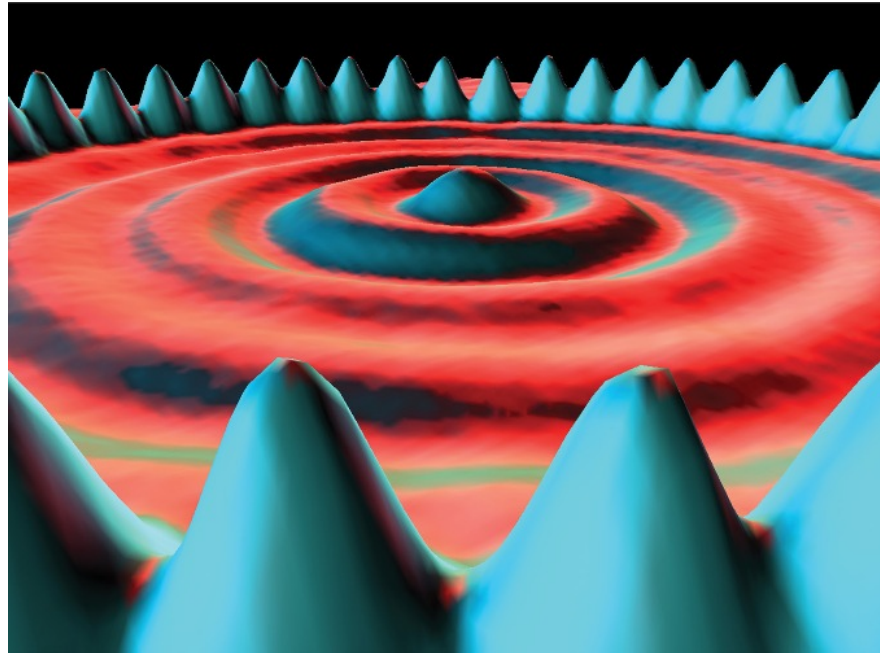


Chapter 39

More About Matter Waves



Lecture 33, 34

Seon-Hee Seo

2016.11.30-12.02

39.2: String Waves and Matter Waves



Confinement of a wave leads to quantization—that is, to the existence of discrete states with discrete energies. The wave can have only those energies.

This observation applies to waves of all kinds, including matter waves.

For matter waves, however, it is more convenient to deal with the energy E of the associated particle than with the frequency f of the wave.

39.3: Energies of a Trapped Electron: One-dimensional trap

An electron can be trapped in the $V = 0$ region.

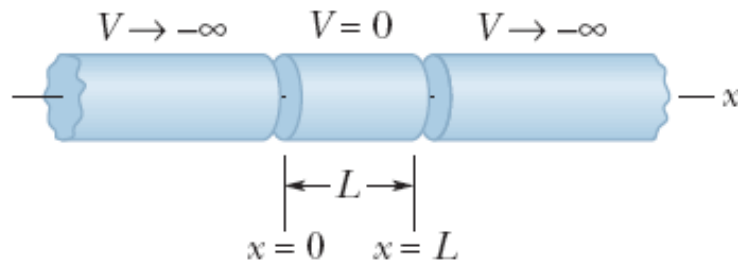


Fig. 39-1 The elements of an idealized “trap” designed to confine an electron to the central cylinder. We take the semi-infinitely long end cylinders to be at an infinitely great negative potential and the central cylinder to be at zero potential.

$$L = \frac{n\lambda}{2}, \quad \text{for } n = 1, 2, 3, \dots$$

Each value of n identifies a state of the oscillating string; the integer n is a **quantum number**.

For each state of the string, the transverse displacement of the string at any position x along the string is given by

$$y_n(x) = A \sin\left(\frac{n\pi}{L}x\right), \quad \text{for } n = 1, 2, 3, \dots,$$

39.3: Energies of a Trapped Electron: Finding the quantized energies

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}.$$

$$L = \frac{n\lambda}{2}, \quad \text{for } n = 1, 2, 3, \dots$$

$$\longrightarrow \lambda = \frac{2L}{n} = \frac{h}{\sqrt{2mE}}$$

$$\longrightarrow E_n = \left(\frac{h^2}{8mL^2} \right) n^2, \quad \text{for } n = 1, 2, 3, \dots$$

An electron can be trapped in the $U = 0$ region.

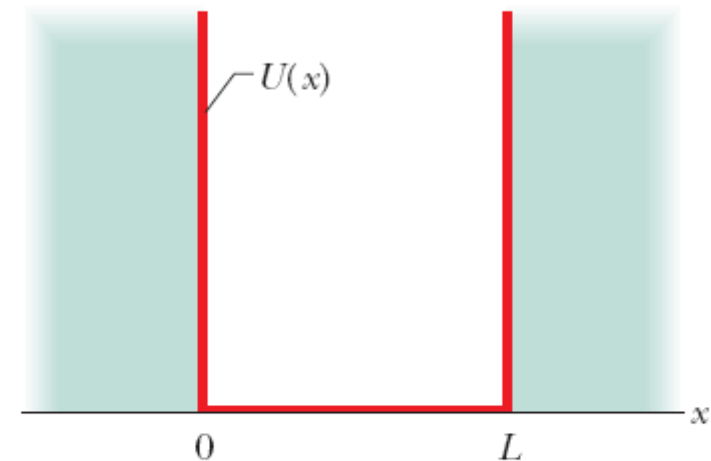


Fig. 39-2 The electric potential energy $U(x)$ of an electron confined to the central cylinder of the idealized trap of Fig. 39-1. We see that $U = 0$ for $0 < x < L$, and $U \rightarrow \infty$ for $x < 0$ and $x > L$.

39.3: Energies of a Trapped Electron: Finding the quantized energies

$$E_n = \left(\frac{h^2}{8mL^2} \right) n^2, \quad \text{for } n = 1, 2, 3, \dots$$

These are the lowest five energy levels allowed the electron.
(No intermediate levels are allowed.)

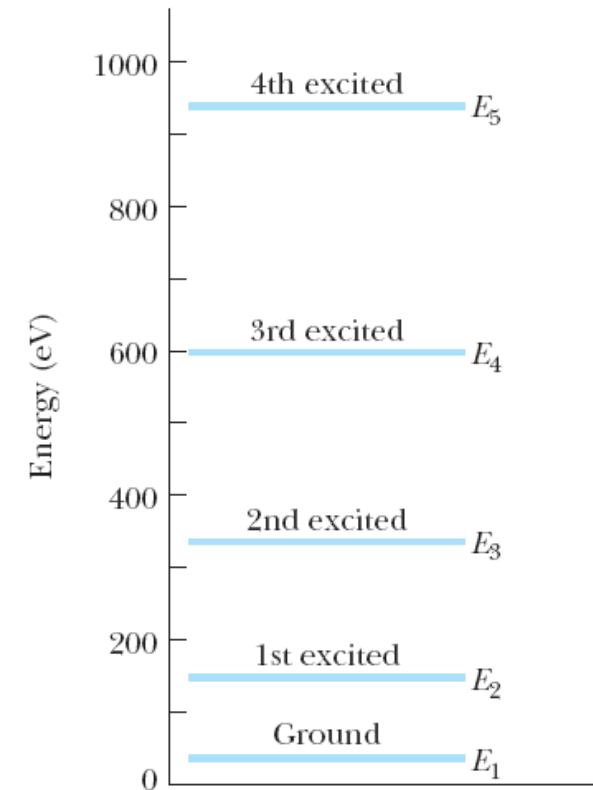


Fig. 39-3 Several of the allowed energies given by Eq. 39-4 for an electron confined to the infinite well of Fig. 39-2. Here width $L = 100$ pm. Such a plot is called an *energy-level diagram*.

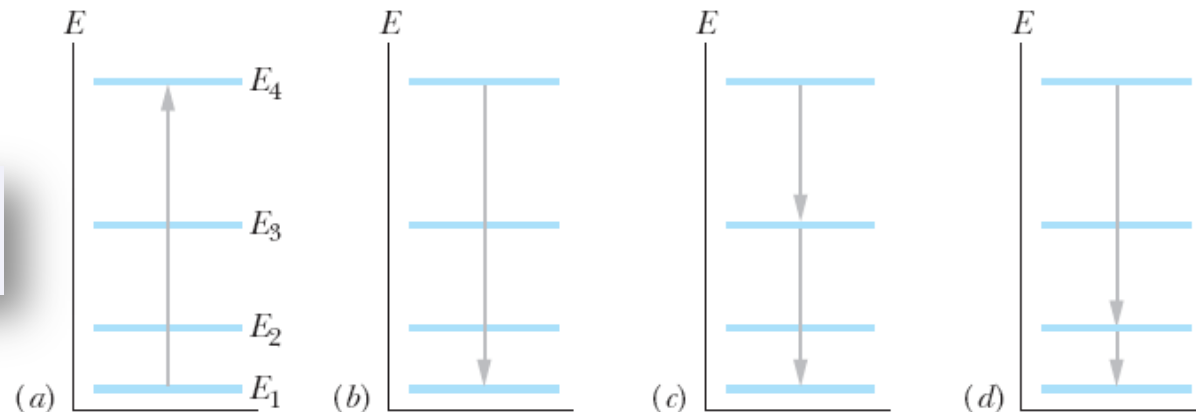
39.3: Energies of a Trapped Electron: Finding the quantized energies

Fig. 39-4 (a) Excitation of a trapped electron from the energy level of its ground state to the level of its third excited state. (b)–(d) Three of four possible ways the electron can de-excite to return to the energy level of its ground state. (Which way is not shown?)

The electron is excited to a higher energy level.

It can de-excite to a lower level in several ways (set by chance).

$$\Delta E = E_{\text{high}} - E_{\text{low}}.$$



If a confined electron is to absorb a photon, the energy hf of the photon must equal the energy difference ΔE between the initial energy level of the electron and a higher level.

$$hf = \Delta E = E_{\text{high}} - E_{\text{low}}.$$

Example, Energy levels in a 1-D infinite potential well:

An electron is confined to a one-dimensional, infinitely deep potential energy well of width $L = 100$ pm.

(a) What is the smallest amount of energy the electron can have?

