(x)(cos\omega t - i\,sin\omega t)$$

$$= \psi(x)e^{-i\omega t}$$

- *quantum wave function*
- *complex number*
- *temporal part always has this form*

For a quantum standing wave, the distribution of matter is time independent or stationary $\Rightarrow$ ***stationary states***.

Quick Recap of Complex Numbers

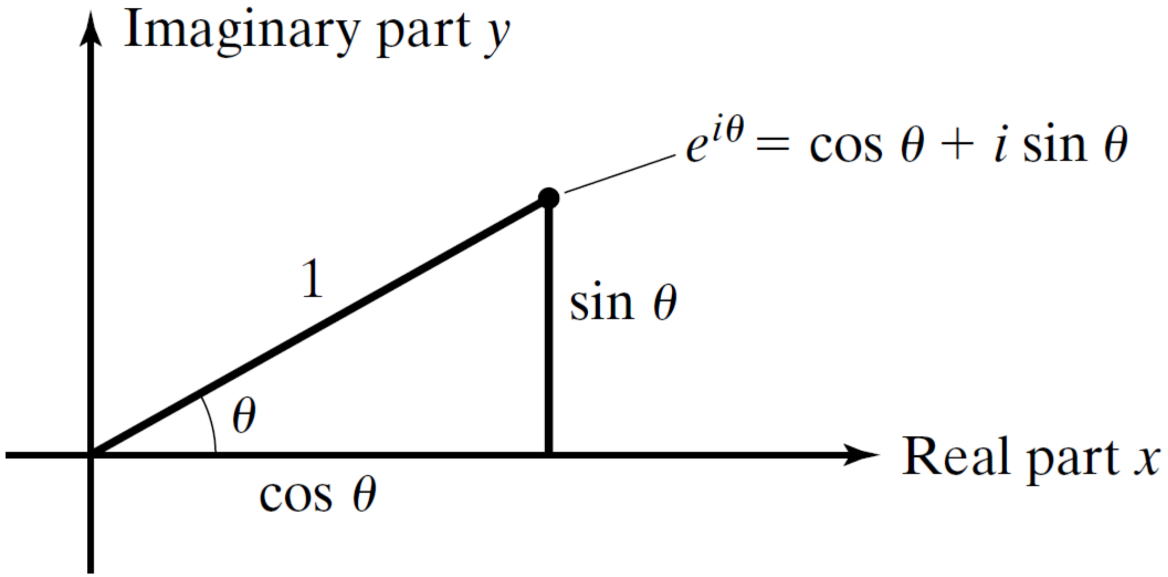


FIGURE 7.4

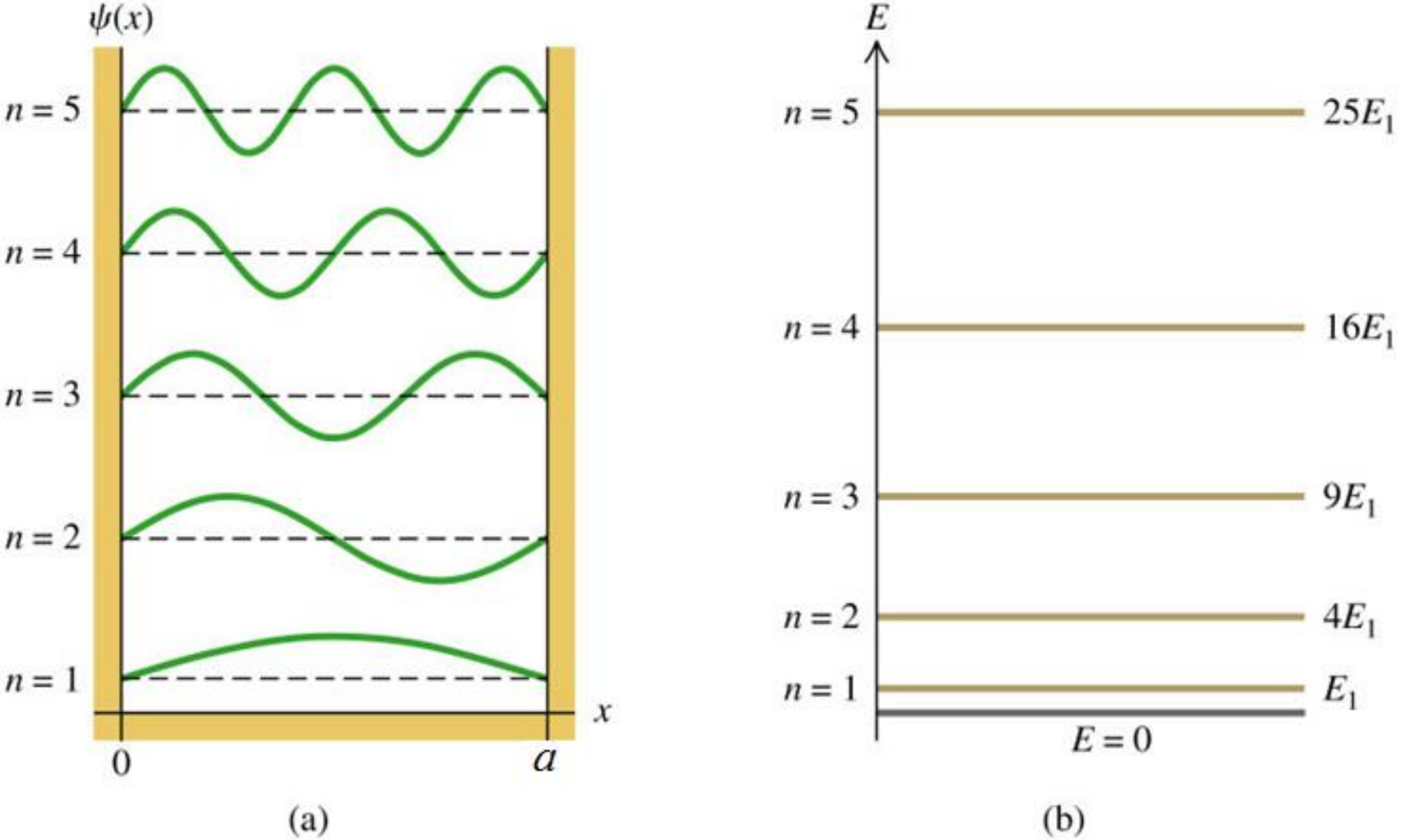
The complex number $e^{i\theta} = \cos\theta + i\sin\theta$ is represented by a point with coordinates $(\cos\theta, \sin\theta)$ in the complex plane. The absolute value of any complex number $z = x + iy$ is defined as $|z| = \sqrt{x^2 + y^2}$. Since $\cos^2\theta + \sin^2\theta = 1$, it follows that $|e^{i\theta}| = 1$.

$$\Psi(x,t) = \psi(x)e^{-i\omega t} \quad (7.11)$$

$$|\Psi(x,t)|^2 = |\psi(x)|^2|e^{-i\omega t}|^2$$

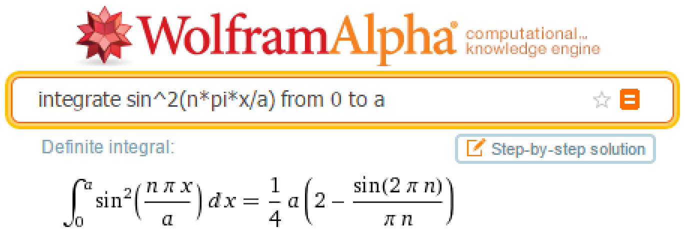
or, since $|e^{-i\omega t}| = 1$, $|\Psi(x,t)|^2 = |\psi(x)|^2$ (for quantum standing waves) (7.12)

