Chapter 41. One-Dimensional Quantum Mechanics

Quantum effects are important in nanostructures such as this tiny sign built by scientists at IBM's research laboratory by moving xenon atoms around on a metal surface.

Chapter Goal: To understand and apply the essential ideas of quantum mechanics.

Chapter 41. One-Dimensional Quantum Mechanics

Topics:

- Schrödinger's Equation: The Law of Psi
- Solving the Schrödinger Equation
- A Particle in a Rigid Box: Energies and Wave Functions
- A Particle in a Rigid Box: Interpreting the Solution
- The Correspondence Principle
- Finite Potential Wells
- Wave-Function Shapes
- The Quantum Harmonic Oscillator
- More Quantum Models
- Quantum-Mechanical Tunneling

The Schrödinger Equation

Consider an atomic particle with mass *m* and mechanical energy *E* in an environment characterized by a potential energy function *U*(*x*).

The Schrödinger equation for the particle's wave function is

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

Conditions the wave function must obey are

1. $\psi(x)$ and $\psi'(x)$ are continuous functions.
2. $\psi(x) = 0$ if x is in a region where it is physically impossible for the particle to be.
3. $\psi(x) \to 0$ as $x \to +\infty$ and $x \to -\infty$.
4. $\psi(x)$ is a normalized function.

Solving the Schrödinger Equation

If a second order differential equation has two independent solutions $\psi_1(x)$ and $\psi_2(x)$, then a *general solution* of the equation can be written as

$$\psi(x) = A\psi_1(x) + B\psi_2(x)$$

where A and B are constants whose values are determined by the boundary conditions.

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

There is a more general form of the Schrodinger equation which includes time dependence and x,y,z coordinates;

We will limit discussion to 1-D solutions

Must know U(x), the potential energy function the particle experiences as it moves.

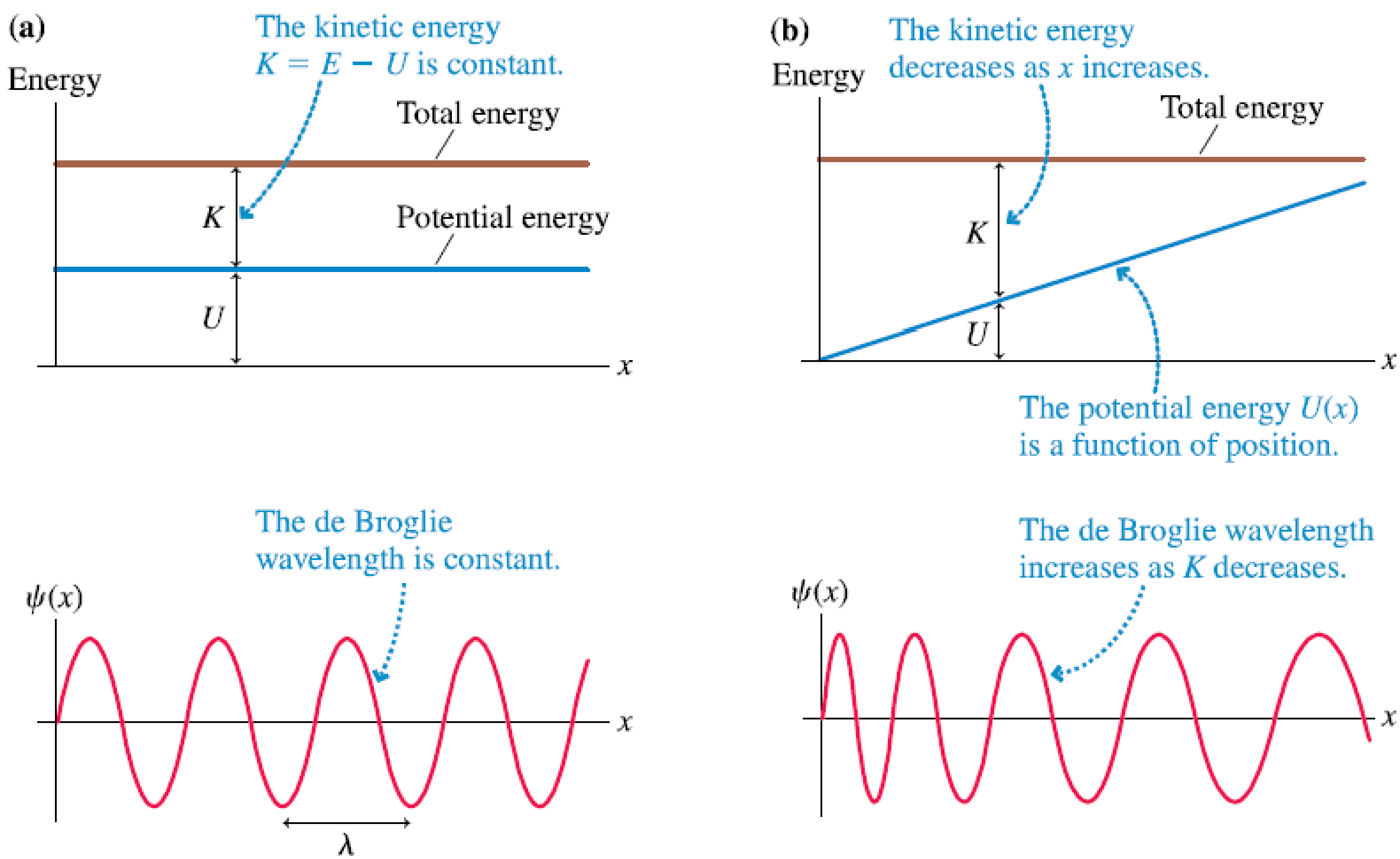
Objective is to solve for ψ(x) and the total energy E=KE + U of the particle.

In ‘bound state’ problems where the particle is trapped (localized in space), the energies will be found to be quantized upon solving the Schrodinger equation.

In ‘unbound states’ where the particle is not trapped, the particle will travel as a traveling wave with an amplitude given by ψ(x)

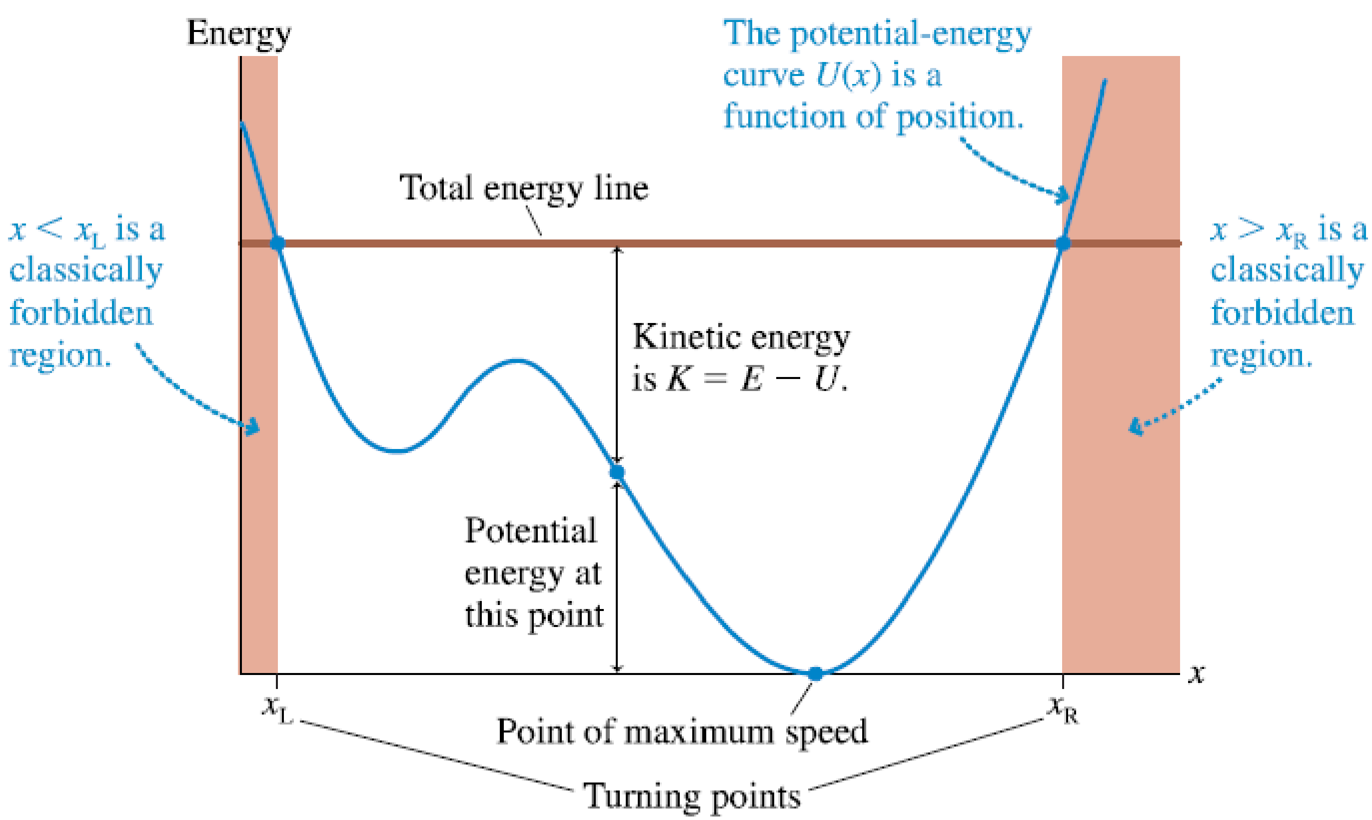
E, KE, and PE

FIGURE 41.1 The de Broglie wavelength changes as a particle's kinetic energy changes.



E, KE, and PE

FIGURE 41.2 Interpreting an energy diagram.



Short "Derivation" of Schrodinger's Equation:

1. $E = KE + PE = \frac{p^2}{2m} + U(x)$

2. For "photon-like" particle: $E = \hbar\omega$ $\quad (E = hf)$

3. De Broglie, $p = \hbar k$ $\quad \left(p = \frac{h}{\lambda}\right)$

Schrodinger: $\psi(\vec{x}) = A e^{i(\vec{k}\cdot\vec{x} - \omega t)}$

Consider only x: $\psi(x) = A e^{i(kx - \omega t)}$, A is generally complex

(Recall that $e^{i\theta} = \cos\theta + i\sin\theta$

$$\frac{\partial \psi}{\partial t} = -iA\omega e^{i(kx-\omega t)} = -i\omega\psi$$

Let: $\omega = \frac{E}{\hbar}$ $\Rightarrow$ $E\psi(x) = i\hbar \frac{\partial \psi}{\partial t}$ $\quad (1)$

$$\frac{\partial \psi}{\partial t} = -iA\omega e^{i(kx-\omega t)} = -i\omega\psi$$

Let: $\omega = \frac{E}{\hbar} \Rightarrow E\psi(x) = i\hbar \frac{\partial \psi}{\partial t}$ ①

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial x}\right) = \frac{\partial}{\partial x}\left[ikAe^{i(kx-\omega t)}\right] = (ik)^2\psi = -k^2\psi$$

$$k^2 = p^2/\hbar \Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar}\psi \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = \frac{p^2}{2m}\psi$$

$$\frac{p^2}{2m} = KE = E - U(x) \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = (E - U(x))\psi \quad ②$$

$$= \underbrace{E\psi}_{i\hbar \frac{\partial \psi}{\partial t}} - U(x)\psi$$

$$\Rightarrow \quad i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + U(x)\psi$$

Schrodinger's Time dependent Equation

$$\Rightarrow \quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + u(x)\psi$$

Schrodinger's Time dependent Equation

$$② \Rightarrow \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = \left(E - u(x)\right)\psi(x)$$