Lowest energy level: Here, the collection of constants in front of n^2 in Eq. 39-4 is evaluated as

$$\begin{aligned}\frac{h^2}{8mL^2} &= \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{s})^2}{(8)(9.11 \times 10^{-31} \text{ kg})(100 \times 10^{-12} \text{ m})^2} \\ &= 6.031 \times 10^{-18} \text{ J.}\end{aligned}\quad (39-7)$$

The smallest amount of energy the electron can have corresponds to the lowest quantum number, which is $n = 1$ for the ground state of the electron. Thus, Eqs. 39-4 and 39-7 give us

$$\begin{aligned}E_1 &= \left(\frac{h^2}{8mL^2}\right)n^2 = (6.031 \times 10^{-18} \text{ J})(1)^2 \\ &\approx 6.03 \times 10^{-18} \text{ J} = 37.7 \text{ eV.}\end{aligned}\quad (\text{Answer})$$

(b) How much energy must be transferred to the electron if it is to make a quantum jump from its ground state to its second excited state?

$$\begin{aligned}\Delta E_{31} &= \left(\frac{h^2}{8mL^2}\right)(3)^2 - \left(\frac{h^2}{8mL^2}\right)(1)^2 \\ &= \frac{h^2}{8mL^2}(3^2 - 1^2) \\ &= (6.031 \times 10^{-18} \text{ J})(8) \\ &= 4.83 \times 10^{-17} \text{ J} = 301 \text{ eV.}\end{aligned}\quad (\text{Answer})$$

Upward jump: The energies E_3 and E_1 depend on the quantum number n , according to Eq. 39-4. Therefore, substituting that equation into Eq. 39-8 for energies E_3 and E_1 and

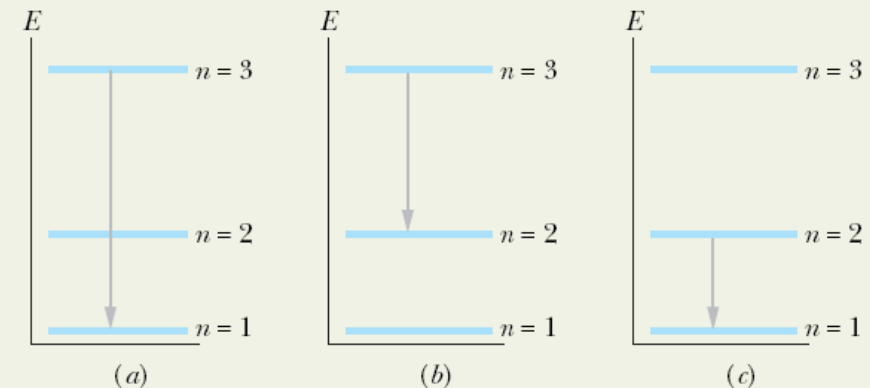


Fig. 39-5 De-excitation from the second excited state to the ground state either directly (a) or via the first excited state (b, c).

Example, Energy levels in a 1-D infinite potential well, cont.

(c) If the electron gains the energy for the jump from energy level E_1 to energy level E_3 by absorbing light, what light wavelength is required?

KEY IDEAS

(1) If light is to transfer energy to the electron, the transfer must be by photon absorption. (2) The photon's energy must equal the energy difference ΔE between the initial energy level of the electron and a higher level, according to Eq. 39-6 ($hf = \Delta E$). Otherwise, a photon *cannot* be absorbed.

Wavelength: Substituting c/λ for f , we can rewrite Eq. 39-6 as

$$\lambda = \frac{hc}{\Delta E}. \quad (39-9)$$

For the energy difference ΔE_{31} we found in (b), this equation gives us

$$\begin{aligned} \lambda &= \frac{hc}{\Delta E_{31}} \\ &= \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{s})(2.998 \times 10^8 \text{ m/s})}{4.83 \times 10^{-17} \text{ J}} \\ &= 4.12 \times 10^{-9} \text{ m}. \end{aligned} \quad (\text{Answer})$$

(d) Once the electron has been excited to the second excited state, what wavelengths of light can it emit by de-excitation?

The direct jump involves the same energy difference ΔE_{31} we found in (c). Then the wavelength is the same as we calculated in (c)—except now the wavelength is for light

that is emitted, not absorbed. Thus, the electron can jump directly to the ground state by emitting light of wavelength

$$\lambda = 4.12 \times 10^{-9} \text{ m}. \quad (\text{Answer})$$

Following the procedure of part (b), you can show that the energy differences for the jumps of Figs. 39-5*b* and *c* are

$$\Delta E_{32} = 3.016 \times 10^{-17} \text{ J} \quad \text{and} \quad \Delta E_{21} = 1.809 \times 10^{-17} \text{ J}.$$

From Eq. 39-9, we then find that the wavelength of the light emitted in the first of these jumps (from $n = 3$ to $n = 2$) is

$$\lambda = 6.60 \times 10^{-9} \text{ m}, \quad (\text{Answer})$$

and the wavelength of the light emitted in the second of these jumps (from $n = 2$ to $n = 1$) is

$$\lambda = 1.10 \times 10^{-8} \text{ m}. \quad (\text{Answer})$$

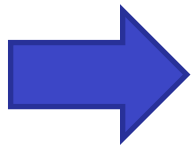
39.4: Wave Functions of a Trapped Electron

Fig. 39-6 The probability density $\psi_n^2(x)$ for four states of an electron trapped in a one-dimensional infinite well; their quantum numbers are $n = 1, 2, 3$, and 15. The electron is most likely to be found where $\psi_n^2(x)$ is greatest and least likely to be found where $\psi_n^2(x)$ is least.

$$\left(\begin{array}{c} \text{probability } p(x) \\ \text{of detection in width } dx \\ \text{centered on position } x \end{array} \right) = \left(\begin{array}{c} \text{probability density } \psi_n^2(x) \\ \text{at position } x \end{array} \right) (\text{width } dx),$$

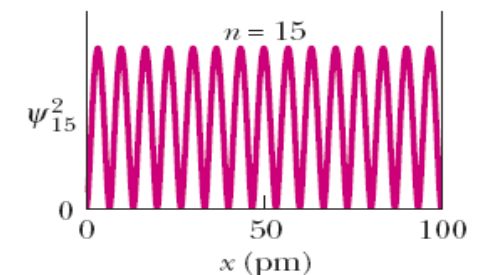
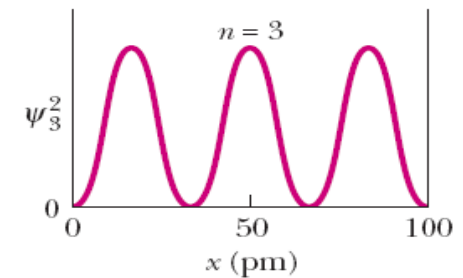
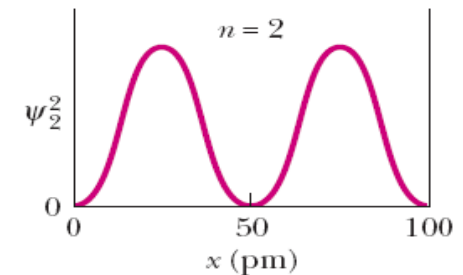
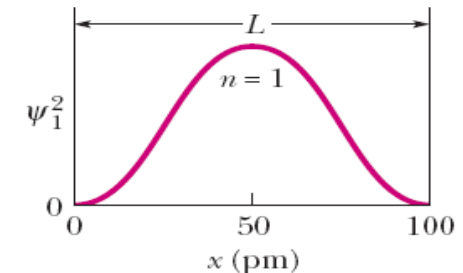
$$p(x) = \psi_n^2(x) dx.$$

$$\psi_n(x) = A \sin\left(\frac{n\pi}{L}x\right), \quad \text{for } n = 1, 2, 3, \dots,$$



$$\begin{aligned} \left(\begin{array}{c} \text{probability of detection} \\ \text{between } x_1 \text{ and } x_2 \end{array} \right) &= \int_{x_1}^{x_2} p(x) \\ &= \int_{x_1}^{x_2} A^2 \sin^2\left(\frac{n\pi}{L}x\right) dx. \end{aligned}$$

The probability density must be zero at the infinite walls.



39.4: Wave Functions of a Trapped Electron

Normalization and Zero-Point Energy

➤ The product $\psi_n^2(x) dx$ gives the probability that an electron in an infinite well can be detected in the interval of the x axis that lies between x and $x + dx$. We know that the electron must be somewhere in the infinite well; so it must be true that

$$\int_{-\infty}^{+\infty} \psi_n^2(x) dx = 1 \quad (\text{normalization equation})$$

$$E_n = \left(\frac{h^2}{8mL^2} \right) n^2, \quad \text{for } n = 1, 2, 3, \dots$$

➤ $n=1$ in the previous equation defines the state of lowest energy for an electron in an infinite potential well, the **ground state**. Therefore in quantum physics confined systems cannot exist in states with zero energy. They must always have a **certain minimum energy** called the **zero-point energy**.

Example, Detection probability in a 1D potential well

A ground-state electron is trapped in the one-dimensional infinite potential well of Fig. 39-2, with width $L = 100$ pm.

(a) What is the probability that the electron can be detected in the left one-third of the well ($x_1 = 0$ to $x_2 = L/3$)?

KEY IDEAS

(1) If we probe the left one-third of the well, there is no guarantee that we will detect the electron. However, we can calculate the probability of detecting it with the integral of Eq. 39-13. (2) The probability very much depends on which state the electron is in—that is, the value of quantum number n .

Calculations: Because here the electron is in the ground state, we set $n = 1$ in Eq. 39-13. We also set the limits of integration as the positions $x_1 = 0$ and $x_2 = L/3$ and set the amplitude constant A as $\sqrt{2/L}$ (so that the wave function is normalized). We then see that

$$\left(\begin{array}{c} \text{probability of detection} \\ \text{in left one-third} \end{array} \right) = \int_0^{L/3} \frac{2}{L} \sin^2 \left(\frac{1\pi}{L} x \right) dx.$$

We could find this probability by substituting 100×10^{-12} m for L and then using a graphing calculator or a computer math package to evaluate the integral. Here, however, we shall evaluate the integral “by hand.” First we switch to a new integration variable y :

$$y = \frac{\pi}{L} x \quad \text{and} \quad dx = \frac{L}{\pi} dy.$$

From the first of these equations, we find the new limits of integration to be $y_1 = 0$ for $x_1 = 0$ and $y_2 = \pi/3$ for $x_2 = L/3$. We then must evaluate

$$\text{probability} = \left(\frac{2}{L} \right) \left(\frac{L}{\pi} \right) \int_0^{\pi/3} (\sin^2 y) dy.$$

Using integral 11 in Appendix E, we then find

$$\text{probability} = \frac{2}{\pi} \left(\frac{y}{2} - \frac{\sin 2y}{4} \right)_0^{\pi/3} = 0.20.$$

Thus, we have

$$\left(\begin{array}{c} \text{probability of detection} \\ \text{in left one-third} \end{array} \right) = 0.20. \quad (\text{Answer})$$

That is, if we repeatedly probe the left one-third of the well, then on average we can detect the electron with 20% of the probes.