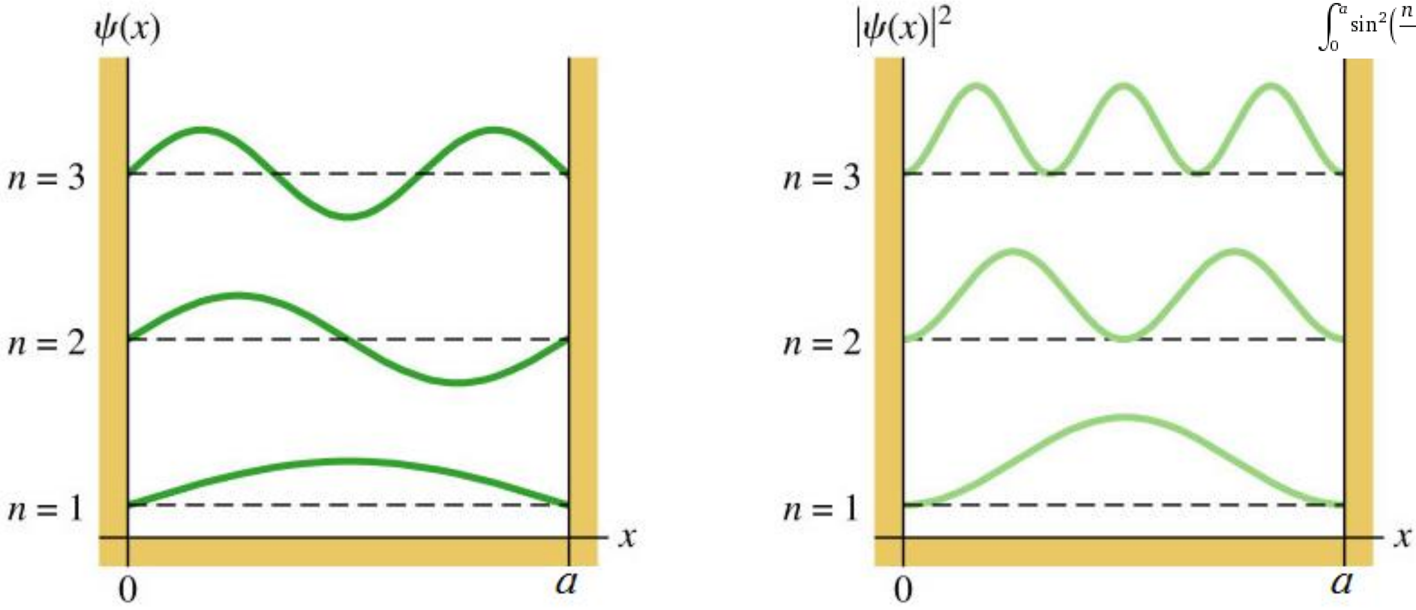
Particle in a Box: Wave Functions and Energy-Level Diagram



$$E = \frac{p^2}{2m} = n^2\left(\frac{\pi^2\hbar^2}{2ma^2}\right), n = 1, 2, 3, \dots$$

Particle in a Box: Probability and Normalization. Expectation Values





(a) (b)

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

$$\psi(x) = \sqrt{\frac{2}{a}} sin\left(\frac{n\pi x}{a}\right), n = 1, 2, 3, \ldots$$

The Schrödinger Wave Equation

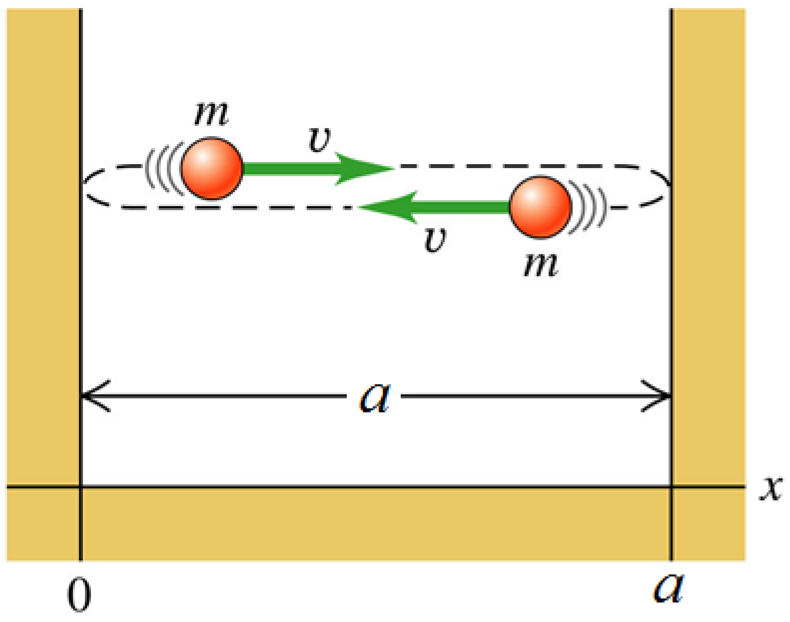
$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

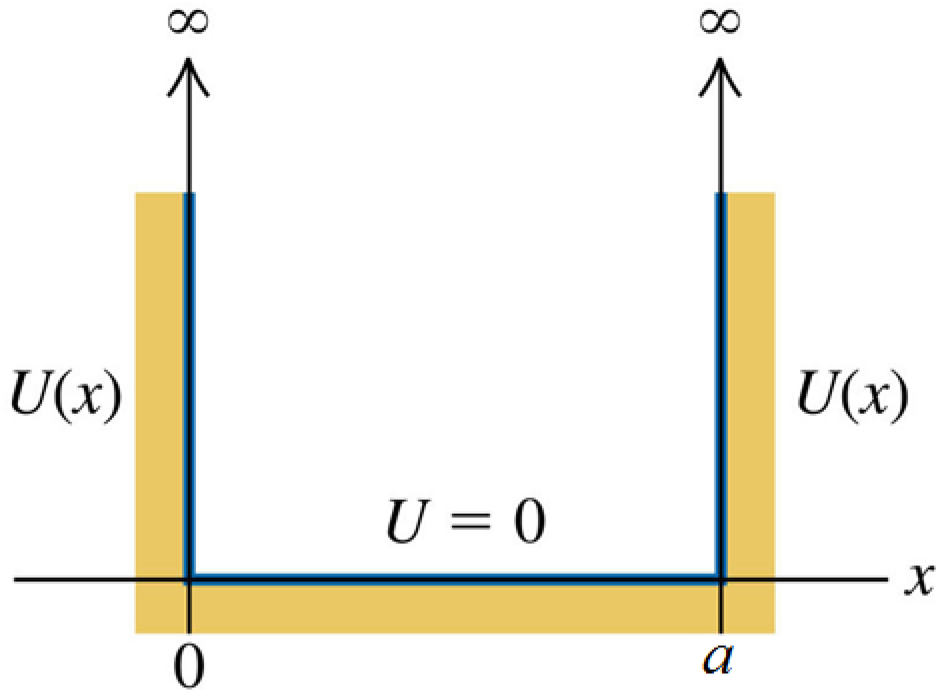
time-dependent Schrödinger Equation

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

time-independent Schrödinger Equation

The Schrödinger Equation and the Infinite Potential Well (i.e., the Rigid Box)