Schrodinger's Time independent Equation

The Schrödinger Equation with Constant potential

Let $\Psi(x,t) = \underbrace{A\, e^{bx}}_{\psi(x)}\, \underbrace{e^{at}}_{\psi(t)}$, $\mathcal{U}(x) = \mathcal{U}$ Constant

$$\boxed{i\hbar \frac{\partial \Psi(x,t)}{\partial t} = E\, \Psi(x,t)} \Rightarrow i\hbar \frac{\partial \psi(t)}{\partial t} = E\, \psi(t) \Rightarrow i\hbar a = E$$

$$\Rightarrow a = -\frac{iE}{\hbar} = -i\omega$$

$$\therefore \psi(t) \approx e^{-i\omega t}$$

Let $\psi(x) = A e^{bx}$ in general (b can be complex)

$$\Rightarrow \quad \frac{\partial^2 \psi}{\partial x^2} = b^2 \psi$$

$$\Rightarrow \quad \boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = (E-U)\psi} \Rightarrow b^2 = \frac{2m}{\hbar^2}(U-E)$$

$$\text{or} \quad \pm b = \begin{cases} i\sqrt{\dfrac{2m}{\hbar^2}|E-U(x)|} & U<E \\ -\sqrt{\dfrac{2m}{\hbar^2}|E-U(x)|} & U>E \end{cases}$$

For $U<E$, $E-U = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m}$

$$\Rightarrow \quad b = \pm i\sqrt{\frac{2m}{\hbar^2}\frac{(\hbar k)^2}{2m}} = \pm ik$$

$$\Rightarrow \quad \psi(x,t) = A e^{\pm ikx - i\omega t} \qquad U<E$$

"+" + "−" x-direction

For $U > E$, KE is negative!, Case of Quantum Tunneling

Let $\frac{2m}{\hbar^2}(U-E) \equiv K$

$$\Rightarrow \quad \Psi(x,t) = A e^{-i\omega t} e^{\pm Kx}$$

Must Have "$-Kx$" for Ψ to be normalizable:

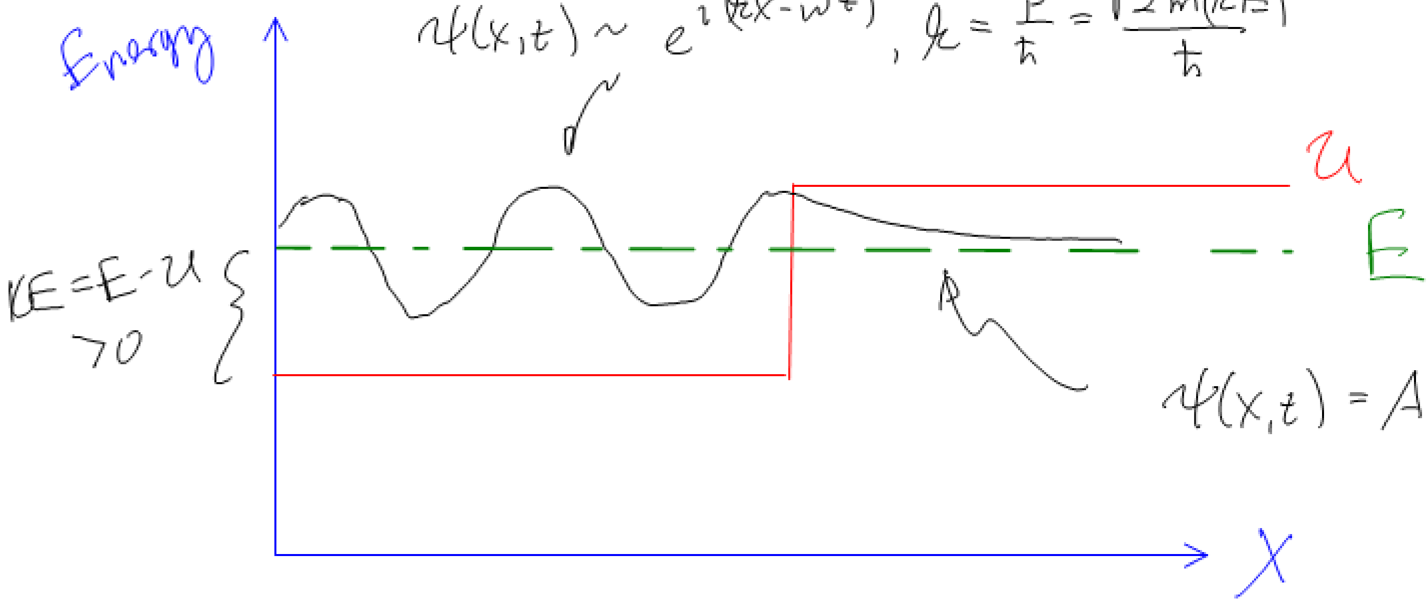
$$\Rightarrow \quad \Psi(x,t) = A e^{-i\omega t} e^{-Kx} \qquad U > E$$

$$\psi(x,t) = A e^{\pm ikx - i\omega t} \qquad U < E$$

"+" & "−" x-direction

$$\psi(x,t) = A e^{-i\omega t} e^{-Kx} \qquad U > E$$

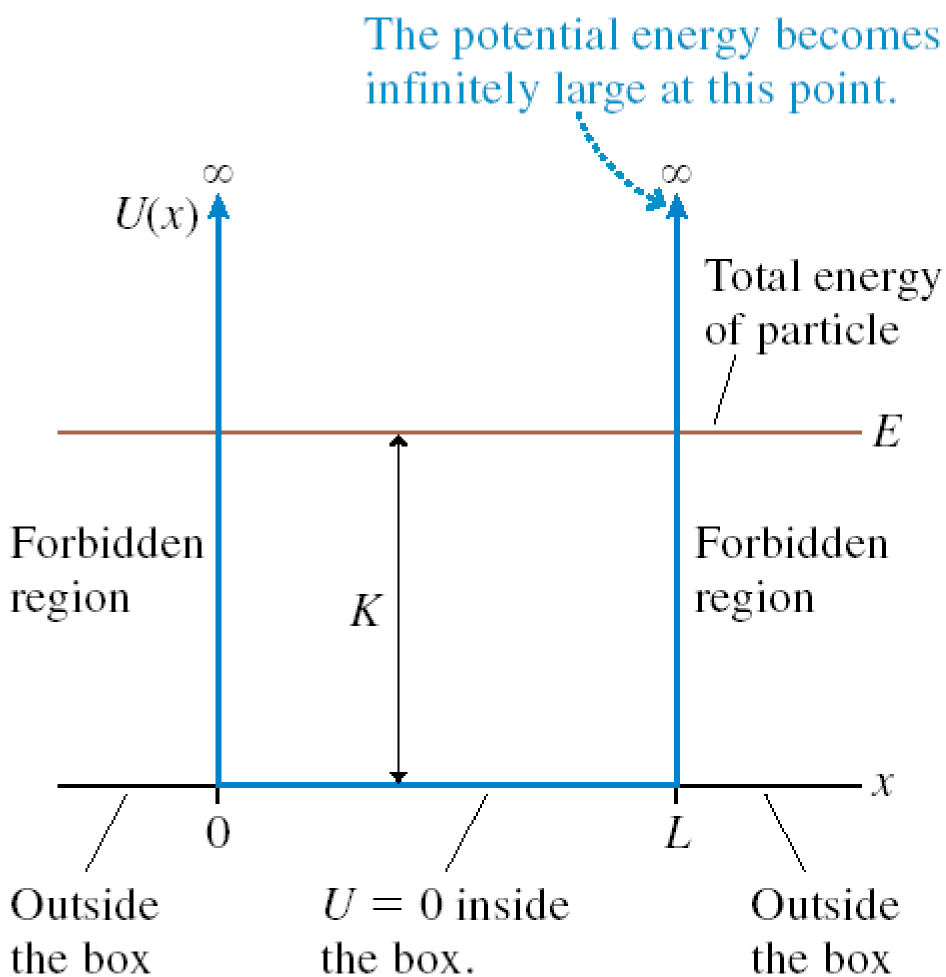
$$\psi(x,t) \sim e^{i(kx-\omega t)}, \quad k = \frac{p}{\hbar} = \frac{\sqrt{2m(KE)}}{\hbar}$$



$$\psi(x,t) = A e^{-i\omega t} e^{-Kx}, \quad U > E$$

A Particle in a Rigid Box

FIGURE 41.4 The energy diagram of a particle in a rigid box of length L.



A Particle in a Rigid Box

Consider a particle of mass *m* confined in a rigid, one-dimensional box. The boundaries of the box are at *x* = 0 and *x* = *L*.

1. The particle can move freely between 0 and *L* at constant speed and thus with constant kinetic energy.
2. No matter how much kinetic energy the particle has, its turning points are at *x* = 0 and *x* = *L.*
3. The regions *x* < 0 and *x* > *L* are forbidden. The particle cannot leave the box.

A potential-energy function that describes the particle in this situation i

$$U_{\text{rigid box}}(x) = \begin{cases} 0 & 0 \le x \le L \\ \infty & x < 0 \quad \text{or} \quad x > L \end{cases}$$

Particle in a rigid Box:

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

for $x \geq 0$, $x \leq L$, $E > U = 0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = (E-U)\psi \qquad \text{Let } \psi(x) = A e^{bx}$$

$$\Rightarrow \quad b = \pm i k \qquad \text{where} \qquad \hbar k = p = \sqrt{2m(KE)} = \sqrt{2m(E-U)}$$

$$\Rightarrow k = \frac{\sqrt{2m(E-\cancel{U})}}{\hbar} \quad 0$$

$$\Rightarrow \psi(x) = A e^{\pm ikx}$$

$$\Rightarrow \psi(x) = A \cos kx \pm B \sin kx \quad , \text{ general Solution}$$

$$\Rightarrow \psi(x) = A \cos kx \pm B \sin kx \quad , \text{ general Solution}$$

Boundary Conditions

$$\psi(x=0) = 0 \Rightarrow \underline{\underline{A = 0}} \quad ; \quad \psi(x=L) = 0 \Rightarrow \pm B \sin kL = 0$$

$$\Rightarrow \sin kL = 0$$

$$\Rightarrow k_n L = n\pi$$

$$\Rightarrow k_n = \frac{n\pi}{L} = \frac{\sqrt{2mE_n}}{\hbar}$$

$$\Rightarrow E_n = \left(\frac{\hbar n\pi}{L}\right)^2 \frac{1}{2m} \quad , \quad \hbar = \frac{h}{2\pi}$$

$$\Rightarrow E_n = \left(\frac{hn}{L}\right)^2 \frac{1}{8m} \quad , \quad \psi_n(x) = B \sin\left(\frac{n\pi}{L} x\right)$$

$$\Rightarrow E_n = \left(\frac{hn}{L}\right)^2 \frac{1}{8m} \quad , \quad \psi_n(x) = B \sin\left(\frac{n\pi}{L} x\right)$$

Normalize wave function to find B:

$$1 = \int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = B^2 \int_0^L (\sin k_n x)^2 dx$$

$$\left.\text{Let } \alpha = k_n x \Rightarrow d\alpha = k_n dx \right] = \frac{B^2}{k_n} \int_0^{n\pi} (\sin \alpha)^2 d\alpha$$

$$\& \quad k_n L = n\pi$$

$$\frac{B^2}{k_n}\int_0^{n\pi}(\sin\alpha)^2\,d\alpha$$

$$\sin\alpha = \mathrm{Im}(e^{i\alpha})$$
$$\sin^2\alpha = [\mathrm{Im}\, e^{i\alpha}]^2$$

$$z = a + ib$$
$$|z|^2 = a^2 + b^2$$
$$= (\mathrm{Re}\, z)^2 + (\mathrm{Im}\, z)^2$$

$$z^2 = a^2 - b^2 - i2ab$$
$$\therefore \mathrm{Re}\left[\left(\frac{|z|^2 - z^2}{2}\right)\right] = b^2 = (\mathrm{Im}\, z)^2$$

$$\therefore \sin^2\alpha = \mathrm{Re}\left[\frac{1 - e^{2i\alpha}}{2}\right]$$

Since $|z|^2 = z^* z = e^{-i\alpha} e^{i\alpha} = 1$

$z^2 = e^{i\alpha} e^{i\alpha} = e^{2i\alpha}$

$\mathrm{Re}\, e^{2i\alpha} = \cos 2\alpha$

$$= \frac{1}{2} - \frac{1}{2}\cos 2\alpha$$
$$= \frac{1}{2}(1 - \cos 2\alpha)$$

$$\int \cos 2\alpha = \frac{1}{2}\sin 2\alpha$$

$$\therefore \frac{B^2}{k_n}\int_0^{n\pi}(\sin\alpha)^2\,d\alpha = \frac{B^2}{k_n}\int_0^{n\pi}\frac{1}{2}(1 - \cos 2\alpha)\,d\alpha$$

$$\Rightarrow E_n = \left(\frac{hn}{L}\right)^2 \frac{1}{8m}, \qquad \psi_n(x) = B \sin\left(\frac{n\pi}{L} x\right)$$