(b) What is the probability that the electron can be detected in the middle one-third of the well?

Reasoning: We now know that the probability of detection in the left one-third of the well is 0.20. By symmetry, the probability of detection in the right one-third of the well is also 0.20. Because the electron is certainly in the well, the probability of detection in the entire well is 1. Thus, the probability of detection in the middle one-third of the well is

$$\begin{aligned} \left(\begin{array}{c} \text{probability of detection} \\ \text{in middle one-third} \end{array} \right) &= 1 - 0.20 - 0.20 \\ &= 0.60. \quad (\text{Answer}) \end{aligned}$$

Example, Detection probability in a 1D potential well

Evaluate the amplitude constant A in Eq. 39-10 for an infinite potential well extending from $x = 0$ to $x = L$.

KEY IDEA

The wave functions of Eq. 39-10 must satisfy the normalization requirement of Eq. 39-14, which states that the probability that the electron can be detected somewhere along the x axis is 1.

Calculations: Substituting Eq. 39-10 into Eq. 39-14 and taking the constant A outside the integral yield

$$A^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1. \quad (39-15)$$

We have changed the limits of the integral from $-\infty$ and $+\infty$ to 0 and L because the wave function is zero outside these new limits (so there's no need to integrate out there).

We can simplify the indicated integration by changing the variable from x to the dimensionless variable y , where

$$y = \frac{n\pi}{L}x, \quad (39-16)$$

hence

$$dx = \frac{L}{n\pi} dy.$$

When we change the variable, we must also change the integration limits (again). Equation 39-16 tells us that $y = 0$ when $x = 0$ and that $y = n\pi$ when $x = L$; thus 0 and $n\pi$ are our new limits. With all these substitutions, Eq. 39-15 becomes

$$A^2 \frac{L}{n\pi} \int_0^{n\pi} (\sin^2 y) dy = 1.$$

We can use integral 11 in Appendix E to evaluate the integral, obtaining the equation

$$\frac{A^2 L}{n\pi} \left[\frac{y}{2} - \frac{\sin 2y}{4} \right]_0^{n\pi} = 1.$$

Evaluating at the limits yields

$$\frac{A^2 L}{n\pi} \frac{n\pi}{2} = 1;$$

thus

$$A = \sqrt{\frac{2}{L}}. \quad (\text{Answer}) \quad (39-17)$$

This result tells us that the dimension for A^2 , and thus for $\psi_n^2(x)$, is an inverse length. This is appropriate because the probability density of Eq. 39-12 is a probability *per unit length*.

39.5: An Electron in a Finite Well

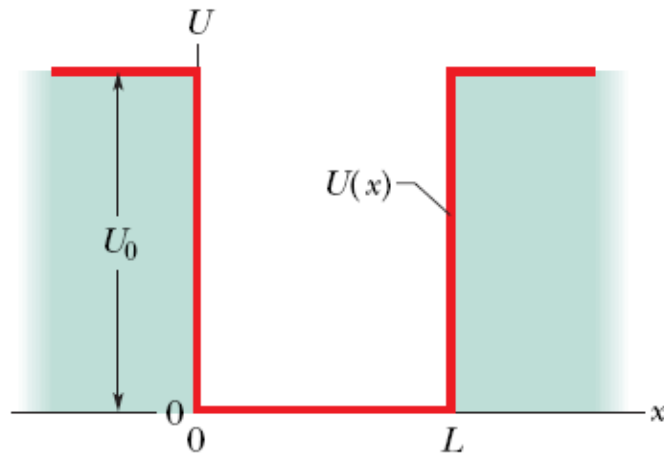


Fig. 39-7 A *finite* potential energy well. The depth of the well is U_0 and its width is L . As in the infinite potential well of Fig. 39-2, the motion of the trapped electron is restricted to the x direction.

To find the wave functions describing the quantum states of an electron in the finite well of Fig. 39-7, one needs to consider Schrödinger's equation.

For motion in one dimension, Schrödinger's equation in the form is:

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} [E - U(x)]\psi = 0.$$

39.5: An Electron in a Finite Well

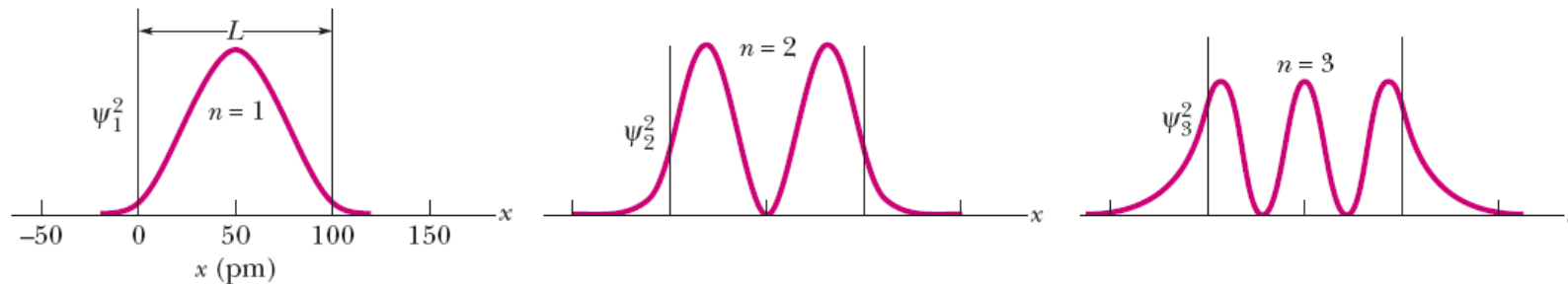


Fig. 39-8 The first three probability densities for an electron confined to a finite potential well of depth $U_0 = 450$ eV and width $L = 100$ pm. Only states $n = 1, 2, 3$, and 4 are allowed.

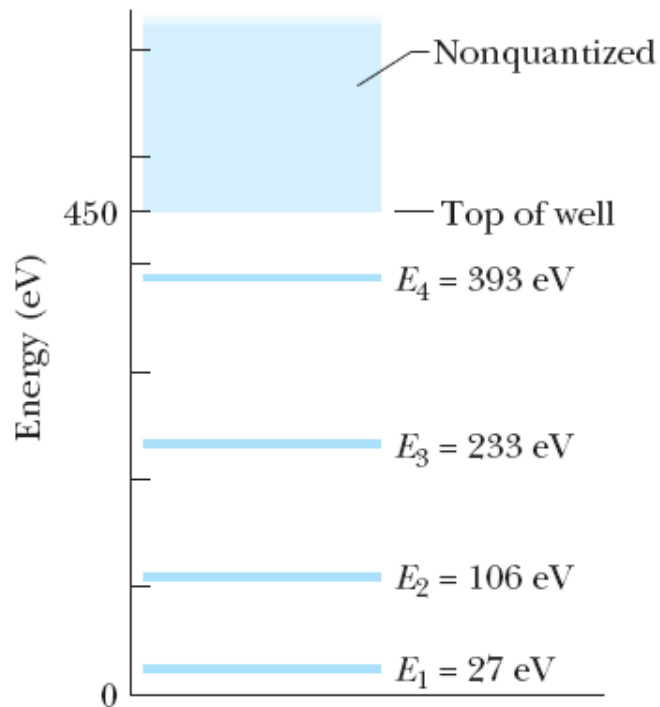


Fig. 39-9 The energy-level diagram corresponding to the probability densities of Fig. 39-8. If an electron is trapped in the finite potential well, it can have only the energies corresponding to $n = 1, 2, 3$, and 4. If it has an energy of 450 eV or greater, it is not trapped and its energy is not quantized.

For a finite well, the electron matter wave penetrates the walls of the well—into a region in which Newtonian mechanics says the electron cannot exist.

However, from the plots in Fig. 39-8, we see there is leakage into the walls, and that the leakage is greater for greater values of quantum number n .

Example, Electron escaping from a finite well

Suppose a finite well with $U_0 = 450$ eV and $L = 100$ pm confines a single electron in its ground state.

(a) What wavelength of light is needed to barely free the electron from the potential well if the electron absorbs a single photon from the light?

Barely escaping: The electron is initially in its ground state, with an energy of $E_1 = 27$ eV. So, to barely become free, it must receive an energy of

$$U_0 - E_1 = 450 \text{ eV} - 27 \text{ eV} = 423 \text{ eV}.$$
$$\frac{hc}{\lambda} = U_0 - E_1,$$

from which we find

$$\begin{aligned}\lambda &= \frac{hc}{U_0 - E_1} \\ &= \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{s})(3.00 \times 10^8 \text{ m/s})}{(423 \text{ eV})(1.60 \times 10^{-19} \text{ J/eV})} \\ &= 2.94 \times 10^{-9} \text{ m} = 2.94 \text{ nm.} \quad (\text{Answer})\end{aligned}$$

Thus, if $\lambda = 2.94$ nm, the electron just barely escapes.

(b) Can the ground-state electron absorb light with $\lambda = 2.00$ nm? If so, what then is the electron's energy?