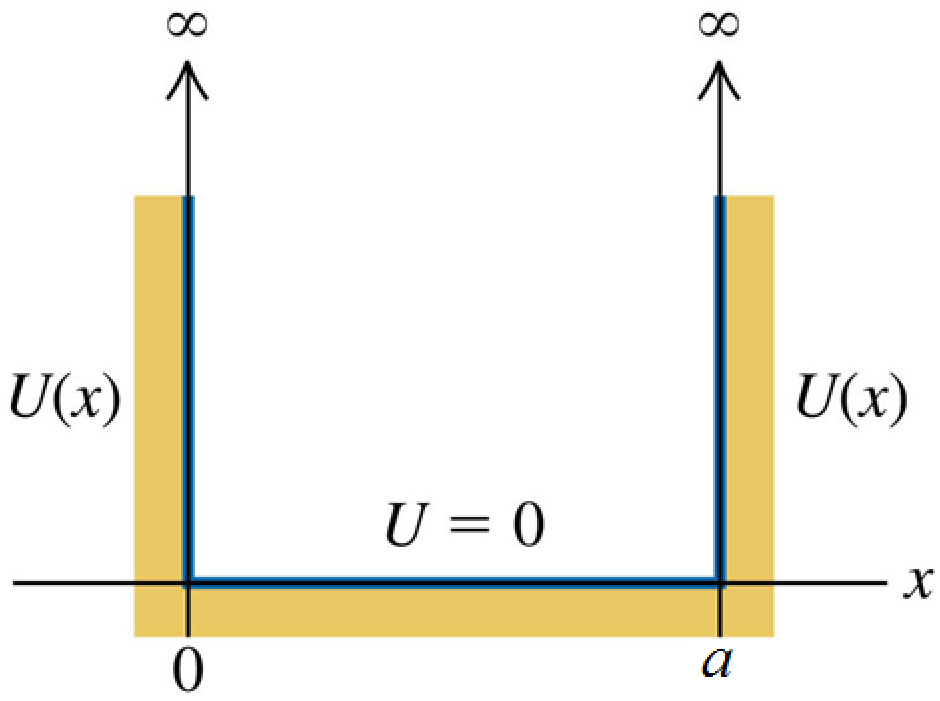
$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[U(x) - E]\psi$$

$$U(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & x < 0 \text{ and } x > a \end{cases}$$

The Schrödinger Equation and the Infinite Potential Well (i.e., the Rigid Box)

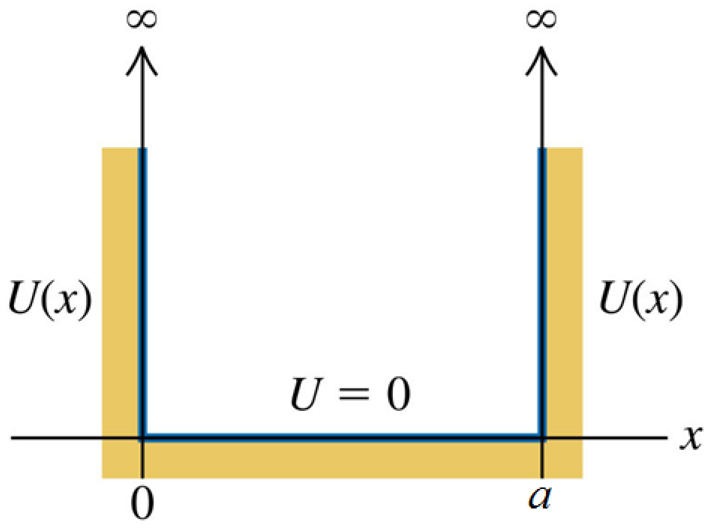
$$\psi' \equiv \frac{d\psi}{dx} \quad \text{and} \quad \psi'' \equiv \frac{d^2\psi}{dx^2}$$

$$\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x) \qquad (7.45)$$



- $\int_{-\infty}^{+\infty} |\psi(x)|^2 = 1$ *normalization*
- $\psi(x) = 0$ *outside the box*
- $\psi(x)$ – *continuous at the walls* $\Rightarrow \psi(0) = \psi(a) = 0$
- $\psi'(x)$ – *continuous everywhere except at the walls*

The Schrödinger Equation and the Infinite Potential Well: E < 0; E = 0; E > 0



$$\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x)$$

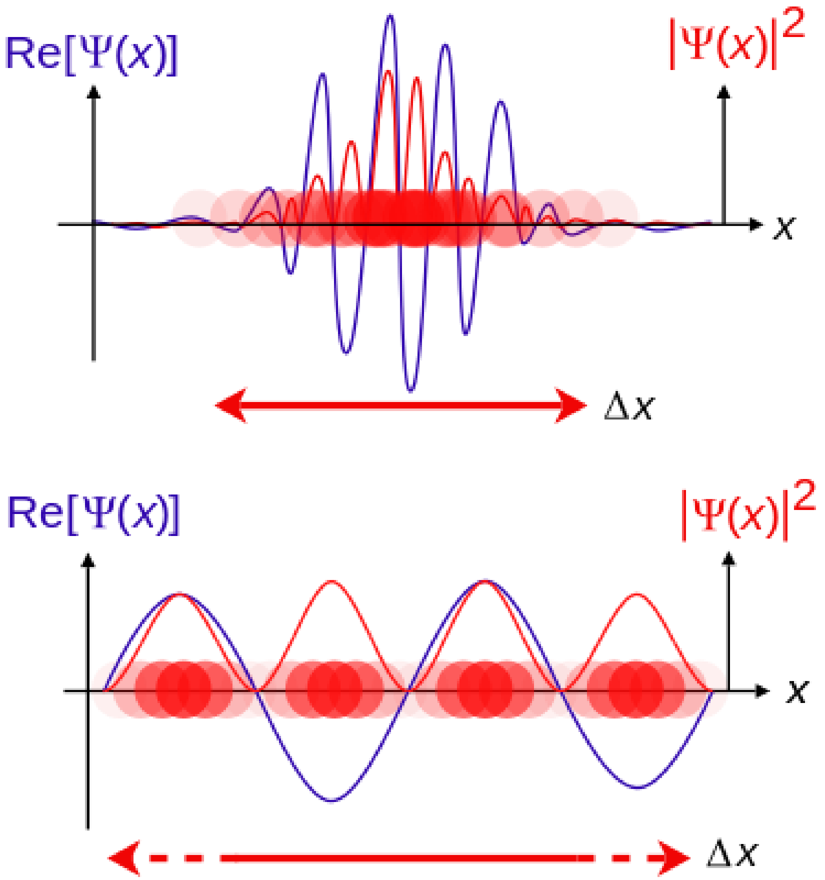
If $E < 0$, the only solution of the Schrödinger equation that satisfies the boundary conditions is the zero function. In other words, with $E < 0$, there can be no standing waves, so negative values of E are not allowed. A similar argument gives the same conclusion for $E = 0$.

$E > 0$ $\qquad k = \frac{\sqrt{2mE}}{\hbar}$ $\qquad \psi''(x) = -k^2\psi(x)$ $\qquad \psi(x) = A \sin kx + B \cos kx$

$$k = \frac{n\pi}{a}$$

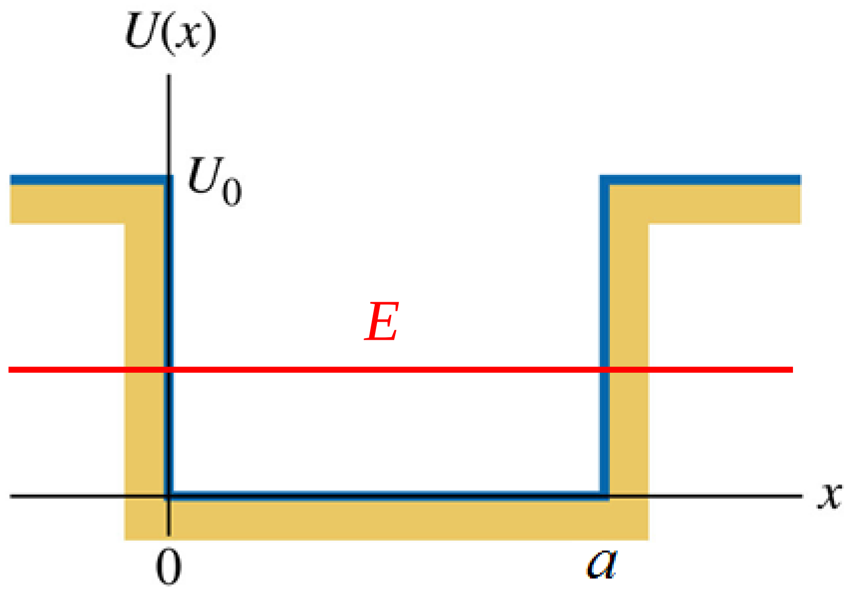
$$E = \frac{\hbar^2 k^2}{2m} = n^2\frac{\pi^2\hbar^2}{2ma^2}$$