Normalize wave function to find B:

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

$$\therefore \frac{B^2}{k_n} \int_0^{n\pi} (\sin\alpha)^2 d\alpha = \frac{B^2}{k_n} \int_0^{n\pi} \frac{1}{2}(1 - \cos 2\alpha) d\alpha$$

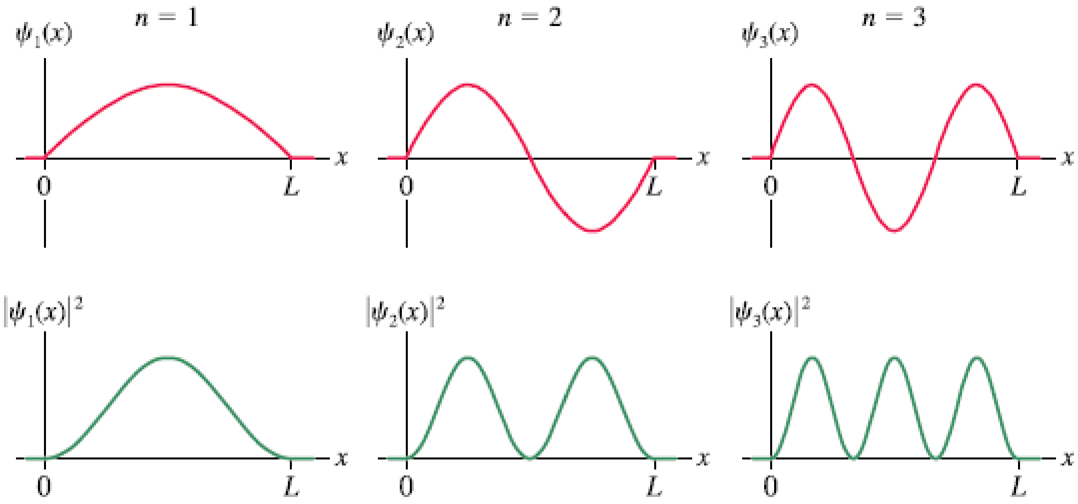
$$= \frac{B^2}{k_n} \left(\frac{\alpha}{2} - \frac{\sin 2\alpha}{4}\right)\Bigg|_0^{n\pi}$$

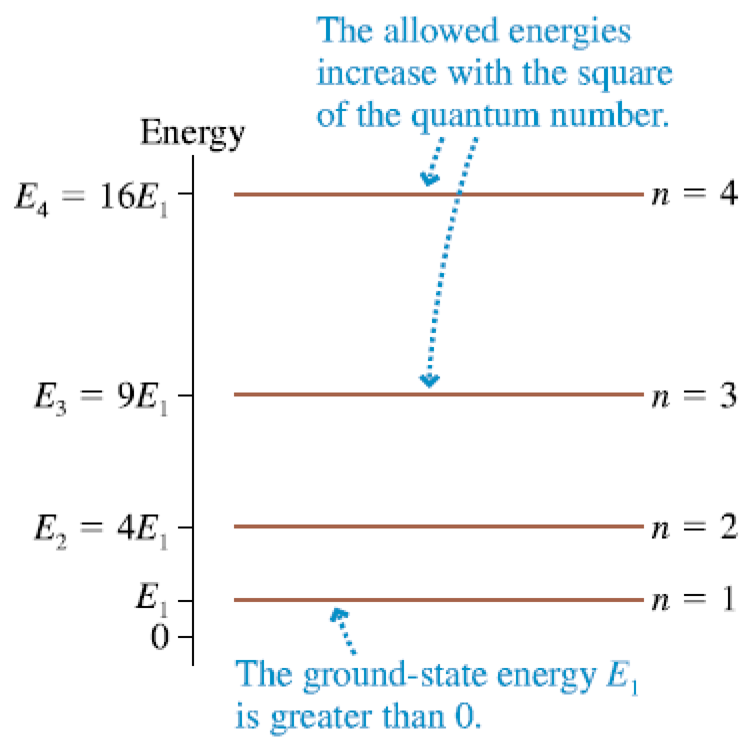
$$= \frac{1}{2} \frac{B^2}{n\pi/L} \left(n\pi - \cancelto{0}{\frac{\sin(2\cdot n\pi)}{2}}\right) = \frac{B^2}{(2/L)} = 1$$

$$\Rightarrow B = \sqrt{\frac{2}{L}}$$

$$\therefore \psi_n = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x & 0 \le x \le L \\ 0 & x \le 0,\ x \ge L \end{cases}$$

FIGURE 41.7 Wave functions and probability densities for a particle in a rigid box of length L.

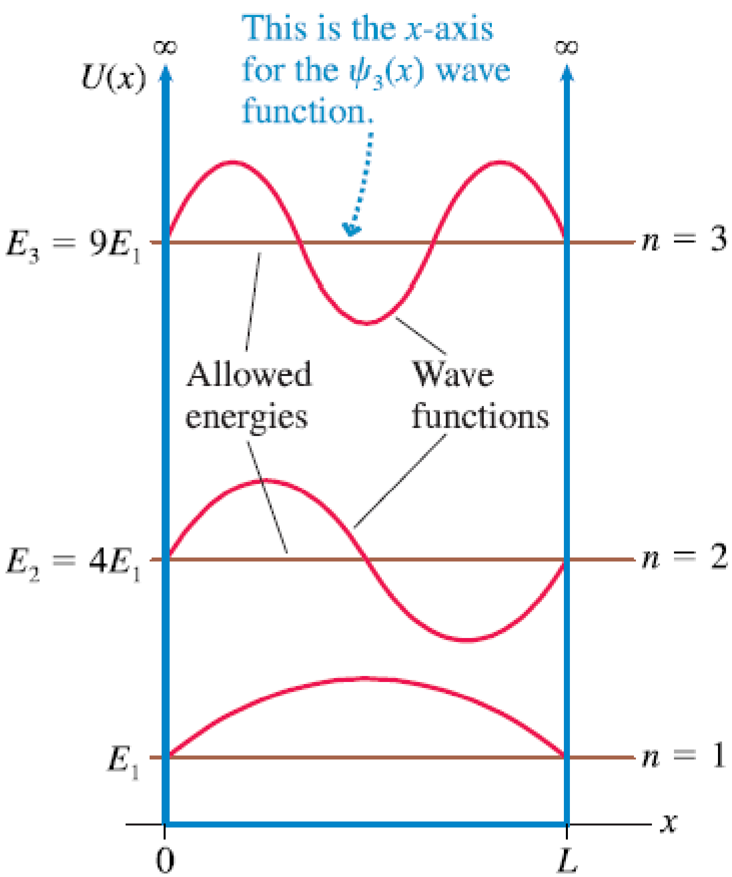




$$\psi_n = \begin{cases} \sqrt{\frac{2}{L}}\, \sin \frac{n\pi}{L} x & 0 \le x \le L \\ 0 & x \le 0,\ x \ge L \end{cases}$$

$$E_n = \left(\frac{hn}{L}\right)^2 \frac{1}{8m}$$

FIGURE 41.8 An alternative way to show the potential-energy diagram, the energies, and the wave functions.



$$E_n = \left(\frac{hn}{L}\right)^2 \frac{1}{8m}$$

Zero point energy: even at T=0K, a confined particle will have a non-zero energy of E1; it is moving

The Correspondence Principle

When wavelength becomes small compared to the size of the box (that is, when either L becomes large or when the energy of the particle becomes large), the particle must behave classically.

For particle in a box:

$$P_{\text{quant}}(x) = |\psi_n(x)|^2 = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right)$$

Classically:

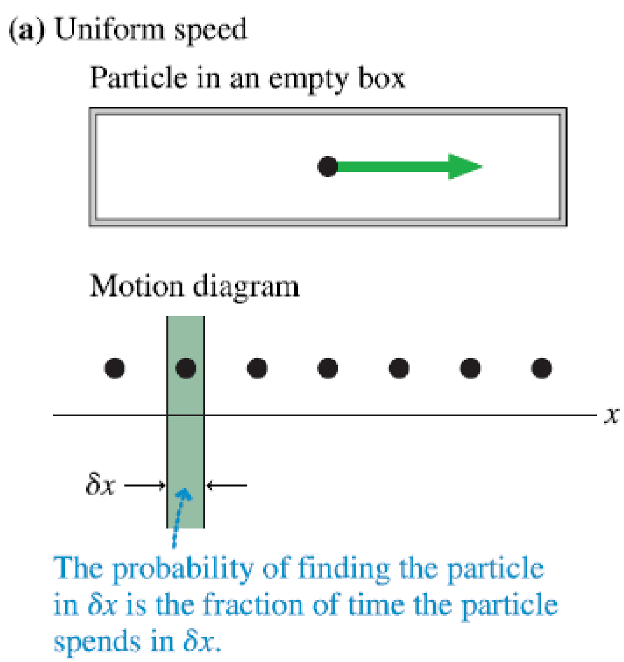
$$\text{Prob}_{\text{class}}(\text{in } \delta x \text{ at } x) = \text{fraction of time spent in } \delta x = \frac{\delta t}{\frac{1}{2}T}$$

$$\text{Prob}_{\text{class}}(\text{in } \delta x \text{ at } x) = \frac{\delta x / v(x)}{\frac{1}{2}T} = \frac{2}{Tv(x)}\delta x$$

$$\text{Prob}_{\text{class}}(\text{in } \delta x \text{ at } x) = P_{\text{class}}(x)\,\delta x$$

$$P_{\text{class}}(x) = \frac{2}{Tv(x)}$$

$$P_{\text{class}}(x) = \frac{2}{(2L/v_0)v_0} = \frac{1}{L}$$



The Correspondence Principle

When wavelength becomes small compared to the size of the box (that is, when either L becomes large or when the energy of the particle becomes large), the particle must behave classically.