More than escaping: The energy transferred to the electron is the photon energy:

$$\begin{aligned}hf &= h \frac{c}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{s})(3.00 \times 10^8 \text{ m/s})}{2.00 \times 10^{-9} \text{ m}} \\ &= 9.95 \times 10^{-17} \text{ J} = 622 \text{ eV.}\end{aligned}$$

From (a), the energy required to just barely free the electron from the potential well is $U_0 - E_1 (= 423 \text{ eV})$. The remainder of the 622 eV goes to kinetic energy. Thus, the kinetic energy of the freed electron is

$$\begin{aligned}K &= hf - (U_0 - E_1) \\ &= 622 \text{ eV} - 423 \text{ eV} = 199 \text{ eV.} \quad (\text{Answer})\end{aligned}$$

39.6: More Electron Traps, Nanocrystallites



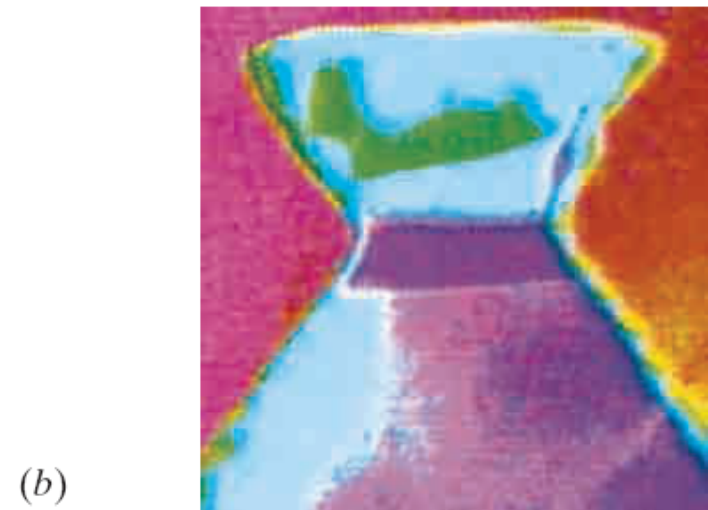
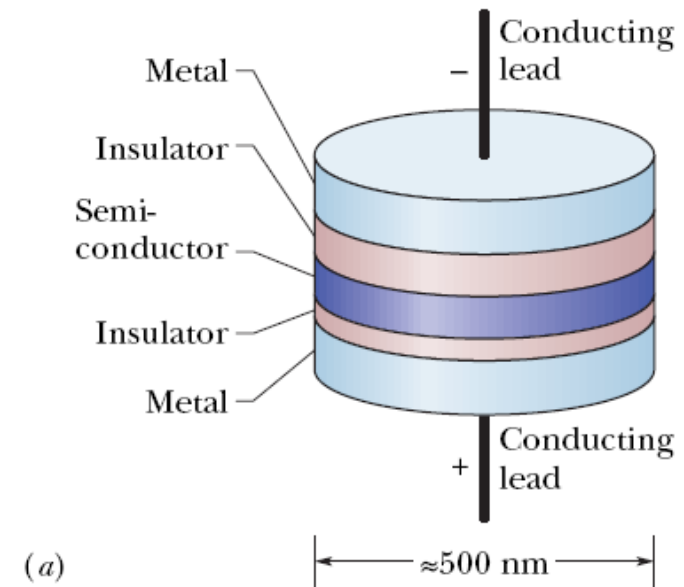
Fig. 39-10 Two samples of powdered cadmium selenide, a semiconductor, differing only in the size of their granules. Each granule serves as an electron trap. The lower sample has the larger granules and consequently the smaller spacing between energy levels and the lower photon energy threshold for the absorption of light. Light not absorbed is scattered, causing the sample to scatter light of greater wavelength and appear red. The upper sample, because of its smaller granules, and consequently its larger level spacing and its larger energy threshold for absorption, appears yellow. (*From Scientific American, January 1993, page 122. Reproduced with permission of Michael Steigerwald, Bell Labs–Lucent Technologies*)

A given nanocrystallite can absorb photons with an energy above a certain threshold energy $E_t (=hf_t)$ and thus wavelengths below a corresponding threshold wavelength

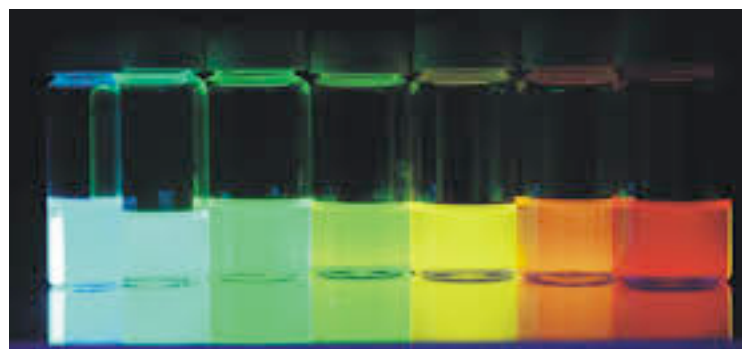
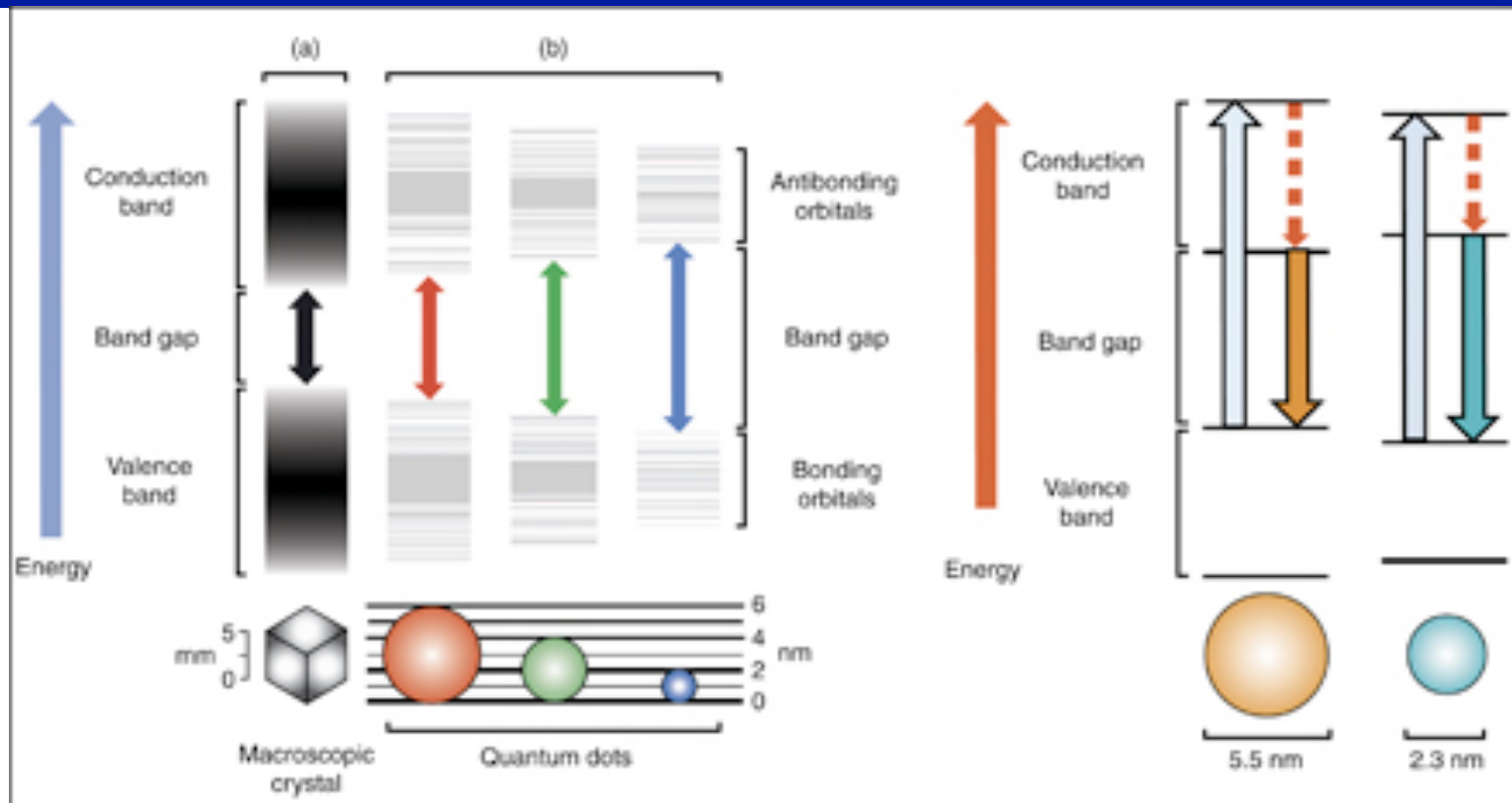
$$\lambda_t = \frac{c}{f_t} = \frac{ch}{E_t}.$$

39.6: More Electron Traps, Quantum Dots

Fig. 39-11 A quantum dot, or “artificial atom.” (a) A central semiconducting layer forms a potential energy well in which electrons are trapped. The lower insulating layer is thin enough to allow electrons to be added to or removed from the central layer by barrier tunneling if an appropriate voltage is applied between the leads. (b) A photograph of an actual quantum dot. The central purple band is the electron confinement region. (From Scientific American, September 1995, page 67. Image reproduced with permission of H. Temkin, Texas Tech University)



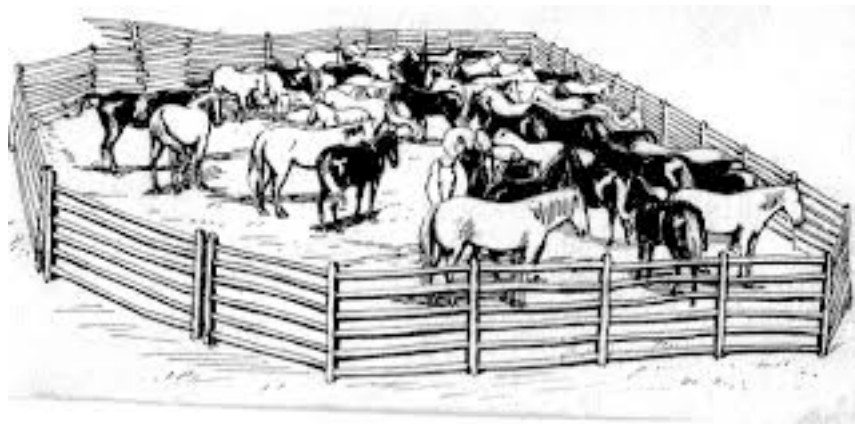
39.6: More Electron Traps, Quantum Dots



2.3 → 5.5
Size (nanometers)