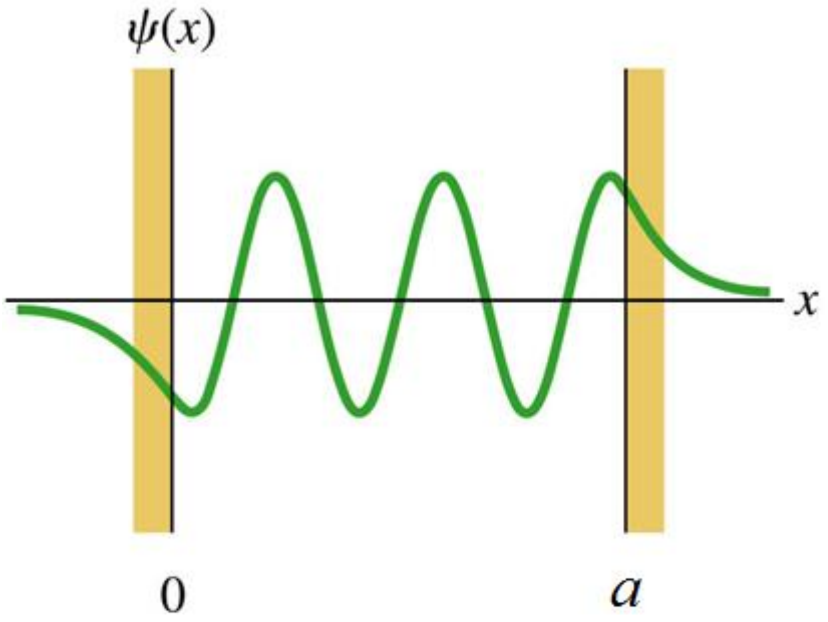
The Free Particle



The energy of a free particle is **not quantized**!

Finite Potential Well





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

$$U(x) = \begin{cases} 0 & 0 \le x \le a \\ U_0 & x < 0 \; and \; x > a \end{cases}$$

- possible wave functions in a finite well
- sinusoidal inside and exponential outside
- $\psi(x) \to 0$ as $x \to \pm\infty$
- joins smoothly at $x = 0$ and $x = a$
- $\psi'(x)$ is continuous at $x = 0$ and $x = a$

Finite Potential Well

- Matching the sinusoidal and exponential functions at the boundary points so that they join smoothly is only possible for certain specific values of E.
- There is no simple formula for the energy levels, as in the case of the infinite well.
- We need to solve a transcendental equation by numerical approximation.
- Each energy level, including the ground level, is lower for a finite well than for the infinitely deep well with the same width.
- The wavelength of the sinusoidal part of each wave function is longer than would be with an infinite well.

Finite Potential Well (Continued)

- A well with finite depth U_0 has only a ***finite number of bound states*** and corresponding energy levels, compared to the infinite number for an infinitely deep well.
- How many levels there are depends on the magnitude of U_0 in comparison with the ground level energy E_∞ for the infinite well. $E_\infty = \dfrac{\pi^2\hbar^2}{2ma^2}$
- When $U_0 \gg E_\infty$ (very deep well) there will be many bound states, and the energies of the lowest few are nearly the same as the energies for the infinitely deep well.
- When U_0 is only a few times as large as E_∞ there will be only a few bound states.
- There is always ***at least one bound state***, no matter how shallow the well.
- When $U_0 < E_\infty$ there is only one bound state (shallow well).
- There is ***no state with $E = 0$*** (as was also the case with the infinite well). Such a state would violate the uncertainty principle.
- In the limit $U_0 \ll E_\infty$ (very shallow or very narrow well) $E \approx 0.68U_0$

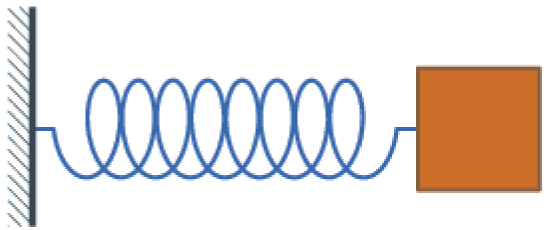
Finite Potential Well (Continued)

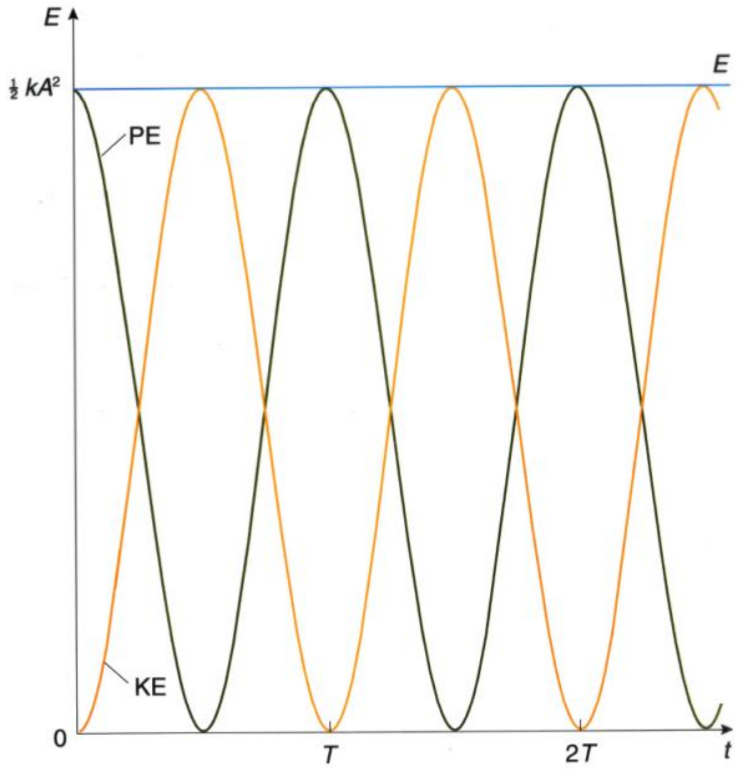
- There are also states for which $E > U_0$. In these states the particle is not bound, but is free to move through all the values of x. Any $E > U_0$ is possible, i.e., there is a **continuum** of energy states, rather than a discrete set.
- The free-particle wave functions are sinusoidal both inside and outside the well.
- The wavelength is shorter inside (or rather above) the well, corresponding to greater kinetic energy in the well than outside.