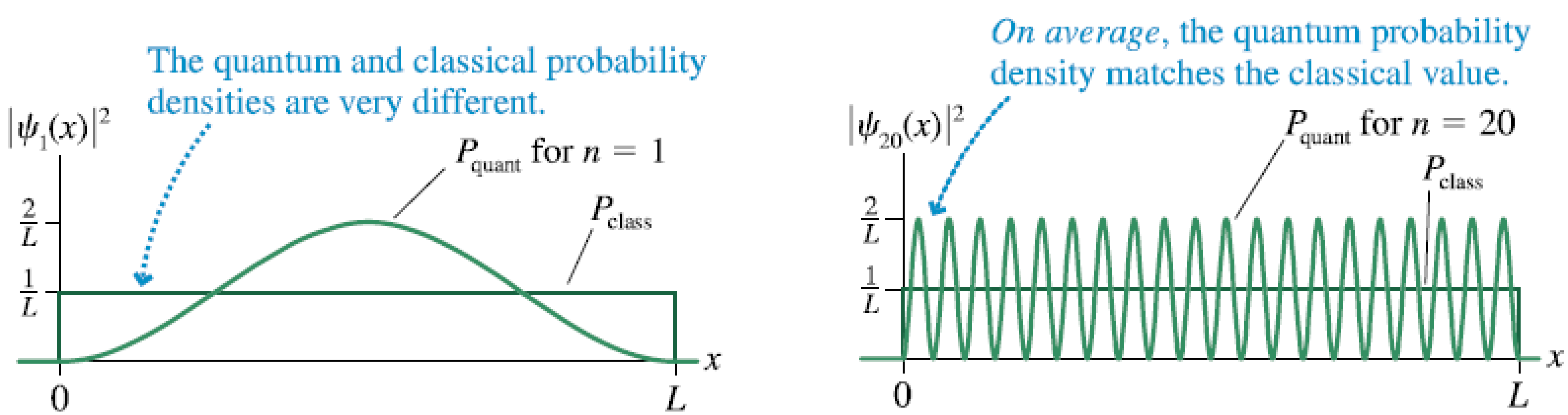
For particle in a box:

$$P_{\text{quant}}(x) = |\psi_n(x)|^2 = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right)$$

Classically:

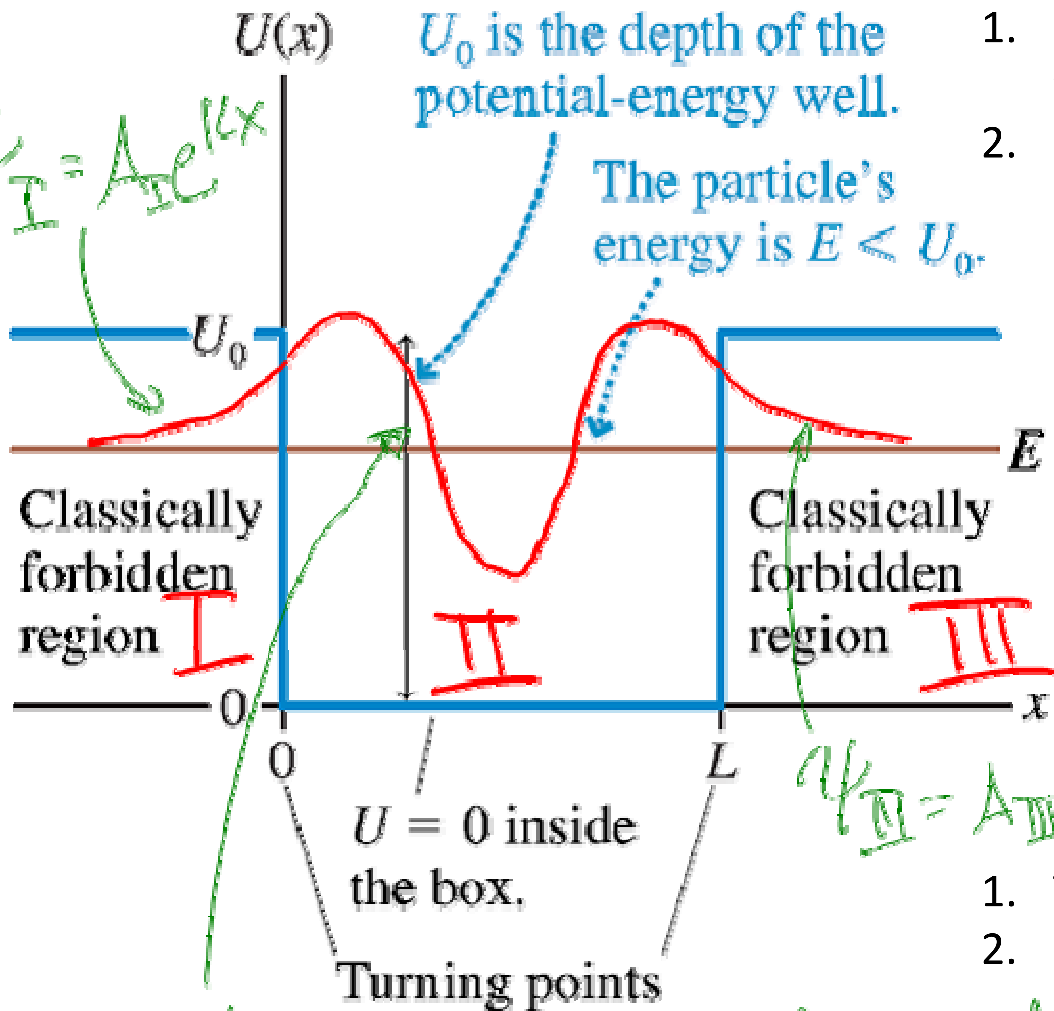
$$P_{\text{class}}(x) = \frac{2}{(2L/v_0)v_0} = \frac{1}{L}$$

FIGURE 41.12 The quantum and classical probability densities for a particle in a box.



Finite Potential well:

(a) $U = 0$ inside the well.



$\psi_I = A_I e^{\kappa x}$

$\psi_{III} = A_{III} e^{-\kappa x}$

$\psi_{II} = A_{II} \cos kx + B_{II} \sin kx$

1. Solve Schrodinger's equation in the three regions (we already did this!)
2. 'Connect' the three regions by using the following boundary conditions:

$$\psi_I(x=0) = \psi_{II}(x=0)$$

$$\psi_{II}(x=L) = \psi_{III}(x=L)$$

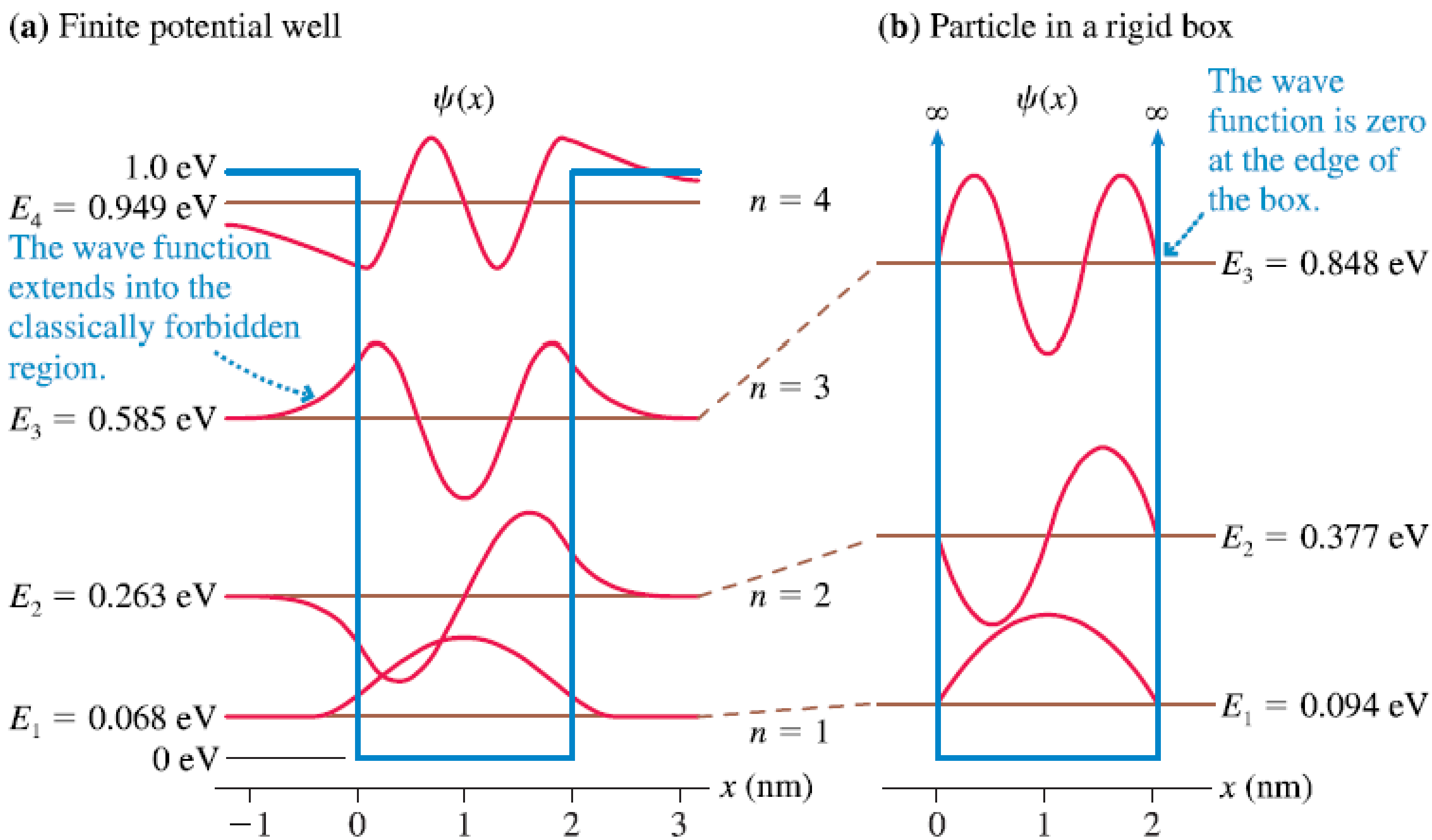
$$\psi_I'(x=0) = \psi_{II}'(x=0)$$

$$\psi_{II}'(x=L) = \psi_{III}'(x=L)$$

1. This will give quantized k's and E's
2. Normalize wave function

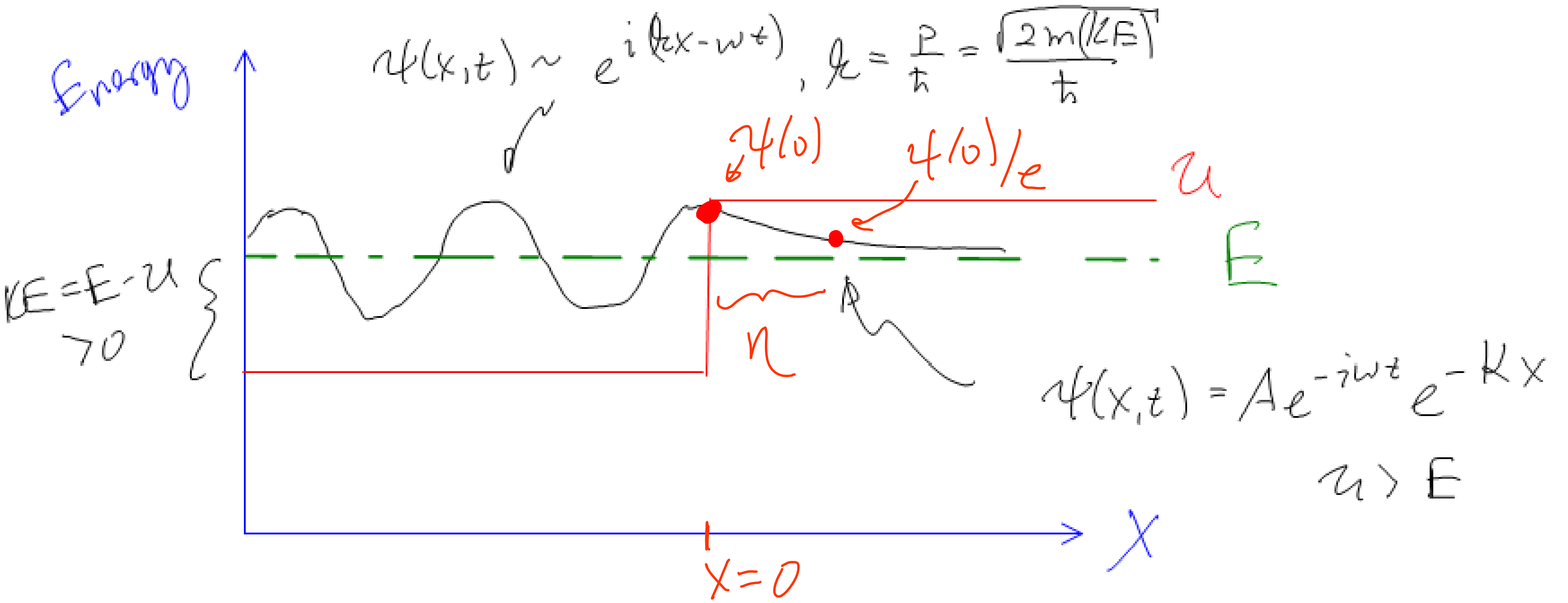
Finite Potential well:

FIGURE 41.14 Energy levels and wave functions for a finite potential well. For comparison, the energies and wave functions are shown for a rigid box of equal width.