39.6: More Electron Traps, Quantum Corrals

Corral



39.6: More Electron Traps, Quantum Corrals

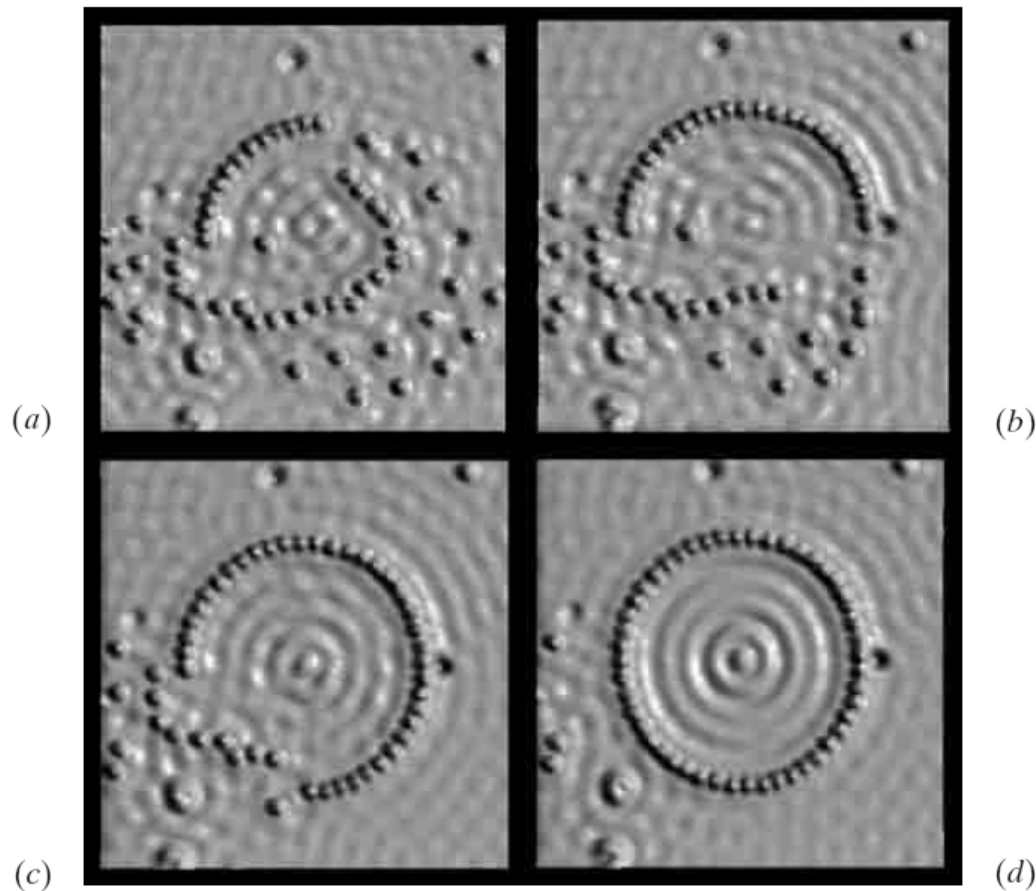
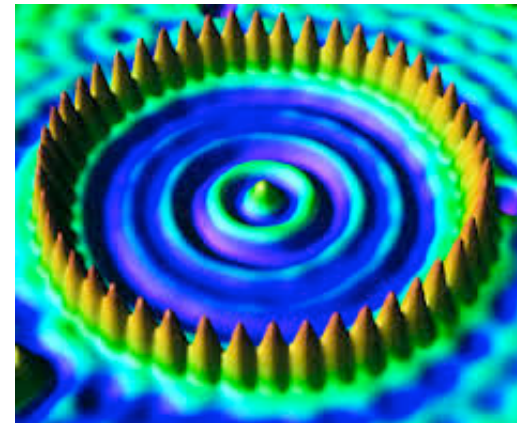


Fig. 39-12 A quantum corral during four stages of construction. Note the appearance of ripples caused by electrons trapped in the corral when it is almost complete. (Courtesy of International Business Machines Corporation, Almaden Research Center)



- Image shows “Quantum corral” of ^{48}Fe atoms on Cu surface
- Low-temperature STM is used for assembly and imaging.
- Can see Schrodinger standing waves.
- Colors are artificial.

39.7: Two- and Three- Dimensional Electron Traps, Rectangular Corral:

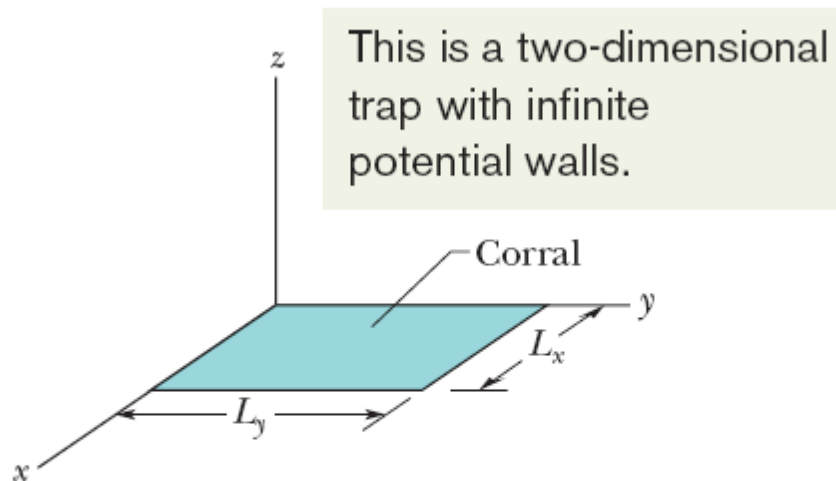


Fig. 39-13 A rectangular corral—a two-dimensional version of the infinite potential well of Fig. 39-2—with widths L_x and L_y .

The normalized wave function:

$$\psi_{n_x, n_y} = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n_x \pi}{L} x\right) \sqrt{\frac{2}{L_y}} \sin\left(\frac{n_y \pi}{L} y\right),$$

See P.12

The energy of the electron:

$$E_{n_x, n_y} = \left(\frac{h^2}{8mL_x^2}\right)n_x^2 + \left(\frac{h^2}{8mL_y^2}\right)n_y^2 = \frac{h^2}{8m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right).$$

39.7: Two- and Three- Dimensional Electron Traps, Rectangular Box:

The energy of an electron trapped in a 3-D infinite potential box:

$$E_{n_x, n_y, n_z} = \frac{h^2}{8m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right).$$

This is a three-dimensional trap with infinite potential walls.

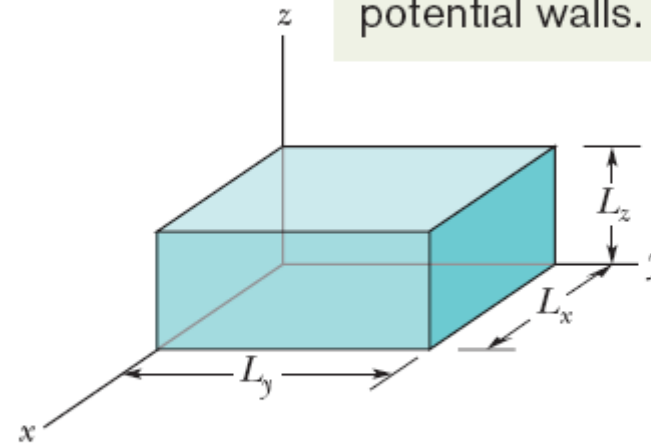


Fig. 39-14 A rectangular box — a three-dimensional version of the infinite potential well of Fig. 39-2 — with widths L_x , L_y , and L_z .

Example, Energy levels in a 2D infinite potential well:

An electron is trapped in a square corral that is a two-dimensional infinite potential well (Fig. 39-13) with widths $L_x = L_y$.

(a) Find the energies of the lowest five possible energy levels for this trapped electron, and construct the corresponding energy-level diagram.

Energy levels: Because the well here is square, we can let the widths be $L_x = L_y = L$. Then Eq. 39-20 simplifies to

$$E_{n_x, n_y} = \frac{h^2}{8mL^2} (n_x^2 + n_y^2). \quad (39-22)$$

The lowest energy states correspond to low values of the quantum numbers n_x and n_y , which are the positive integers 1, 2, ..., ∞ . Substituting those integers for n_x and n_y in Eq. 39-22, starting with the lowest value 1, we can obtain the energy values as listed in Table 39-1. There we can see that

Table 39-1

Energy Levels

n_x	n_y	Energy ^a	n_x	n_y	Energy ^a
1	3	10	2	4	20
3	1	10	4	2	20
2	2	8	3	3	18
1	2	5	1	4	17
2	1	5	4	1	17
1	1	2	2	3	13
			3	2	13

^aIn multiples of $h^2/8mL^2$.

These are the lowest five energy levels allowed the electron. Different quantum states may have the same energy.

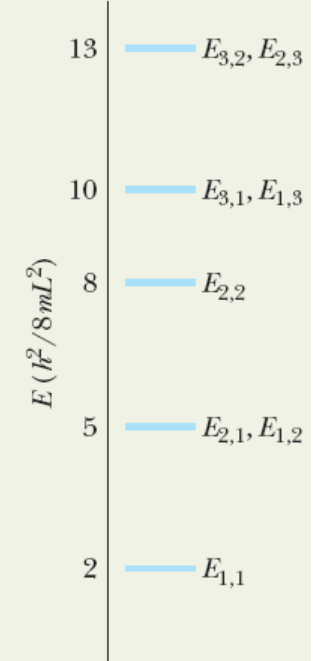


Fig. 39-15 Energy-level diagram for an electron trapped in a square corral.

several of the pairs of quantum numbers (n_x, n_y) give the same energy. For example, the (1, 2) and (2, 1) states both have an energy of $5(h^2/8mL^2)$. Each such pair is associated with degenerate energy levels. Note also that, perhaps surprisingly, the (4, 1) and (1, 4) states have less energy than the (3, 3) state.

From Table 39-1 (carefully keeping track of degenerate levels), we can construct the energy-level diagram of Fig. 39-15.

Example, Energy levels in a 2D infinite potential well, cont.:

(b) As a multiple of $h^2/8mL^2$, what is the energy difference between the ground state and the third excited state?

Energy difference: From Fig. 39-15, we see that the ground state is the (1, 1) state, with an energy of $2(h^2/8mL^2)$. We also see that the third excited state (the third state up from the ground state in the energy-level diagram) is the degenerate (1, 3) and (3, 1) states, with an energy of $10(h^2/8mL^2)$. Thus, the difference ΔE between these two states is

$$\Delta E = 10\left(\frac{h^2}{8mL^2}\right) - 2\left(\frac{h^2}{8mL^2}\right) = 8\left(\frac{h^2}{8mL^2}\right).$$

(Answer)

These are the lowest five energy levels allowed the electron. Different quantum states may have the same energy.

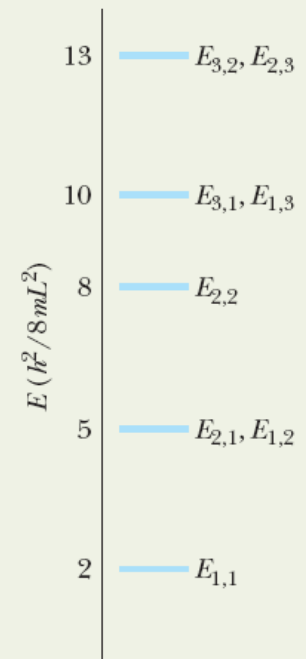
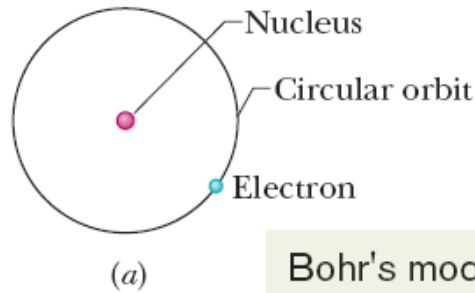


Fig. 39-15 Energy-level diagram for an electron trapped in a square corral.