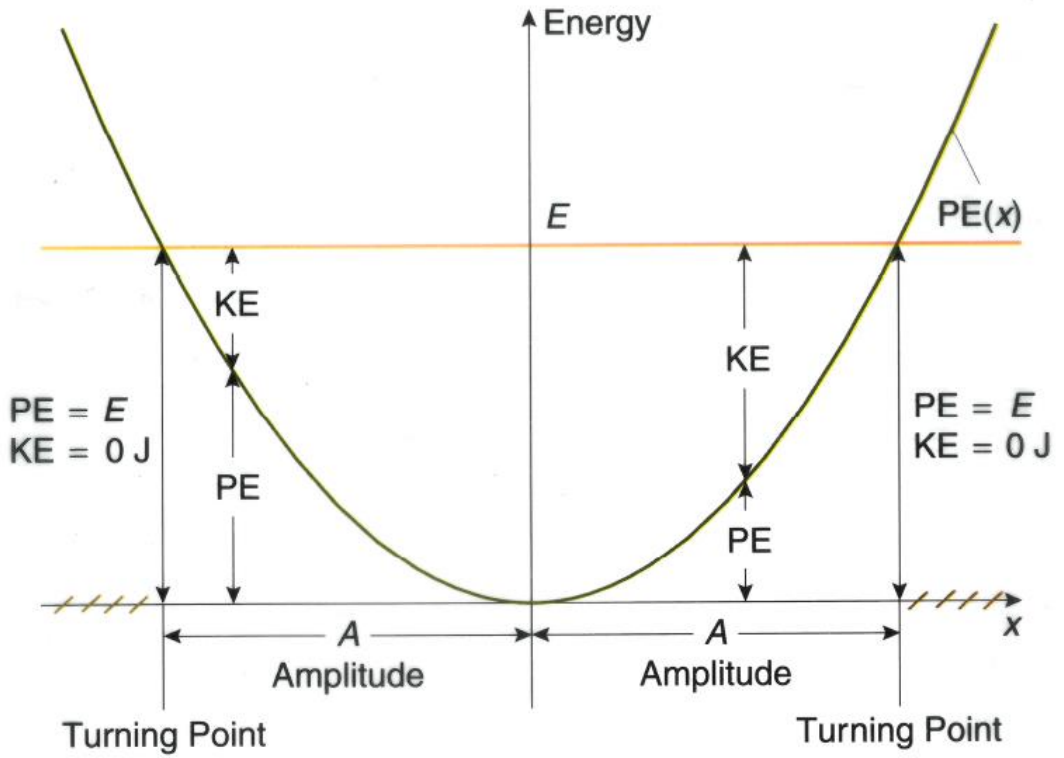
Practical applications of the finite square well:

- Electron inside a metallic sheet
- The 3-D version ($U = 0$ inside a spherical region of radius R and $U = U_0$ outside) provides a simple model for the interaction of a neutron with the nucleus in neutron-scattering experiments (the “crystal-ball” model of the nucleus.)

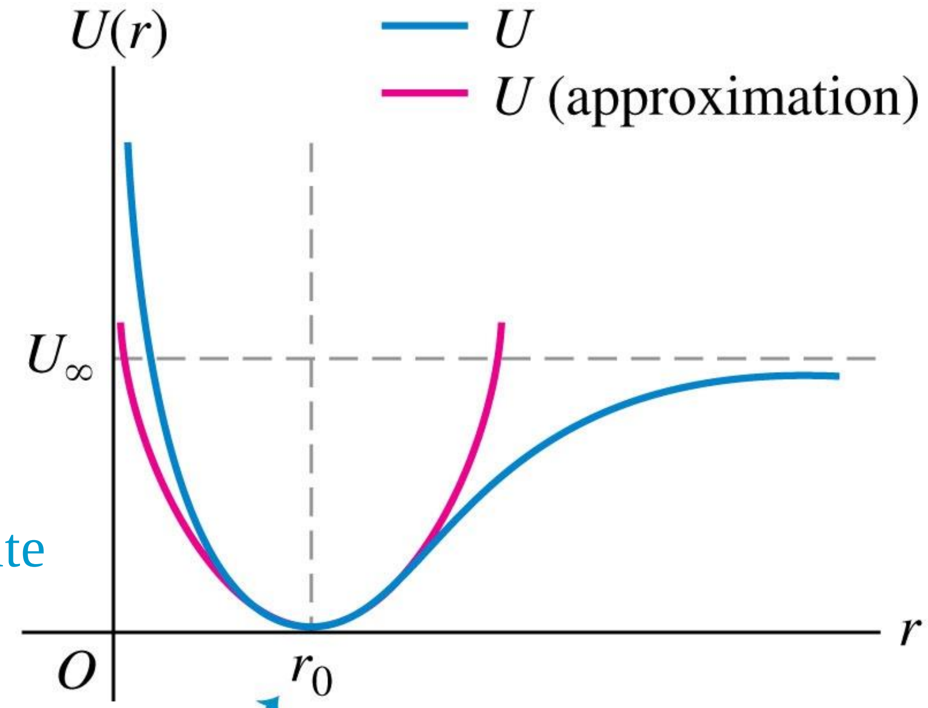
The Simple Harmonic Oscillator







A potential energy function describing the interaction of two atoms in a diatomic molecule



Potential energy needed to dissociate the molecule

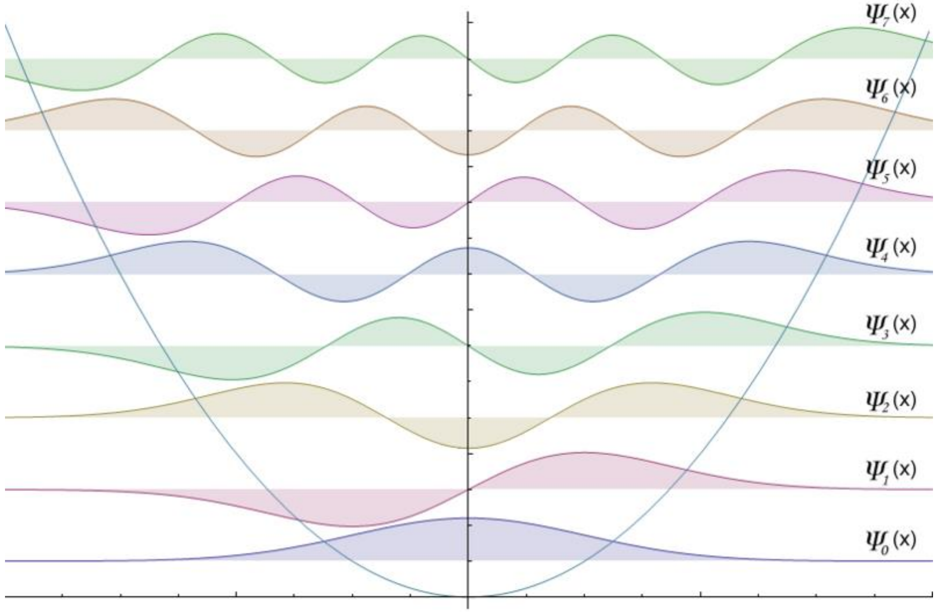
When r is near r_0, the potential-energy curve is approximately parabolic (as shown by the red curve) and the system behaves approximately like a harmonic oscillator.

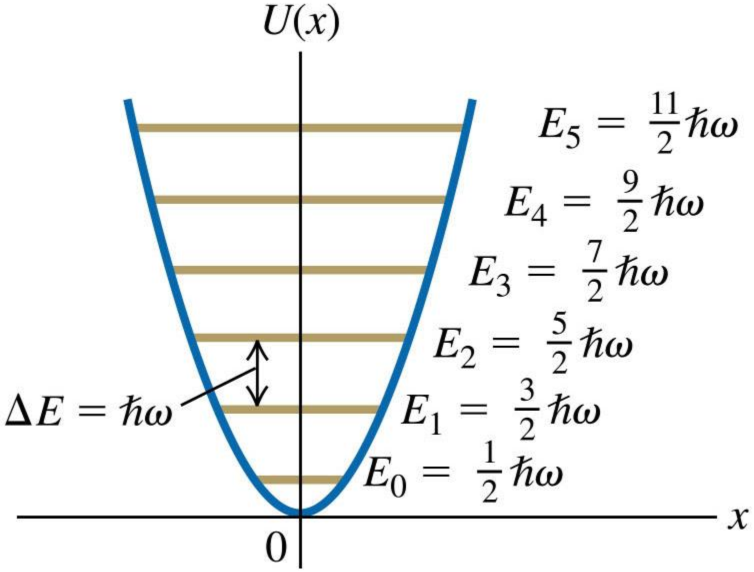
Wave Functions and Energy Levels of the Simple Harmonic Oscillator

$$\psi_n(x) = C_n H_n(x) e^{-\alpha x^2/2} \qquad \alpha^2 = \frac{mk}{\hbar^2}$$