Finite number of bound states, energy spacing smaller since wave function more spread out (like bigger L), wave functions extend into classically forbidden region

Classically forbidden region – penetration depth



$$\psi(x,t) = A\, e^{-i\omega t}\, e^{\pm Kx} \qquad \frac{2m}{\hbar^2}(U-E) \equiv K$$

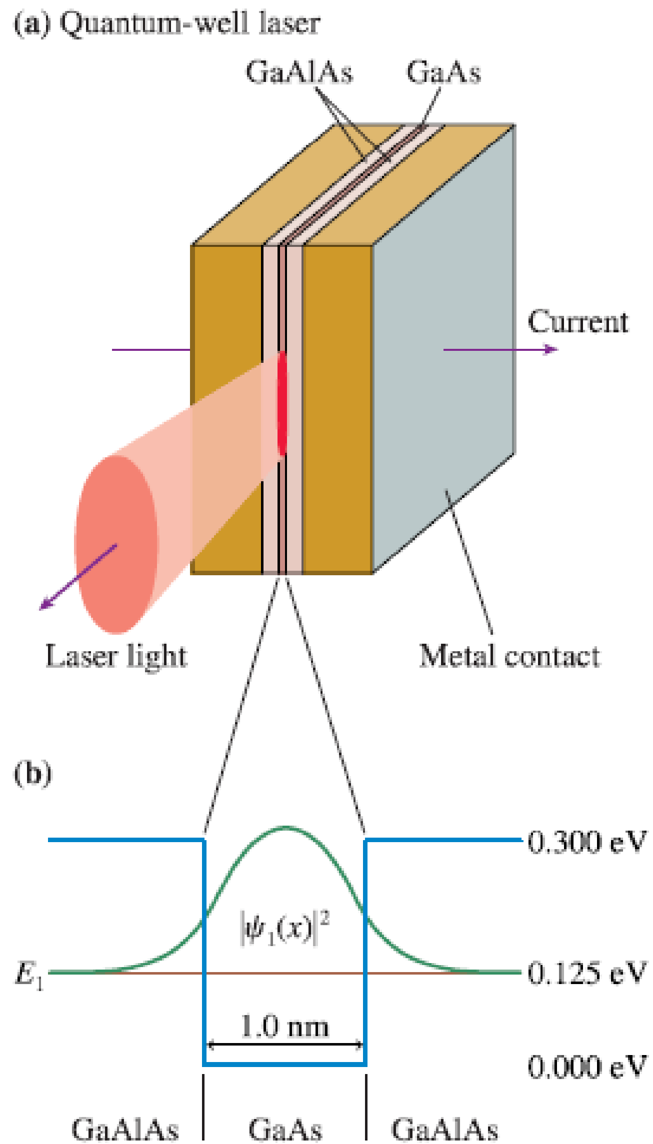
$$\psi(x) \propto e^{-Kx} \quad \therefore \text{ Define } \psi(\eta) = \underbrace{\psi(0)\, e^{-1}} = e^{-K\eta}$$

$$\Rightarrow \eta = \frac{1}{K} = \frac{\hbar}{\sqrt{2m(U-E)}}$$

$\hookrightarrow$ η is the point where ψ falls to $1/e$

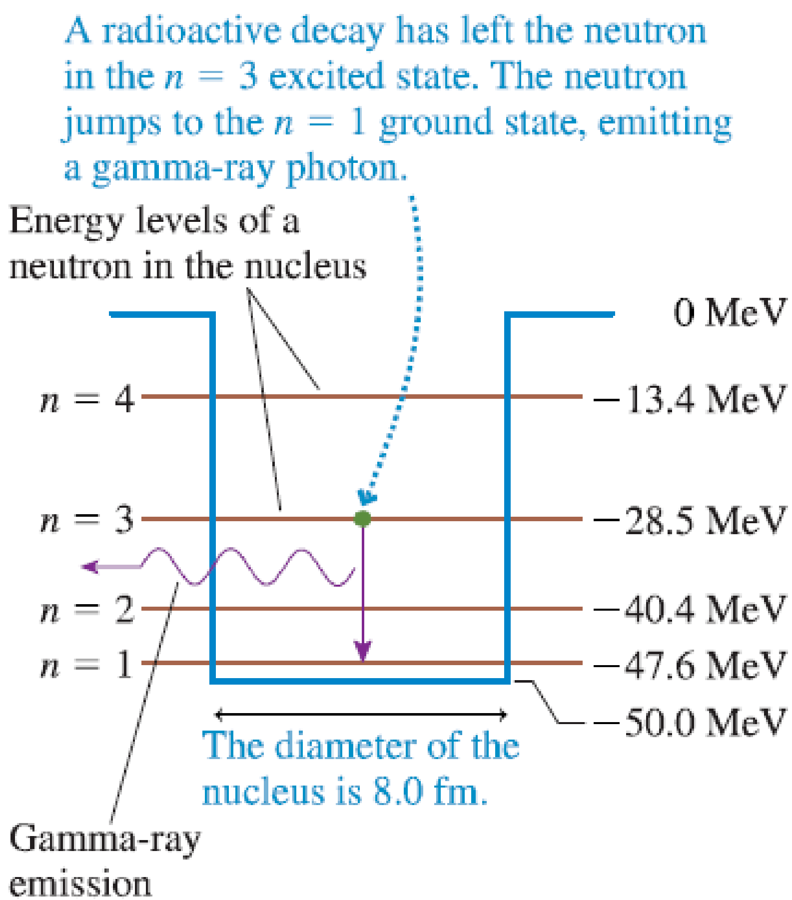
Finite Potential well example – Quantum well lasers

FIGURE 41.16 A semiconductor diode laser with a single quantum well.



Finite Potential well example – 1-D model of nucleus

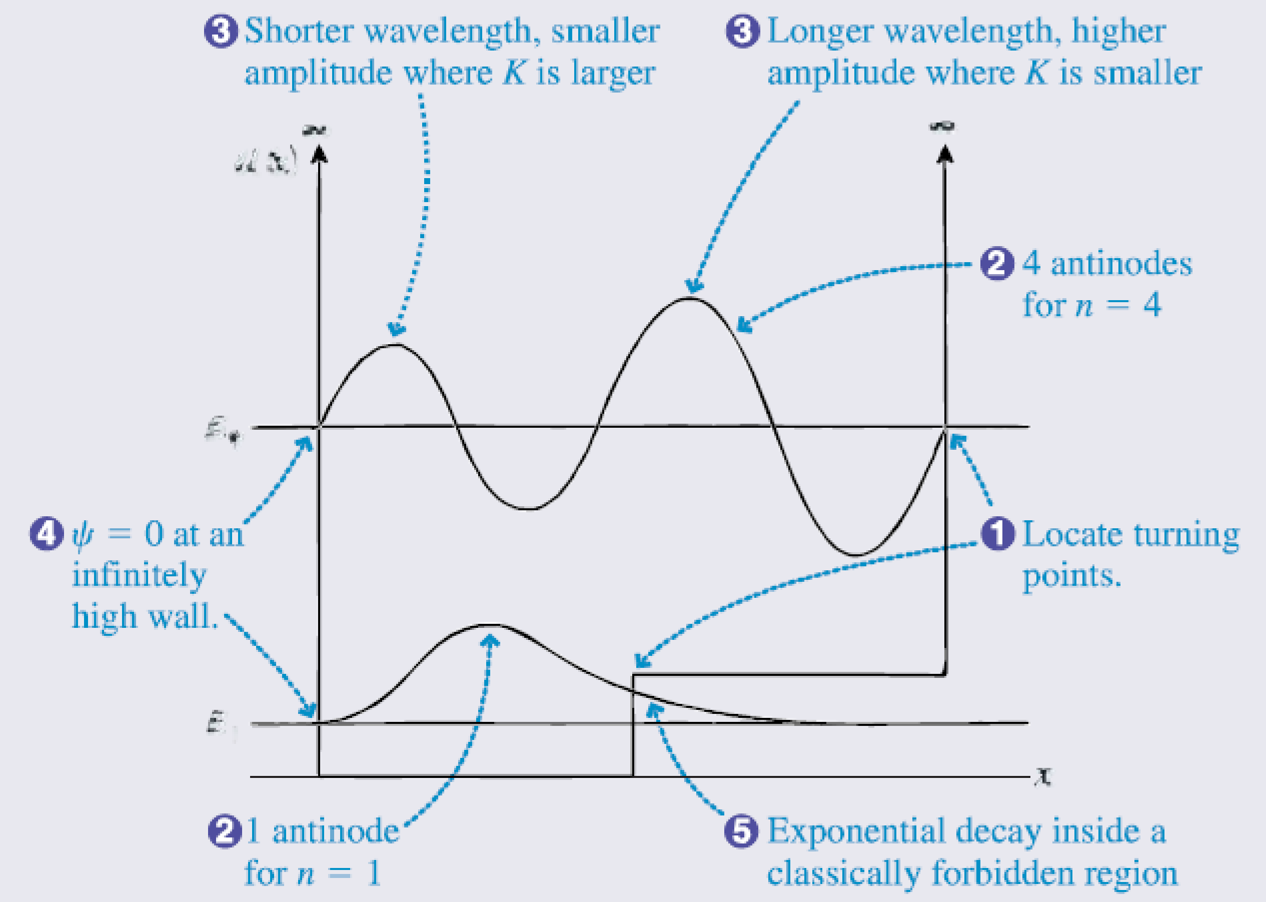
FIGURE 41.17 There are four allowed energy levels for a neutron in this nuclear potential well.



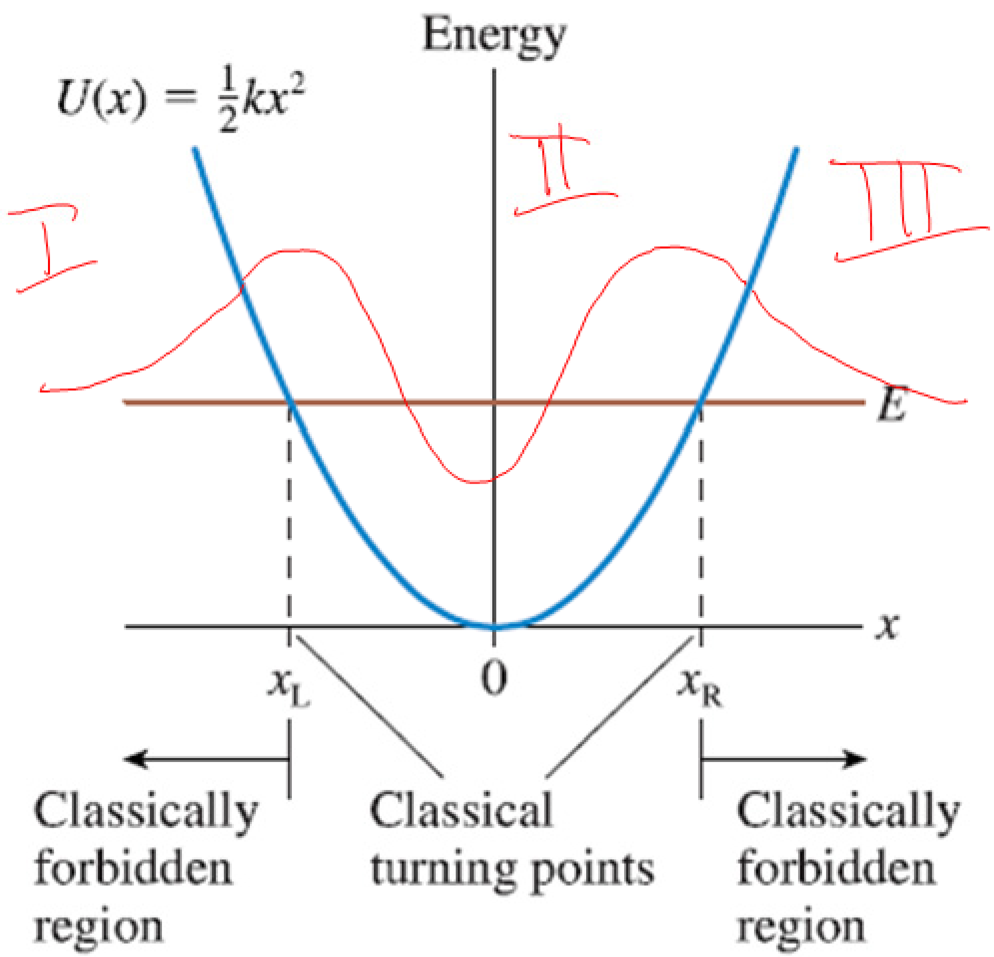
Qualitative wave function shapes

Exponential decay if U>E, oscillatory if E>U i.e. positive KE, KE~p^2 ~$1/\lambda^2$, Amplitude~1/v~1/Sqrt[KE] (particle moving slower means more likely to be in that place)

FIGURE 41.19 The $n = 1$ and $n = 4$ wave functions.