39.8: The Bohr Model of the Hydrogen Atom



Bohr's model for hydrogen resembles the orbital model of a planet around a star.

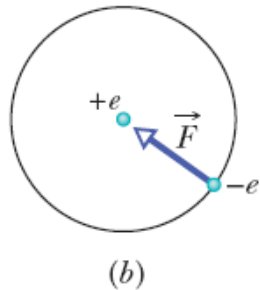


Fig. 39-16 (a) Circular orbit of an electron in the Bohr model of the hydrogen atom. (b) The Coulomb force \vec{F} on the electron is directed radially inward toward the nucleus.

$$F = k \frac{|q_1||q_2|}{r^2},$$

$$-\frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} = m \left(-\frac{v^2}{r} \right),$$

The angular momentum: $\ell = rmv \sin \phi$, $\leftarrow \vec{L} = \vec{r} \times \vec{p}$
 $= rmv \sin 90^\circ$

For quantization of l , $rmv = n\hbar$,

$$v = \frac{n\hbar}{rm}.$$

$$\rightarrow r = \frac{h^2\epsilon_0}{\pi me^2} n^2, \quad \text{for } n = 1, 2, 3, \dots$$

$$\rightarrow r = an^2, \quad \text{for } n = 1, 2, 3, \dots,$$

$$a = \frac{h^2\epsilon_0}{\pi me^2} = 5.291\,772 \times 10^{-11} \text{ m} \approx 52.92 \text{ pm}.$$

Bohr radius

39.8: The Bohr Model of the Hydrogen Atom, Orbital energy is quantized

$$E = K + U$$

$$= \frac{1}{2}mv^2 + \left(-\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \right).$$

→ $E = -\frac{1}{8\pi\epsilon_0} \frac{e^2}{r}.$

$$\left[\begin{array}{l} -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} = m \left(-\frac{v^2}{r} \right), \\ \longrightarrow \frac{1}{2}mv^2 = \frac{1}{8\pi\epsilon_0} \cdot \frac{e^2}{r} \end{array} \right.$$

$$r = \frac{h^2\epsilon_0}{\pi me^2} n^2, \quad \text{for } n = 1, 2, 3, \dots$$

→ $E_n = -\frac{me^4}{8\epsilon_0^2 h^2} \frac{1}{n^2}, \quad \text{for } n = 1, 2, 3, \dots,$

→ $E_n = -\frac{2.180 \times 10^{-18} \text{ J}}{n^2} = -\frac{13.61 \text{ eV}}{n^2}, \quad \text{for } n = 1, 2, 3, \dots$

$$1 \text{ J} = 6.242 \times 10^{18} \text{ eV}$$

39.8: The Bohr Model of the Hydrogen Atom, Energy Changes:

$$hf = \Delta E = E_{\text{high}} - E_{\text{low}}.$$



$$\frac{1}{\lambda} = -\frac{me^4}{8\varepsilon_0^2 h^3 c} \left(\frac{1}{n_{\text{high}}^2} - \frac{1}{n_{\text{low}}^2} \right).$$



$$\frac{1}{\lambda} = R \left(\frac{1}{n_{\text{low}}^2} - \frac{1}{n_{\text{high}}^2} \right),$$

$$R = \frac{me^4}{8\varepsilon_0^2 h^3 c} = 1.097\,373 \times 10^7 \text{ m}^{-1} \quad (\text{Rydberg Constant})$$

39.9: Schrodinger's Equation and The Hydrogen Atom

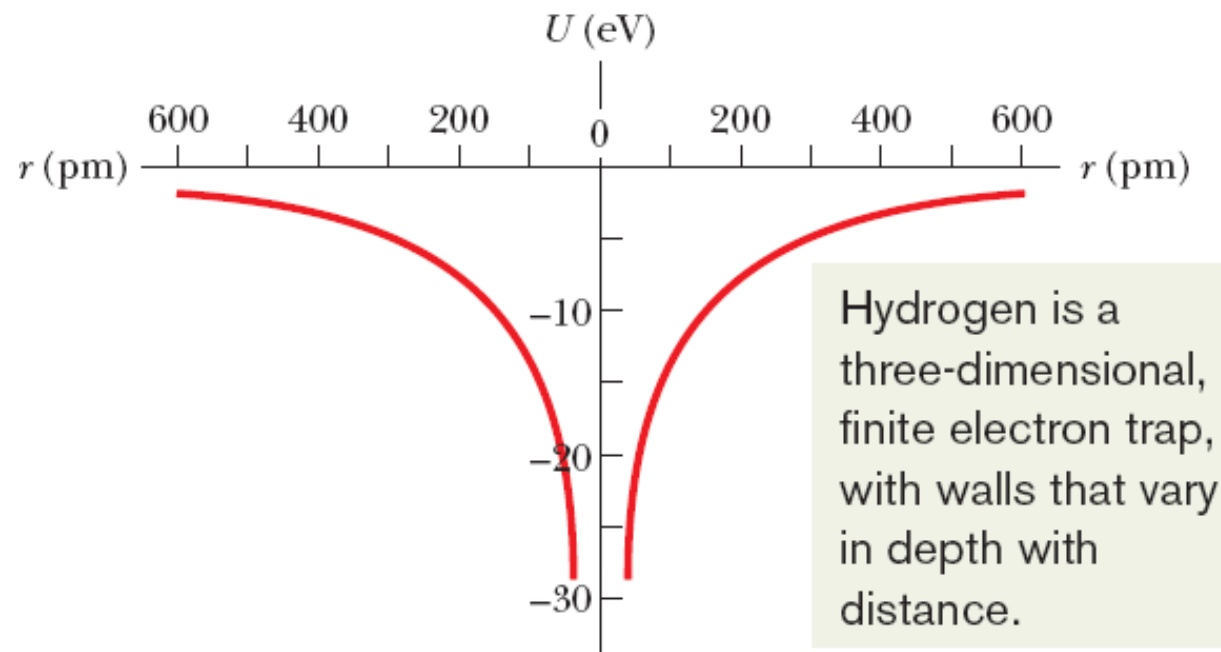


Fig. 39-17 The potential energy U of a hydrogen atom as a function of the separation r between the electron and the central proton. The plot is shown twice (on the left and on the right) to suggest the three-dimensional spherically symmetric trap in which the electron is confined.

39.9: Schrodinger's Equation and The Hydrogen Atom

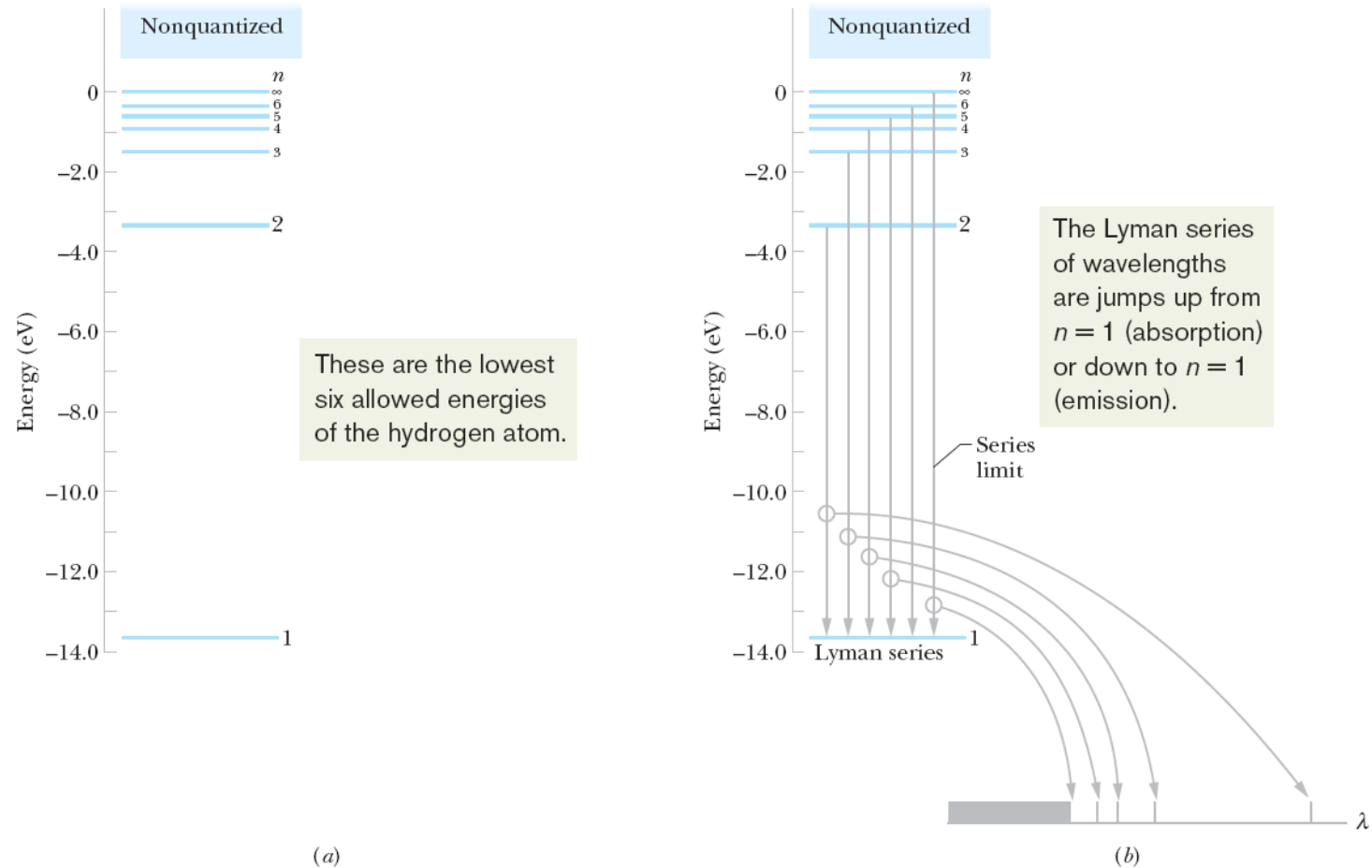
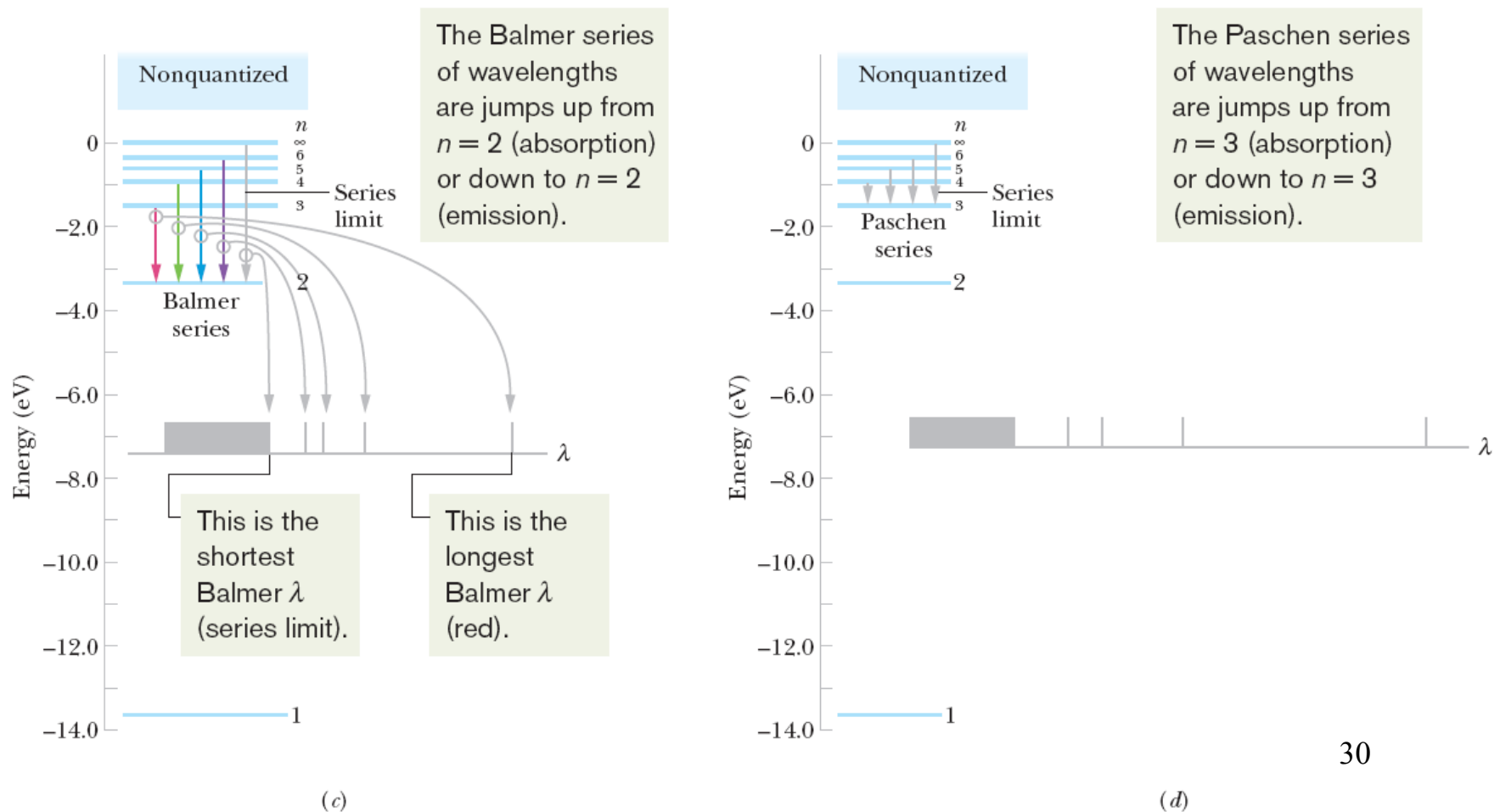