$H_0(x) = 1$
$H_1(x) = 2x$
$H_2(x) = 4x^2 - 2$
$H_3(x) = 8x^3 - 12x$
$H_4(x) = 16x^4 - 48x^2 + 12$
$H_5(x) = 32x^5 - 160x^3 + 120x$
$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120$
$H_7(x) = 128x^7 - 1344x^5 + 3360x^3 - 1680x$

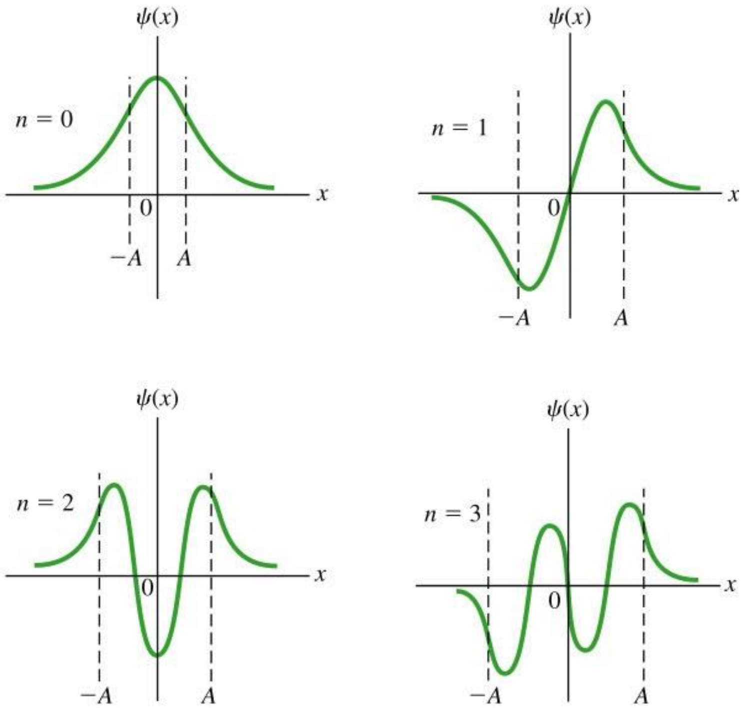
Hermite Polynomials

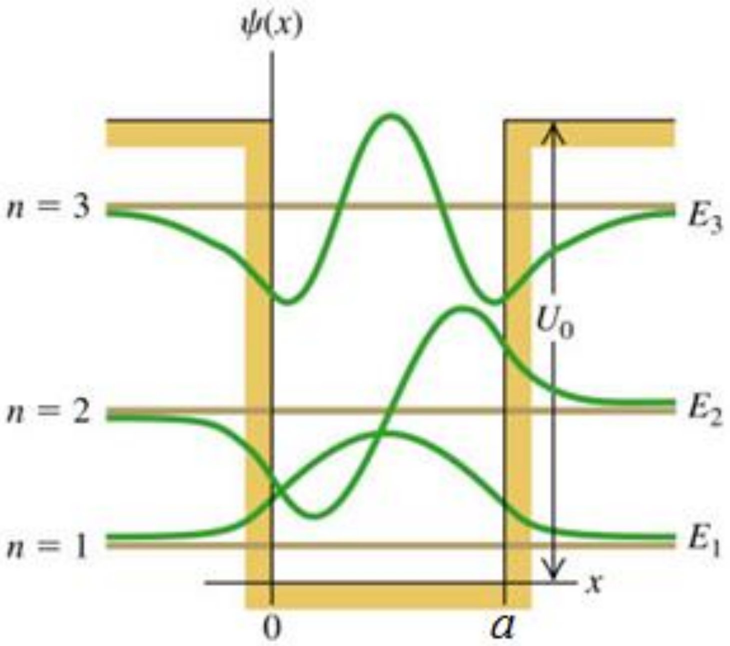




$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad n = 0, 1, 2, \ldots \quad \omega = \sqrt{\frac{k}{m}}$$

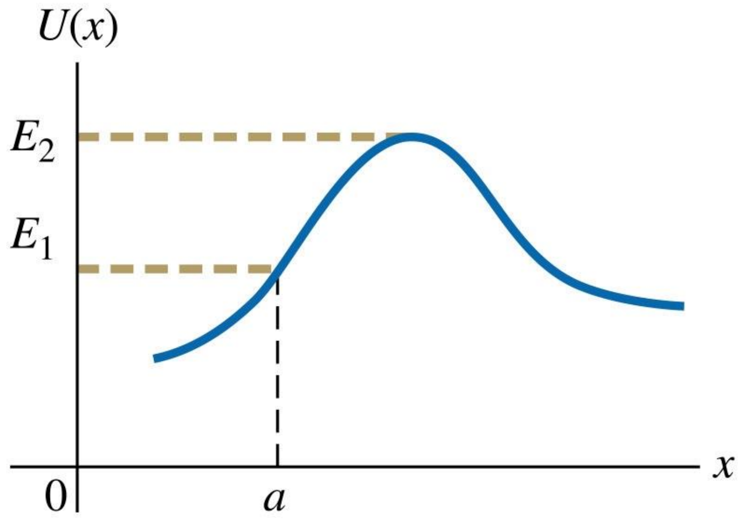
SHO vs. the Finite Well

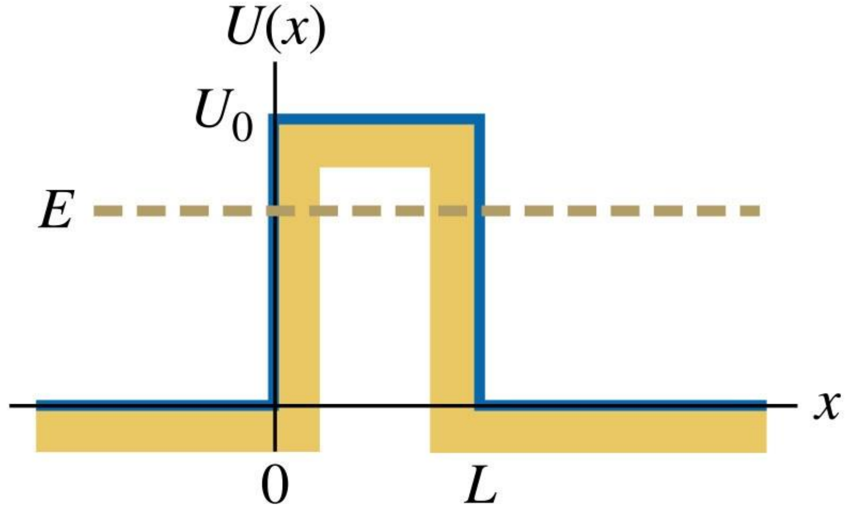




- A is the amplitude of a Newtonian oscillator with the same total energy.
- Each wave function penetrates somewhat into the classically forbidden regions |x| > A.
- The total number of finite maxima and minima for each function is n+1, one more than the quantum number.
- Notice the similarity of these wave functions to those of the finite well.
- The wave functions with higher energy spread out farther than x = 0, just as the classical turning points x = A move farther out when E increases.