Harmonic Oscillator



1. Solve Schrodinger's equation in the three regions (we already did this!)
2. 'Connect' the three regions by using the following boundary conditions:

$$\psi_{I}(x=x_L) = \psi_{II}(x=x_L)$$

$$\psi_{II}(x=x_R) = \psi_{III}(x=x_R)$$

$$\psi'_{I}(x=x_L) = \psi'_{II}(x=x_L)$$

$$\psi'_{II}(x=x_R) = \psi'_{III}(x=x_R)$$

3. This will give quantized k's and E's
4. Normalize wave function

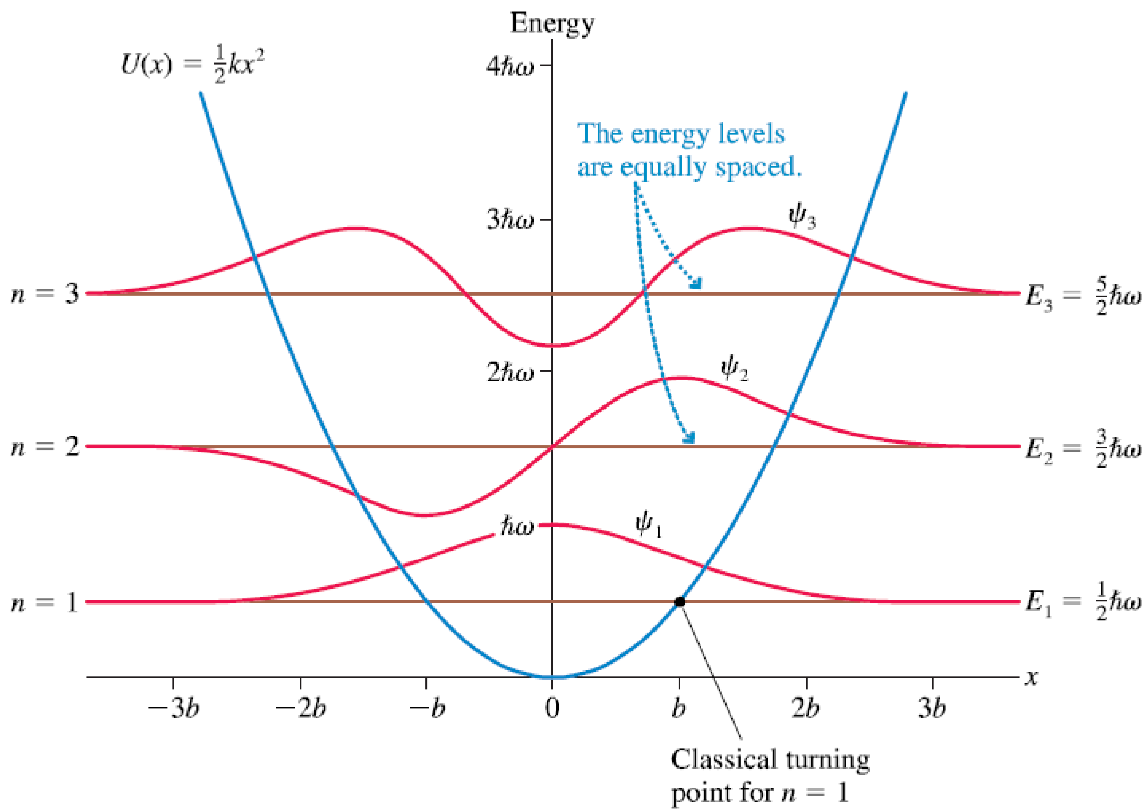
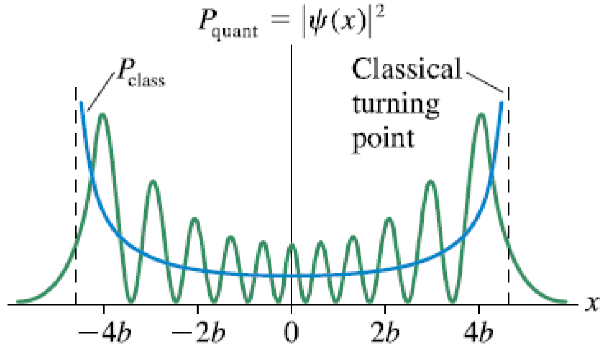


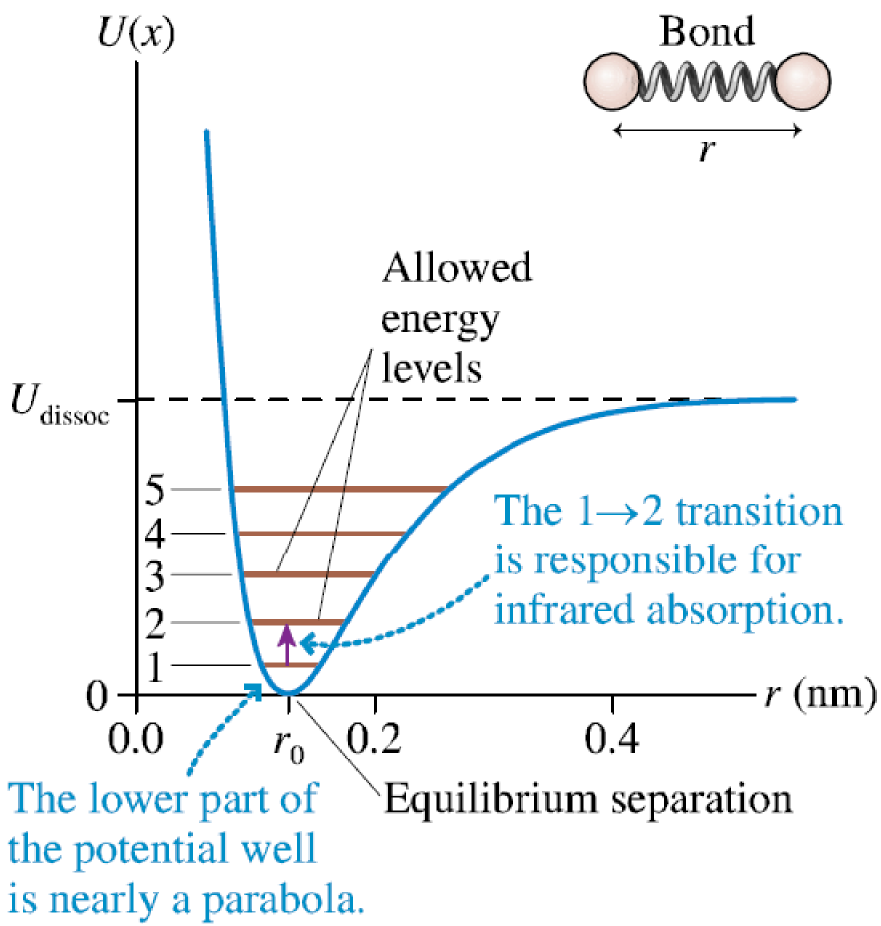
FIGURE 41.22 The quantum and classical probability densities for the $n = 11$ state of a quantum harmonic oscillator.



$$E_n = \left(n - \frac{1}{2}\right)\hbar\omega \qquad n = 1, 2, 3, \ldots$$

Molecular vibrations - Harmonic Oscillator

FIGURE 41.23 The potential energy of a molecular bond and a few of the allowed energies.



E = total energy of the two interacting atoms, NOT of a single particle
U = potential energy between the two atoms

The potential U(x) is shown for two atoms. There exist an equilibrium separation.

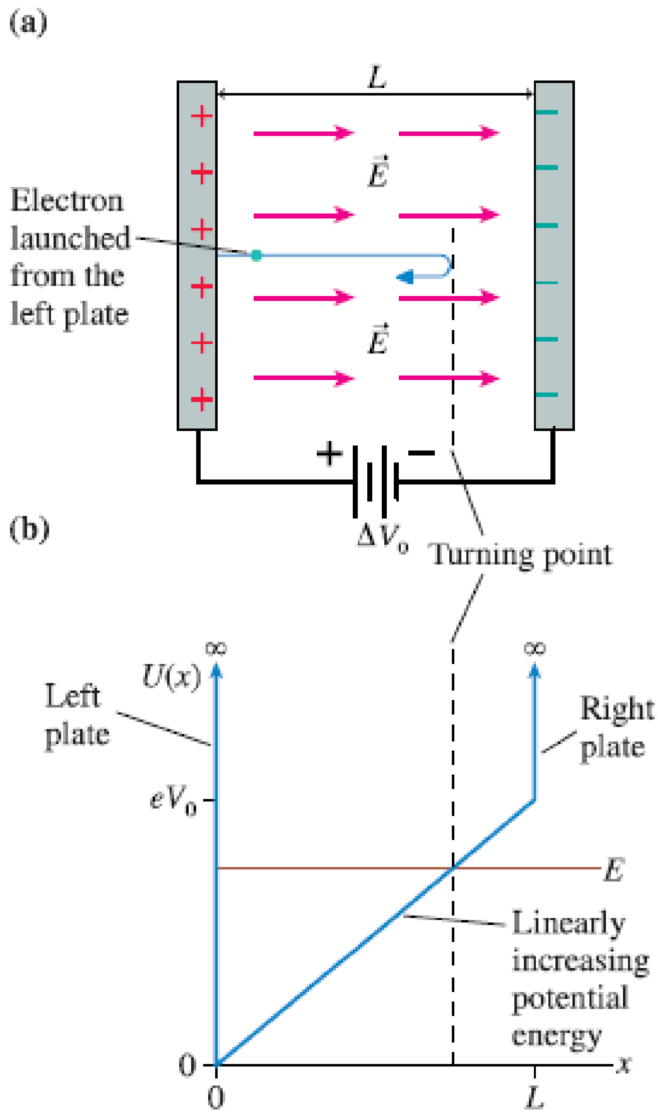
At low energies, this dip looks like a parabola → Harmonic oscillator solution.

Allowed (total) vibrational energies:

$$E_{\mathrm{vib}} \approx \left(n - \frac{1}{2}\right)\hbar\omega \qquad n = 1, 2, 3, \ldots$$

Particle in a capacitor

FIGURE 41.25 An electron in a capacitor.