Fig. 39-18 (a) An energy-level diagram for the hydrogen atom. Some of the transitions for (b) the **Lyman series**. For each, the longest four wavelengths and the series-limit wavelength are plotted on a wavelength axis. Any wavelength shorter than the series-limit wavelength is allowed.

39.9: Schrodinger's Equation and The Hydrogen Atom

Fig. 39-18 Some of the transitions for (c) the **Balmer series**, and (d) the **Paschen series**. For each, the longest four wavelengths and the series-limit wavelength are plotted on a wavelength axis. Any wavelength shorter than the series-limit wavelength is allowed.



39.9: Schrodinger's Equation and The Hydrogen Atom

Each set of quantum numbers (n, l, m_l) identifies the wave function of a particular quantum state. The quantum number n , is called the **principal quantum number**. The **orbital quantum number** l is a measure of the magnitude of the angular momentum associated with the quantum state. The **orbital magnetic quantum number** m_l is related to the orientation in space of this angular momentum vector.

The restrictions on the values of the quantum numbers for the hydrogen atom, as listed in Table 39-2, are not arbitrary but come out of the solution to Schrödinger's equation.

Table 39-2

Quantum Numbers for the Hydrogen Atom

Symbol	Name	Allowed Values
n	Principal quantum number	$1, 2, 3, \dots$
ℓ	Orbital quantum number	$0, 1, 2, \dots, n - 1$
m_ℓ	Orbital magnetic quantum number	$-\ell, -(\ell - 1), \dots, +(\ell - 1), +\ell$

39.9: The Wave Functions of the Hydrogen Atom's Ground State

The wave function for the ground state of the hydrogen atom, obtained by solving the three-dimensional Schrödinger equation and normalizing is

$$\psi(r) = \frac{1}{\sqrt{\pi}a^{3/2}} e^{-r/a} \quad (\text{ground state}) \quad \text{where } a \text{ is the Bohr radius.}$$

The probability that an electron can be detected in any given (infinitesimal) volume element dV located at radius r , of width dr , from the center of the atom is

$$\psi^2(r) dV = \frac{4}{a^3} e^{-2r/a} r^2 dr. \quad \text{in which } 4\pi r^2 \text{ is the surface area of the inner shell}$$

and dr is the radial distance between the two shells.

The **radial probability density** $P(r)$ is a linear probability density such that

$$P(r) dr = \psi^2(r) dV.$$

This leads to:

$$P(r) = \frac{4}{a^3} r^2 e^{-2r/a} \quad (\text{radial probability density, hydrogen atom ground state}).$$

39.9: The Wave Functions of the Hydrogen Atom's Ground State

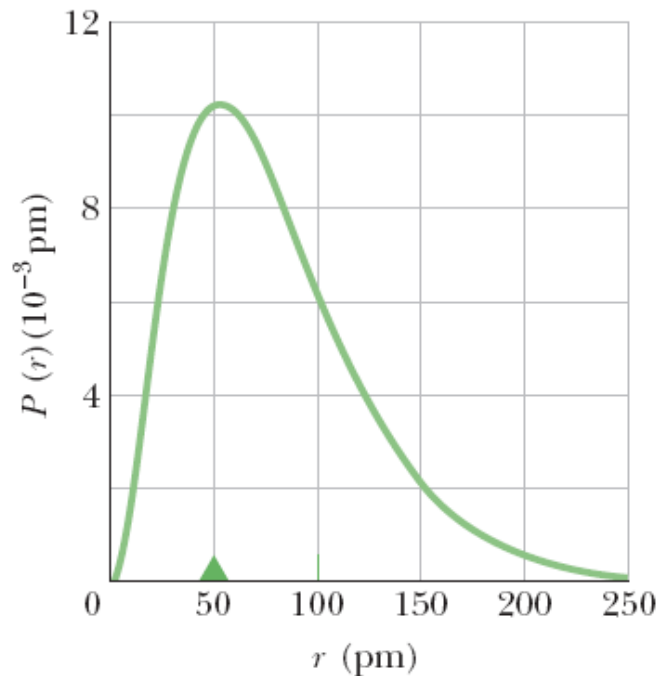


Fig. 39-19 A plot of the radial probability density $P(r)$ for the ground state of the hydrogen atom. The triangular marker is located at one Bohr radius from the origin, and the origin represents the center of the atom.

$$\int_0^{\infty} P(r) dr = 1.$$

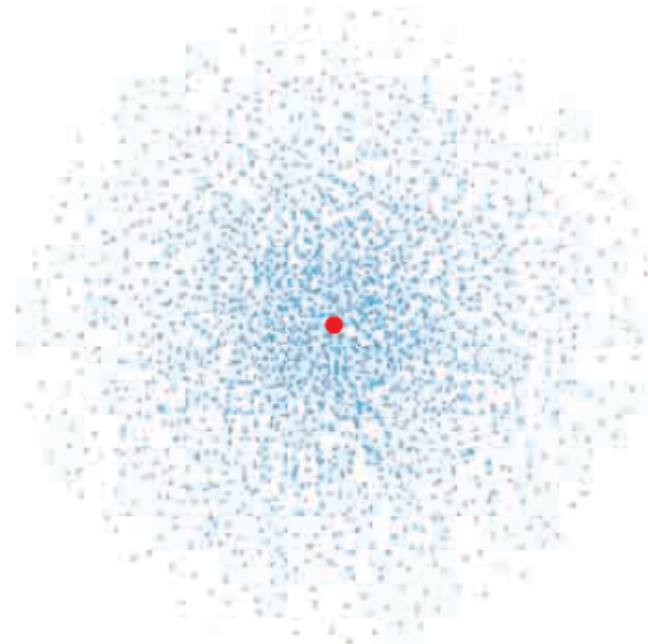


Fig. 39-20 A “dot plot” showing the volume probability density $\psi^2(r)$ —not the *radial* probability density $P(r)$ —for the ground state of the hydrogen atom. The density of dots drops exponentially with increasing distance from the nucleus, which is represented here by a red spot.

Example, Probability of detection of an electron in a hydrogen atom:

Show that the radial probability density for the ground state of the hydrogen atom has a maximum at $r = a$.

KEY IDEAS

(1) The radial probability density for a ground-state hydrogen atom is given by Eq. 39-44,

$$P(r) = \frac{4}{a^3} r^2 e^{-2r/a}.$$

(2) To find the maximum (or minimum) of any function, we must differentiate the function and set the result equal to zero.

If we set the right side equal to zero, we obtain an equation that is true if $r = a$, so that the term $(a - r)$ in the middle of the equation is zero. In other words, dP/dr is equal to zero

Calculation: If we differentiate $P(r)$ with respect to r , using derivative 7 of Appendix E and the chain rule for differentiating products, we get

$$\begin{aligned}\frac{dP}{dr} &= \frac{4}{a^3} r^2 \left(\frac{-2}{a} \right) e^{-2r/a} + \frac{4}{a^3} 2r e^{-2r/a} \\ &= \frac{8r}{a^3} e^{-2r/a} - \frac{8r^2}{a^4} e^{-2r/a} \\ &= \frac{8}{a^4} r(a - r) e^{-2r/a}.\end{aligned}$$

when $r = a$. (Note that we also have $dP/dr = 0$ at $r = 0$ and at $r = \infty$. However, these conditions correspond to a *minimum* in $P(r)$, as you can see in Fig. 39-19.)