Potential Barriers



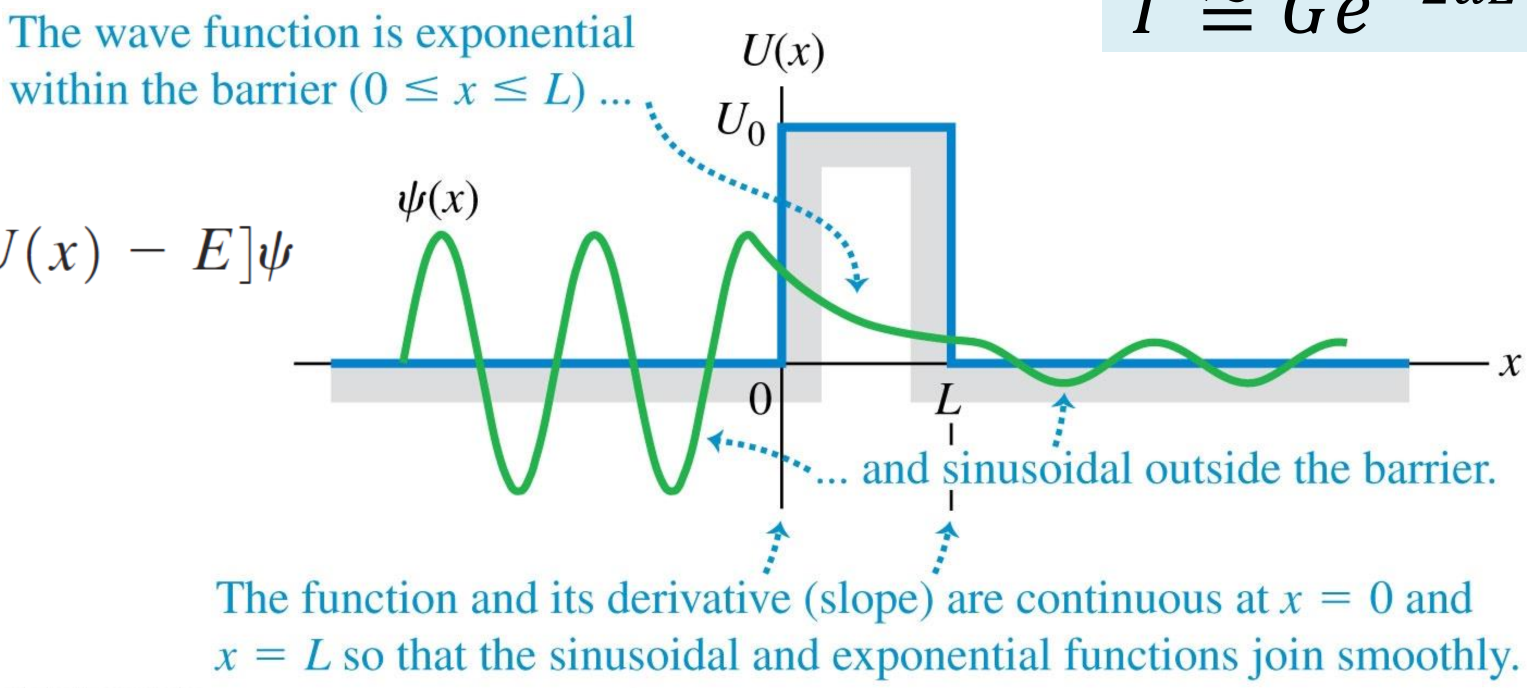


- the “opposite” of a potential well
- a potential energy function with a maximum
- the penetration of a potential barrier is called “tunneling”
- no loss of energy occurs during the process!

Potential Barriers and Tunneling

$$T \cong Ge^{-2\alpha L}$$ transmission coefficient

$$\psi''(x) = \frac{2m}{\hbar^2}[U(x) - E]\psi$$



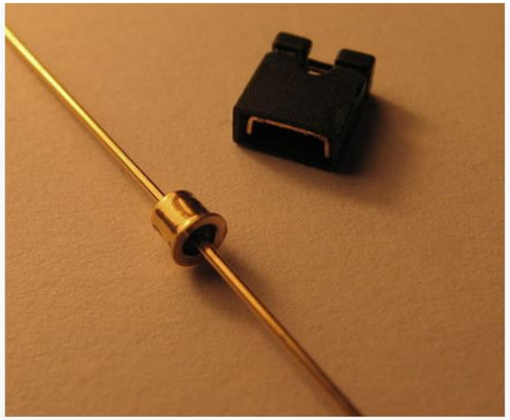
$$\alpha = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

$$G = 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right)$$

A 2.0 eV electron encounters a barrier with height 5.0 eV. What is the probability that it will tunnel through the barrier if the barrier width is a) 1.00 nm; b) 0.50 nm (roughly ten and five atomic diameters, respectively)?

Applications of Tunneling: Tunnel Diode

The tunnel diode is a semiconductor device in which electrons tunnel through a potential barrier. The current can be switched on and off very quickly (within a few picoseconds) by varying the height of the barrier.



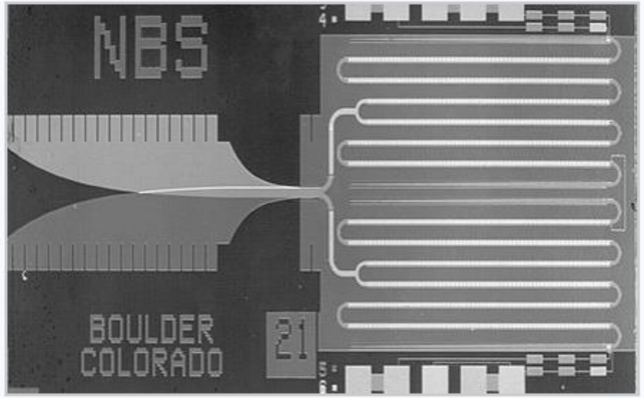
1N3716 tunnel diode (with 0.1" jumper for scale)

Type	Passive
Working principle	Quantum mechanical effect called tunneling
Invented	Leo Esaki Yuriko Kurose[1] Takashi Suzuki[2][3]
First production	Sony
Pin configuration	anode and cathode