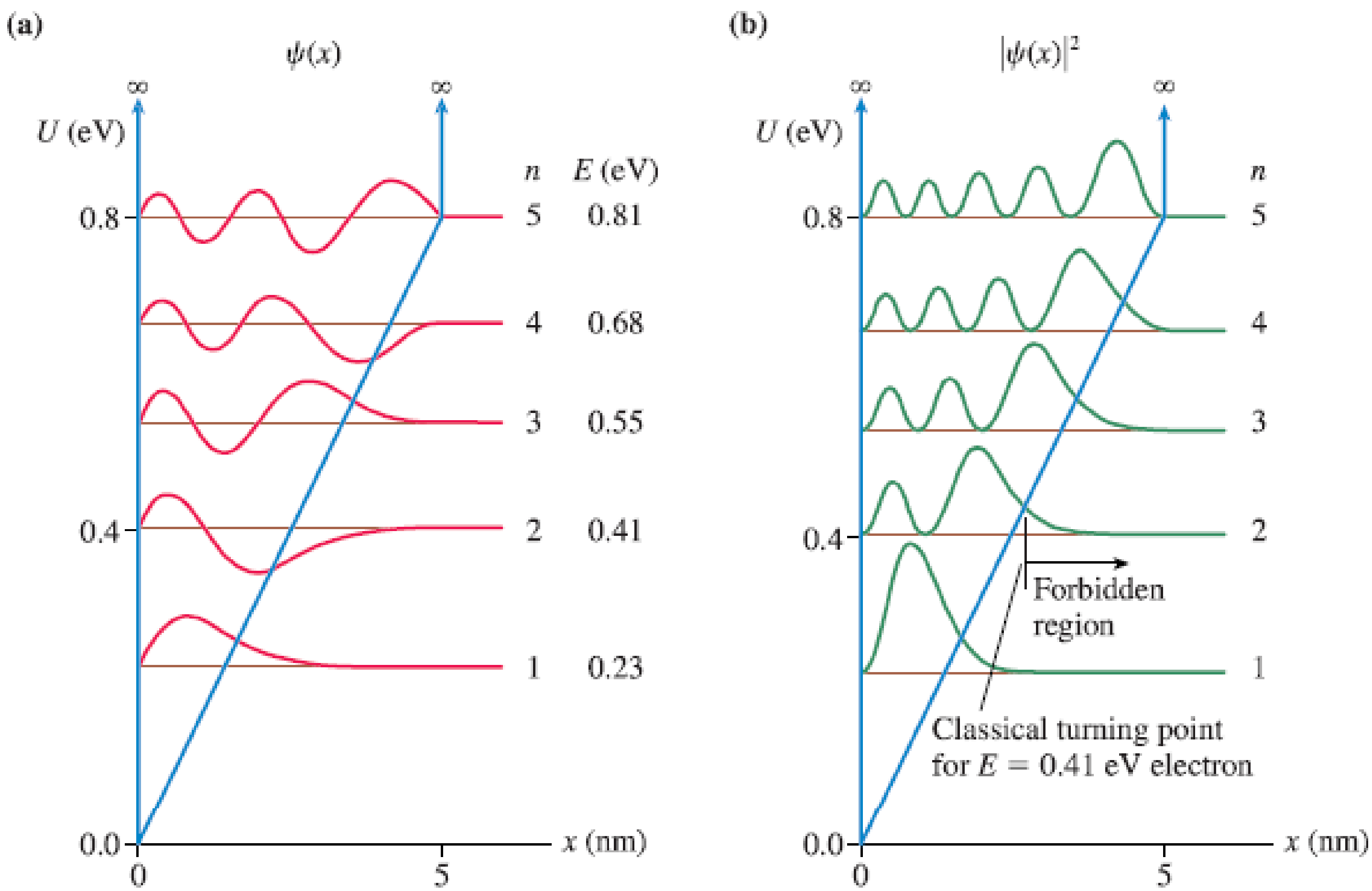
$$V(x) = -Ex = -\frac{\Delta V_0}{L}x$$

The electron, with charge $q = -e$, has potential energy

$$U(x) = qV(x) = +\frac{e\,\Delta V_0}{L}x \qquad 0 < x < L$$

Particle in a capacitor

FIGURE 41.26 Energy levels, wave functions, and probability densities for an electron in a 5.0-nm-wide capacitor with a 0.80 V potential difference.



Covalent Bond: H2+ (single electron)

FIGURE 41.27 A molecule can be modeled as two closely spaced potential wells, one representing each atom.

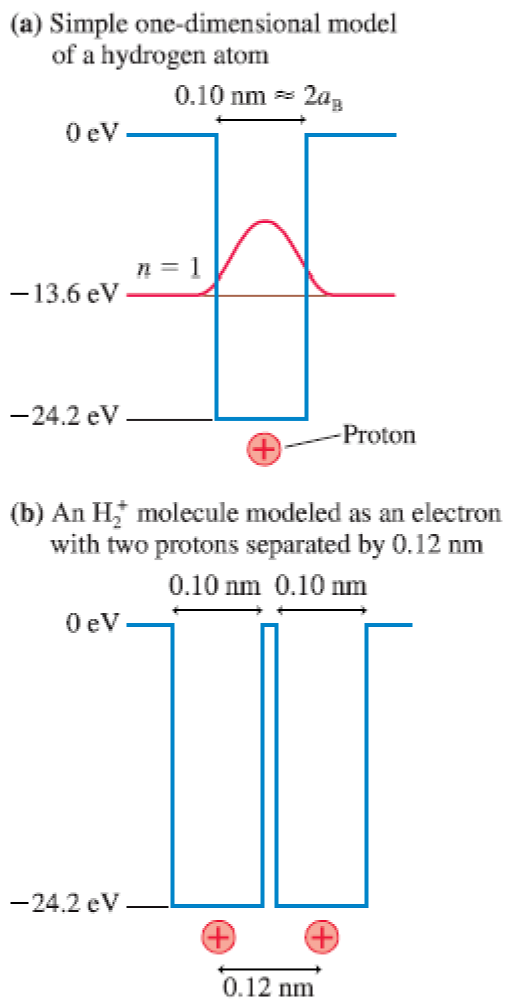
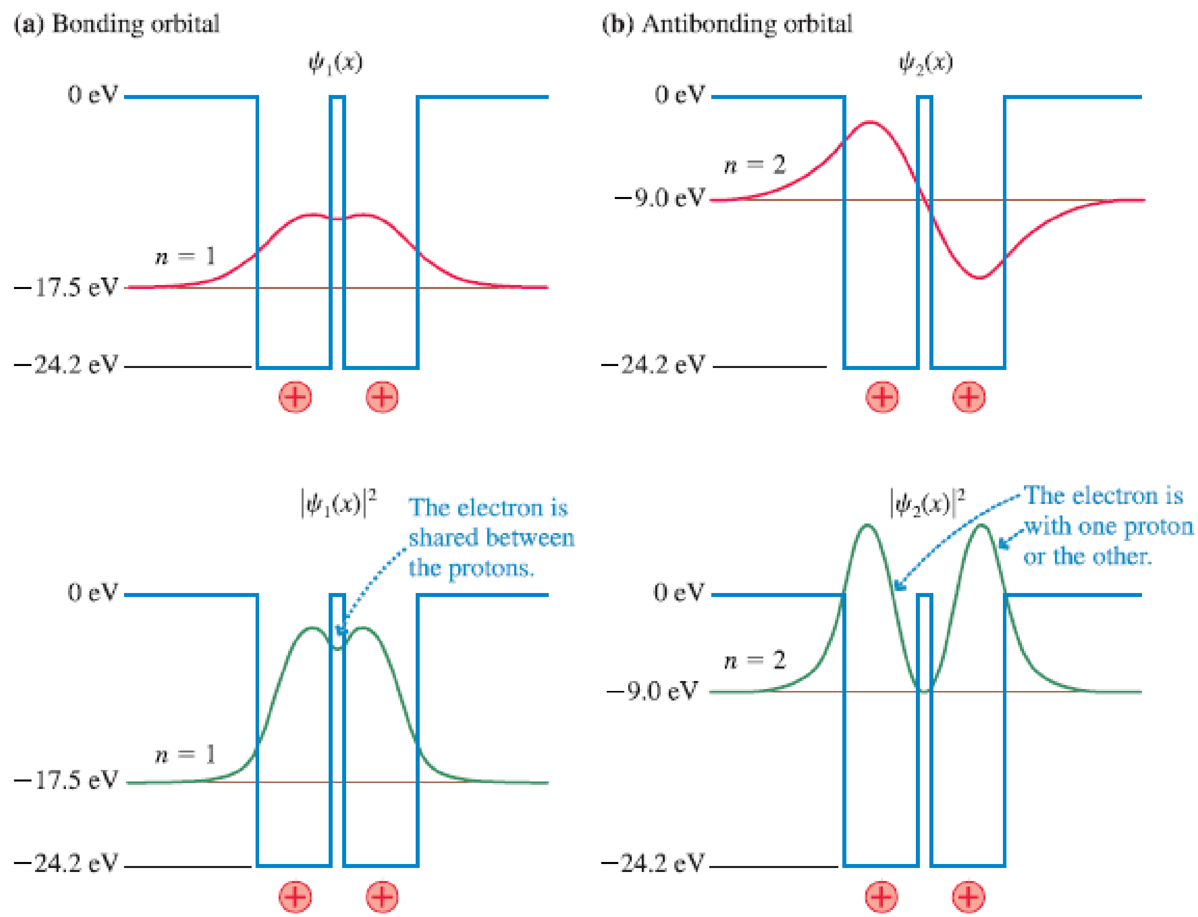
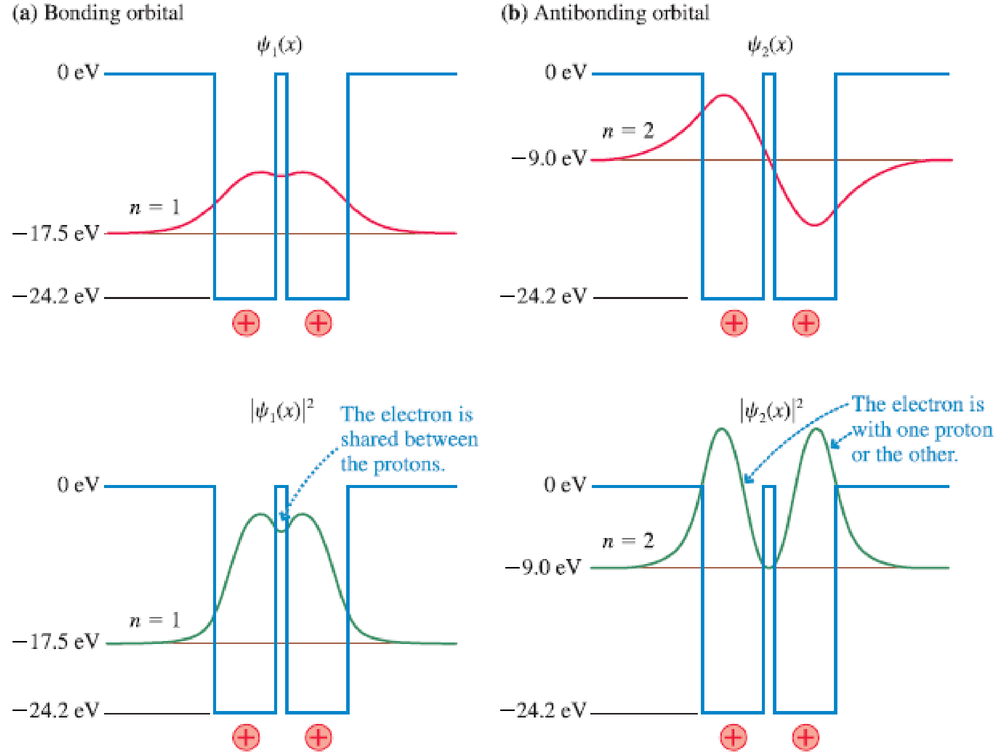


FIGURE 41.28 The wave functions and probability densities of the electron in H_2^+.