Example, Light emission from a hydrogen atom:

(a) What is the wavelength of light for the least energetic photon emitted in the Lyman series of the hydrogen atom spectrum lines?

KEY IDEAS

- (1) For any series, the transition that produces the least energetic photon is the transition between the home-base level that defines the series and the level immediately above it.
(2) For the Lyman series, the home-base level is at $n = 1$ (Fig. 39-18*b*). Thus, the transition that produces the least energetic photon is the transition from the $n = 2$ level to the $n = 1$ level.

Calculations: From Eq. 39-33 the energy difference is

$$\Delta E = E_2 - E_1 = -(13.60 \text{ eV}) \left(\frac{1}{2^2} - \frac{1}{1^2} \right) = 10.20 \text{ eV}.$$

Then from Eq. 39-6 ($\Delta E = hf$), with c/λ replacing f , we have

$$\begin{aligned} \lambda &= \frac{hc}{\Delta E} = \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{s})(3.00 \times 10^8 \text{ m/s})}{(10.20 \text{ eV})(1.60 \times 10^{-19} \text{ J/eV})} \\ &= 1.22 \times 10^{-7} \text{ m} = 122 \text{ nm}. \end{aligned} \quad (\text{Answer})$$

Light with this wavelength is in the ultraviolet range.

(b) What is the wavelength of the series limit for the Lyman series?

KEY IDEA

The series limit corresponds to a jump between the home-base level ($n = 1$ for the Lyman series) and the level at the limit $n = \infty$.

Calculations: Now that we have identified the values of n for the transition, we could proceed as in (a) to find the corresponding wavelength λ . Instead, let's use a more direct procedure. From Eq. 39-36, we find

$$\begin{aligned} \frac{1}{\lambda} &= R \left(\frac{1}{n_{\text{low}}^2} - \frac{1}{n_{\text{high}}^2} \right) \\ &= 1.097\,373 \times 10^7 \text{ m}^{-1} \left(\frac{1}{1^2} - \frac{1}{\infty^2} \right), \end{aligned}$$

which yields

$$\lambda = 9.11 \times 10^{-8} \text{ m} = 91.1 \text{ nm}. \quad (\text{Answer})$$

Light with this wavelength is also in the ultraviolet range.

39.9: Hydrogen Atom States with $n = 2$

Table 39-3

Quantum Numbers for Hydrogen Atom States with $n = 2$

n	ℓ	m_ℓ
2	0	0
2	1	+1
2	1	0
2	1	-1

39.9: Hydrogen Atom States with $n = 2$

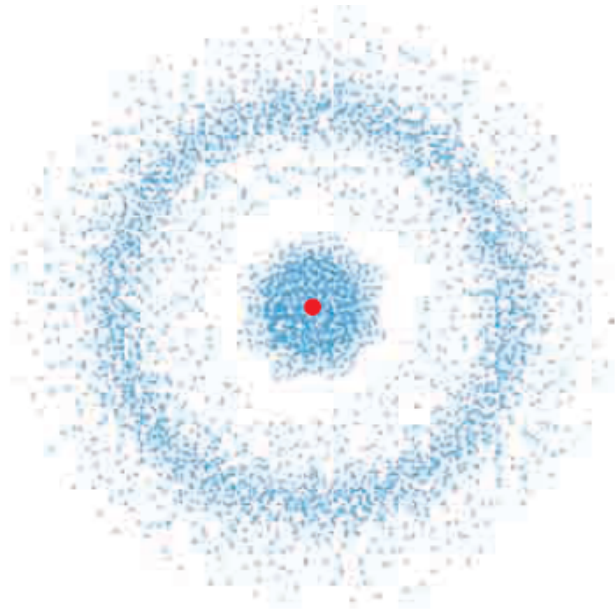


Fig. 39-21 A dot plot showing the volume probability density $\psi^2(r)$ for the hydrogen atom in the quantum state with $n = 2$, $\ell = 0$, and $m_\ell = 0$. The plot has spherical symmetry about the central nucleus. The gap in the dot density pattern marks a spherical surface over which $\psi^2(r) = 0$.

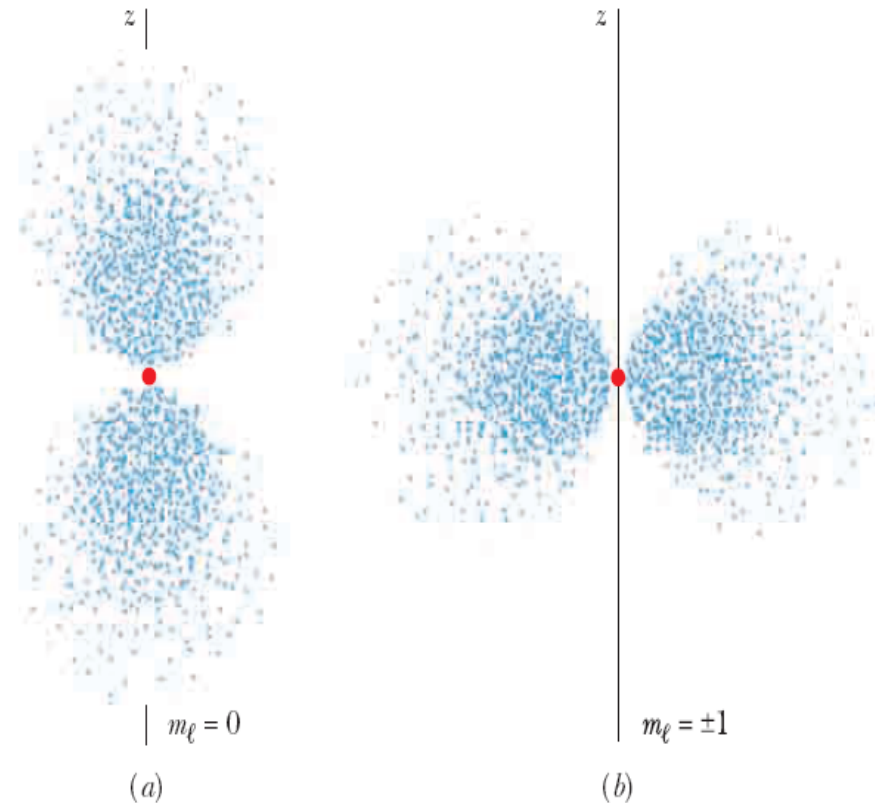


Fig. 39-23 Dot plots of the volume probability density $\psi^2(r, \theta)$ for the hydrogen atom in states with $n = 2$ and $\ell = 1$. (a) Plot for $m_\ell = 0$. (b) Plot for $m_\ell = +1$ and $m_\ell = -1$. Both plots show that the probability density is symmetric about the z axis.

39.9: Hydrogen Atom States with large n

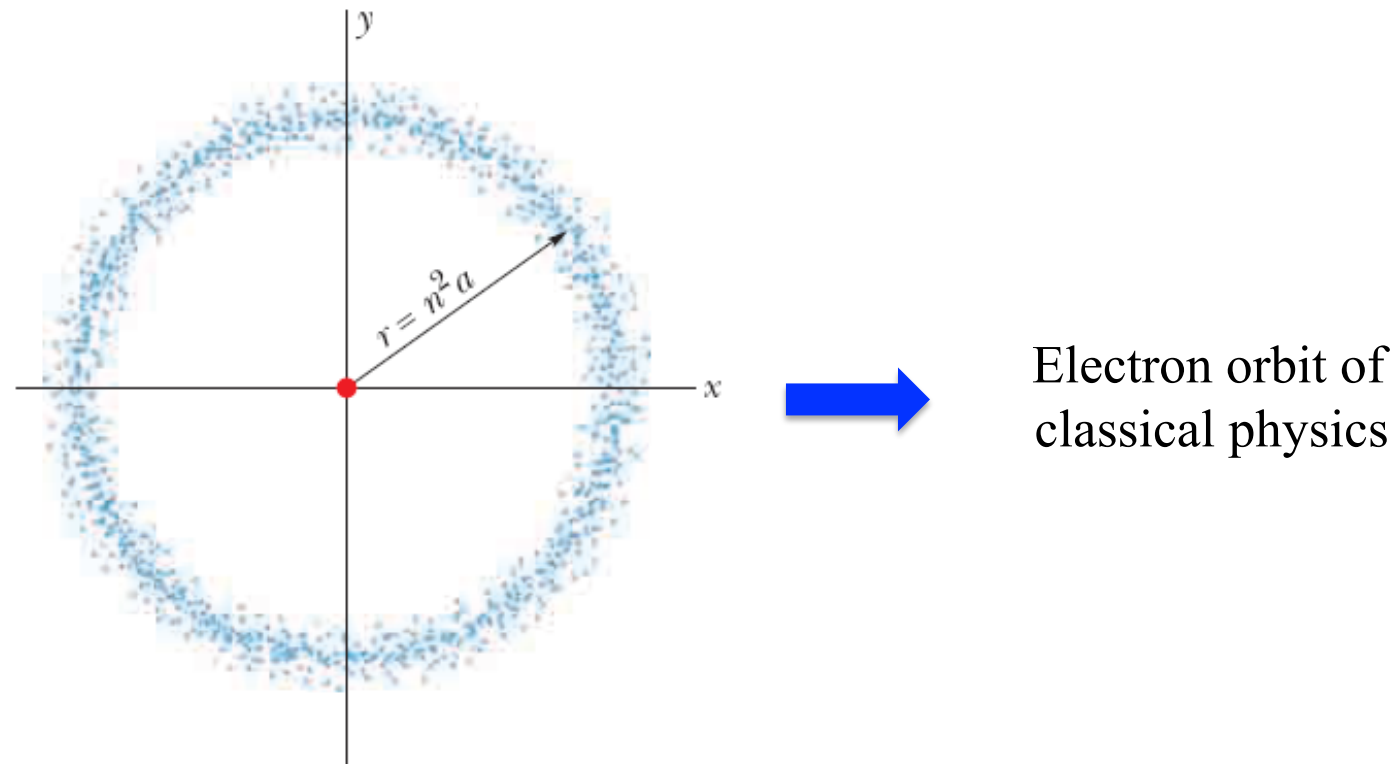


Fig. 39-24 A dot plot of the radial probability density $P(r)$ for the hydrogen atom in a quantum state with a relatively large principal quantum number — namely, $n = 45$ — and angular momentum quantum number $\ell = n - 1 = 44$. The dots lie close to the xy plane, the ring of dots suggesting a classical electron orbit.