Electronic symbol

Applications of Tunneling: Josephson Junction

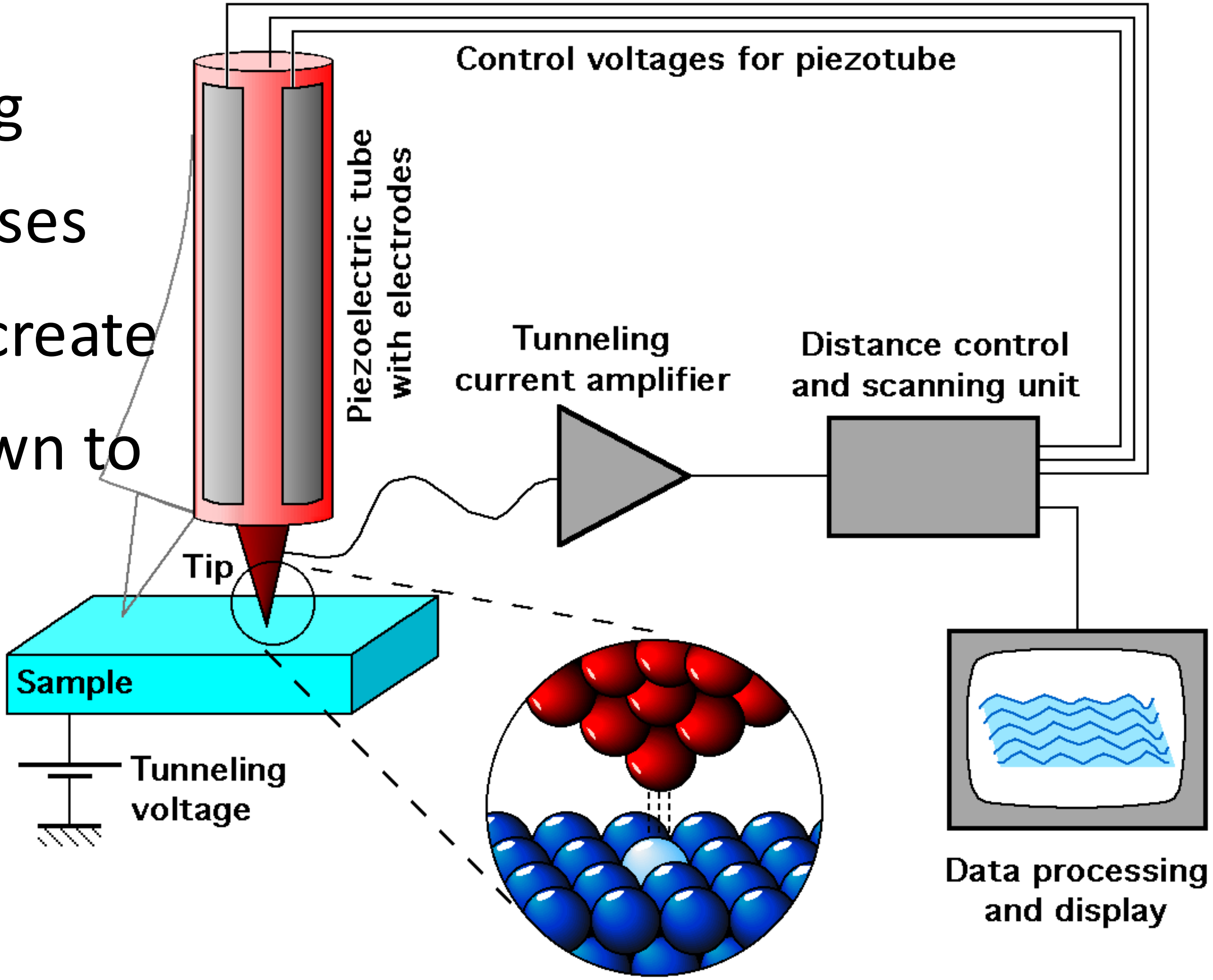
The Josephson junction consists of two superconductors separated by an oxide layer a few atoms thick (1 to 2 nm). Electron pairs in the superconductors can tunnel through the barrier layer, giving such a device unusual circuit properties. Josephson junctions are useful for establishing precise voltage standards and measuring tiny magnetic fields.



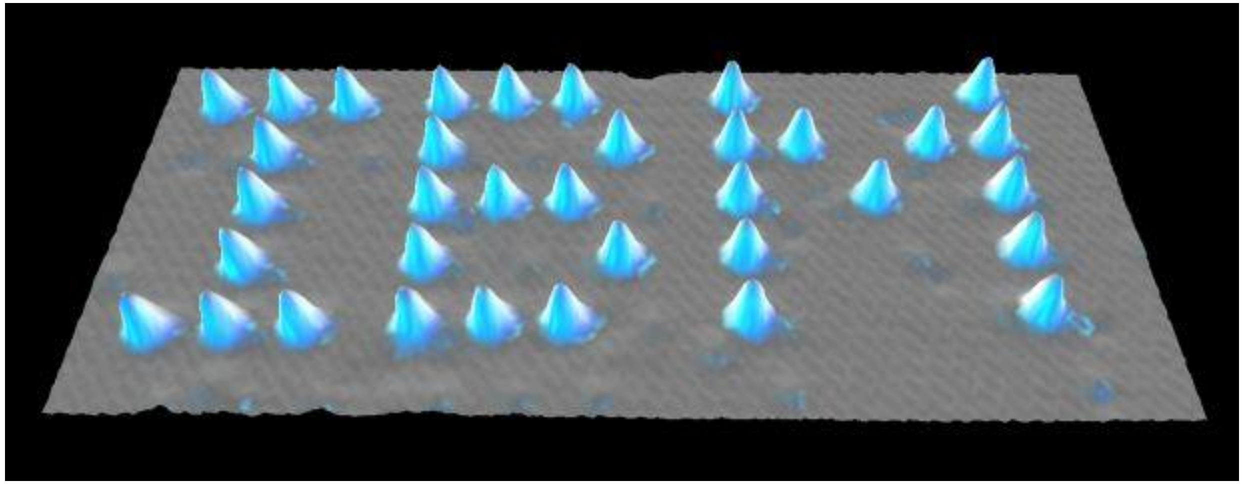
Josephson junction array chip developed by the National Institute of Standards and Technology as a standard volt

Applications of Tunneling: [Scanning Tunneling Microscope (STM)]

The scanning tunneling electron microscope uses electron tunneling to create images of surfaces down to the scale of individual atoms.



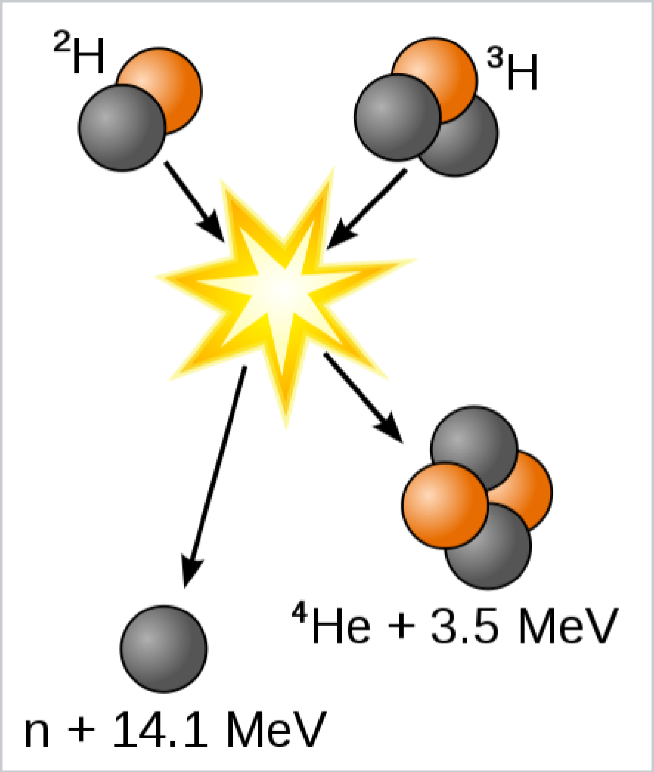
The Smallest-Ever Publicity Stunt



For 22 h over Nov. 9 and 10, 1989, Donald M. Eigler and Erhard K. Schweizer used the ultrasharp tip of a scanning tunneling microscope (STM) to pick up 35 xenon atoms and spell *IBM* in 5 nm tall letters on a cold nickel surface (shown). By the end of the experiment, the IBM team recorded a microscope image of the masterpiece—published several months later (*Nature* 1990, DOI: **10.1038/344524a0**)—that created a scientific sensation and was displayed in newspapers around the globe.

Applications of Tunneling: Nuclear Fusion

In the realm of nuclear physics, a nuclear reaction can occur when two nuclei tunnel through the barrier caused by their electrical repulsion and approach each other closely enough for the attractive nuclear force to cause them to fuse. Fusion reactions occur in the cores of stars, including the sun; without tunneling, the sun wouldn't shine.



Fusion of deuterium with tritium creating helium-4, freeing a neutron, and releasing 17.59 MeV as kinetic energy of the products while a corresponding amount of mass disappears, in agreement with *kinetic E* = Δmc^2, where Δm is the decrease in the total rest mass of particles.[1]

Applications of Tunneling: [Alpha Emission (Alpha Decay)]

The emission of alpha particles from unstable nuclei also involves tunneling. An alpha particle at the surface of a nucleus encounters a potential barrier that results from the combined effects of the attractive nuclear force and the electric repulsion of the remaining part of the nucleus. The alpha particle tunnels through this barrier. Because the tunneling probability depends so critically on the barrier height and width, the lifetimes of alpha-emitting nuclei vary over an extremely wide range.