Covalent Bond: H2+ (single electron)

FIGURE 41.28 The wave functions and probability densities of the electron in H_2^+.

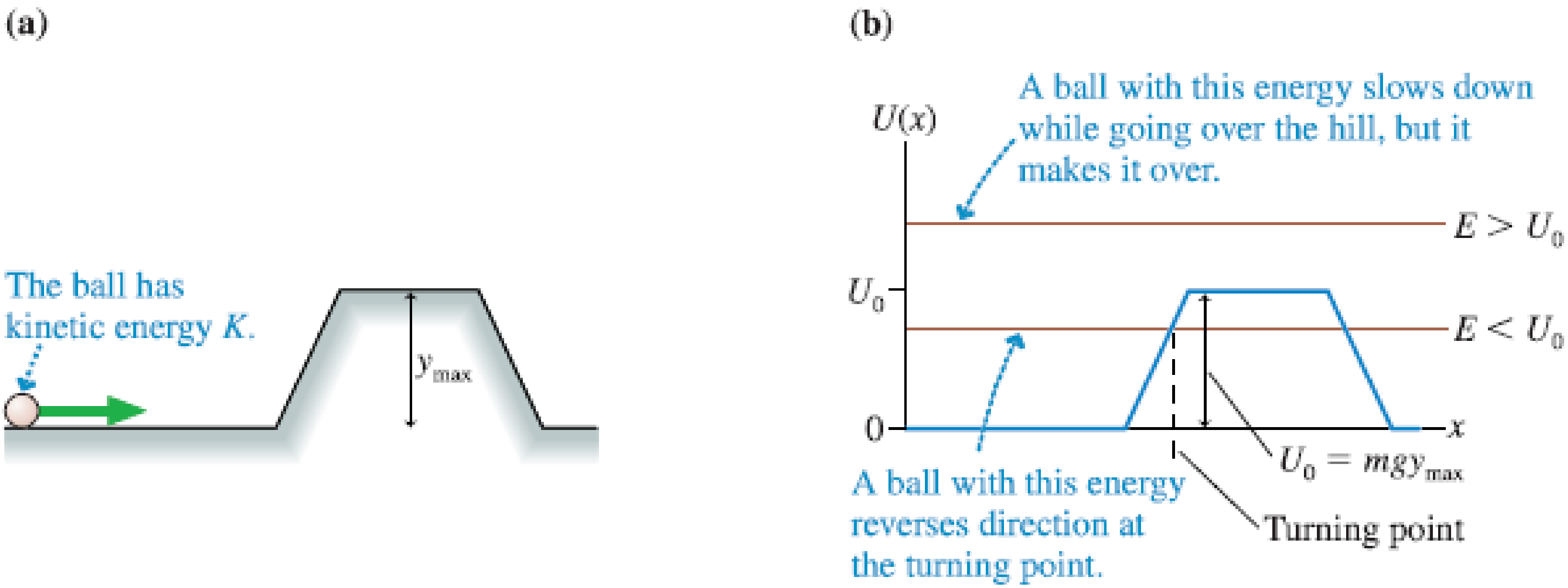


To learn the consequences of these wave functions we need to calculate the total energy of the molecule: $E_{mol} = E_{p-p} + E_{elec}$. The $n = 1$ and $n = 2$ energies shown in Figure 41.28 are the energies E_{elec} of the electron. At the same time, the protons repel each other and have electric potential energy E_{p-p}. It's not hard to calculate that $E_{p-p} = 12.0$ eV for two protons separated by 0.12 nm. Thus

$$E_{mol} = E_{p-p} + E_{elec} = \begin{cases} 12.0\text{ eV} - 17.5\text{ eV} = -5.5\text{ eV} & n = 1 \\ 12.0\text{ eV} - \ \ 9.0\text{ eV} = +3.0\text{ eV} & n = 2 \end{cases}$$

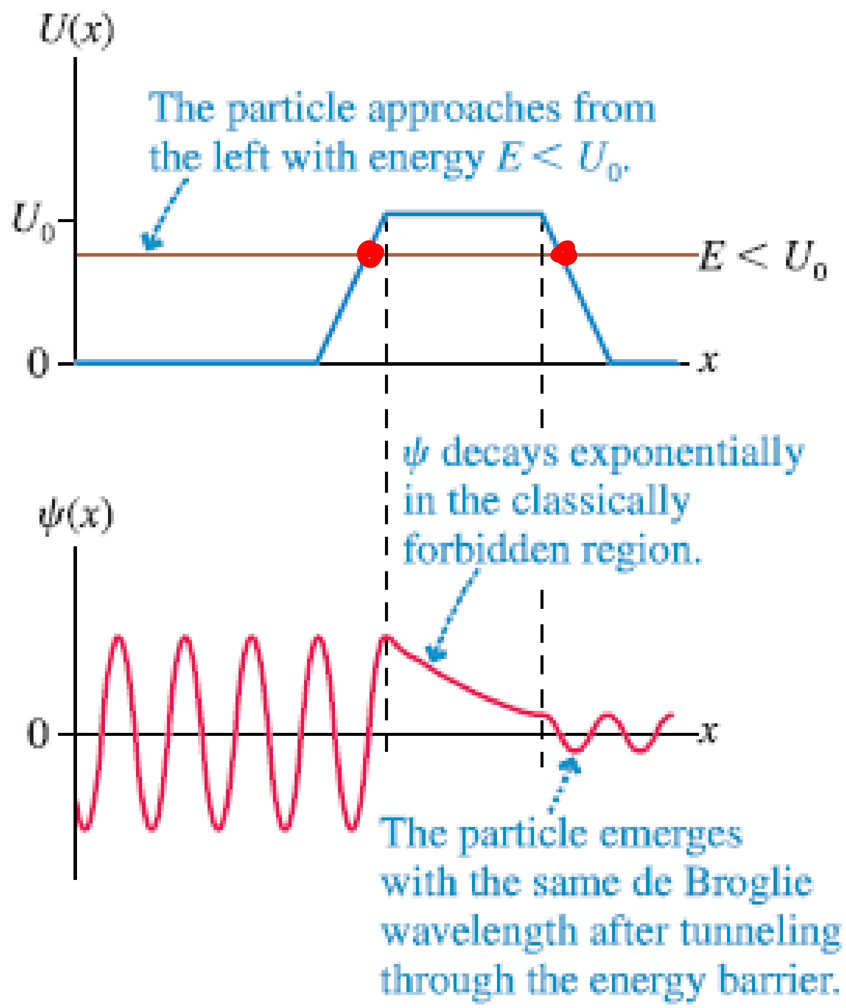
Quantum Tunneling

FIGURE 41.29 A hill is an energy barrier to a rolling ball.



Quantum Tunneling

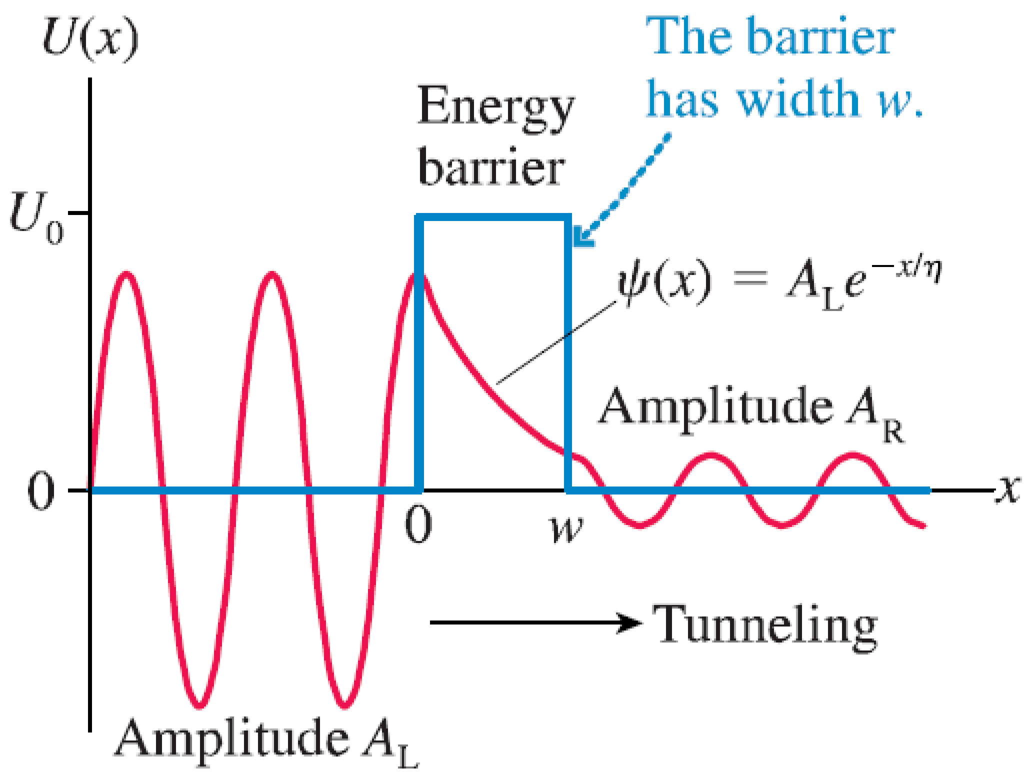
FIGURE 41.30 A quantum particle can penetrate through the energy barrier.



Pic is a little wrong. ψ exp. decays when $E < U_0$

Quantum Tunneling

FIGURE 41.31 Tunneling through an idealized energy barrier.



$$A_R = \psi_{in}(\text{at } x = w) = A_L e^{-w/\eta}$$

$$P_{tunnel} = \frac{|A_R|^2}{|A_L|^2} = (e^{-w/\eta})^2 = e^{-2w/\eta}$$

Quantum Tunneling – Resonant tunneling

FIGURE 41.34 Electron potential energy in a resonant tunneling diode.

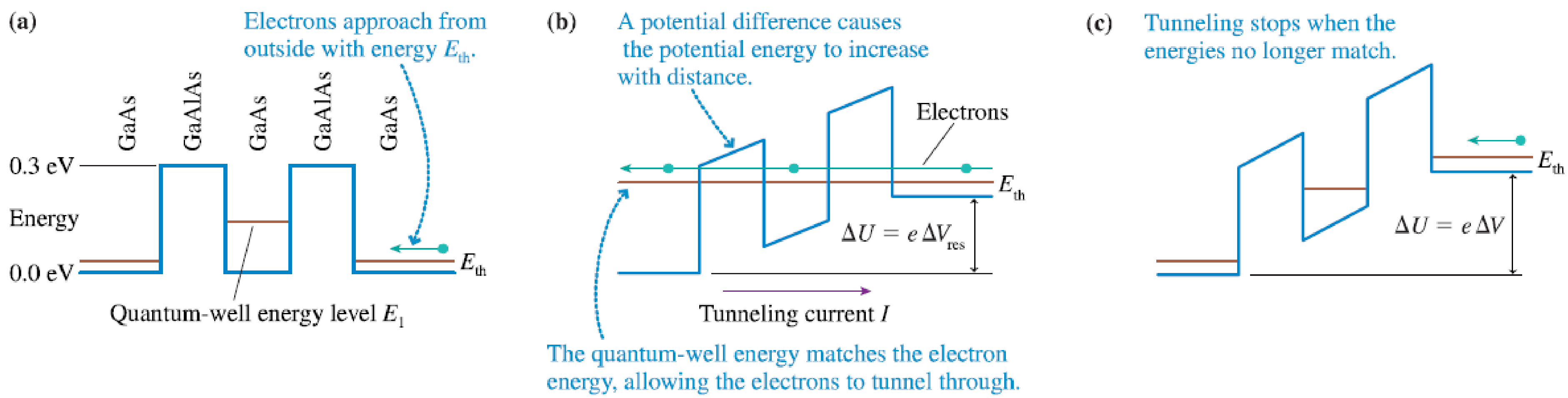


FIGURE 41.35 Experimental measurement of the current-voltage characteristics of a resonant tunneling diode.