Quantum States (Chs. 38, 39)

TODAY:

1. **Particle in a trap.**
2. **Potential Well.**
3. **Hydrogen Atom**

Review: Photons

Light interacts with matter by means of energetic particles called ***photons***. Each photon has energy $E = hf$, where f is the frequency of the light, and h is Planck's Constant. $\boldsymbol{h = 6.63 \times 10^{-34}\ Js}$

This means $\lambda = c/f = hc/E$ with $hc = 1243\ eV \cdot nm$

For example a photon with energy **3 eV** has $\lambda = 414\ nm$ **(violet)** while a photon with energy **2 eV** has $\lambda = 622\ nm$ **(red)**.

Review: Free Electrons

An electron wave determines the probability of detecting an electron.

A free electron traveling with momentum p has a simple wavefunction and wavelength:

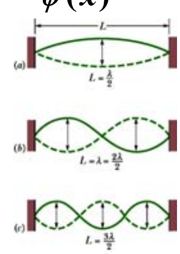
$$\psi = \psi_0 \sin(kx - \omega t) \quad with \quad \lambda = h/p$$

But what about an electron that is bound inside an atom or a solid? It is not moving in a straight line with a constant momentum. How do we determine its wavefunction and its energy?

Review: Bound Electrons

The deBroglie wave for a trapped electron is just like the standing waves on a string, and there are the same allowed wavelengths.

$\psi(x)$



This gives the allowed energies:
wavelength $\Rightarrow$ momentum
momentum $\Rightarrow$ energy

$$\lambda = \frac{2L}{n} \qquad p = \frac{h}{\lambda} = \frac{nh}{2L}$$

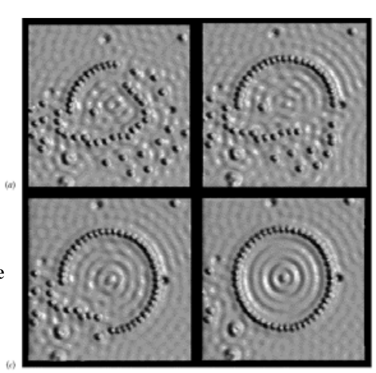
$$E = \frac{p^2}{2m} = \frac{n^2 h^2}{8mL^2} = n^2 E_0$$

Quantization!

Do such electron traps exist?

Textbook Chapter 39 Section 6 describes several kinds of "nanostructures" which can confine an electron to a nanometer sized region.

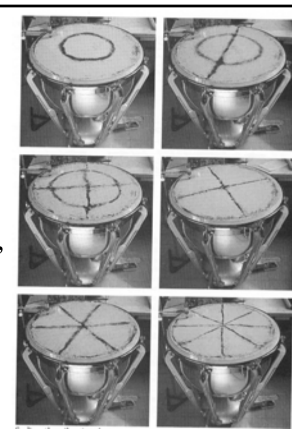
The "quantum corral" made by IBM arranges iron atoms on a copper surface. The ripples are the standing electron waves.



Oscillations in 2 and 3 dimensions

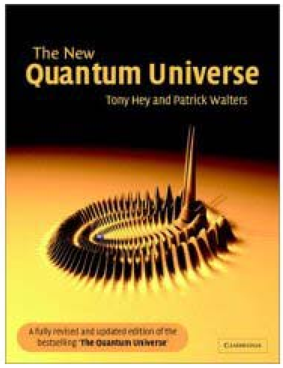
For this vibrating drum, need 2 "quantum numbers", one for the radial and one for the angular oscillations.

For trap in 3 dimensions, need 3 quantum numbers.



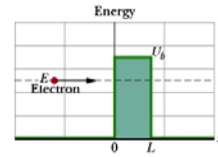
Hey and Walters

Very good paperback, $24.41 at Amazon.com

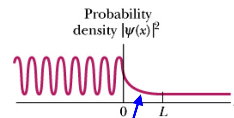


Barrier Penetration

An electron (or any other particle) can "tunnel" through a potential energy barrier that's too high for it to go over. (Chapter 38 Section 9)

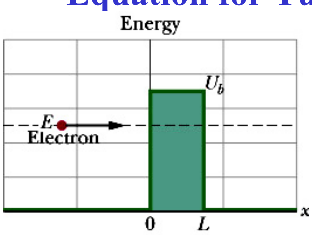


In the "classically forbidden" region, ψ is ***exponentially decreasing*** instead of oscillating.



$$\psi(x) = \psi_0 e^{-r/a}$$

Equation for Tunneling



For e in forbidden region ($0<x<L$) we have

$$\psi = \psi_0 e^{-bx}$$

This means probability of getting through is

T = transmission coefficient = ?

$$T = \frac{\psi(L)^2}{\psi(0)^2} = e^{-2bL}$$

Here $b = \sqrt{\frac{2m}{\hbar^2}[U_b - E]}$

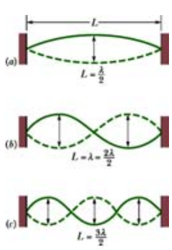
So this means a small change in U_b or L makes a big difference in the current.

Summary: Quantum States and Energy Levels

THREE EXAMPLES:

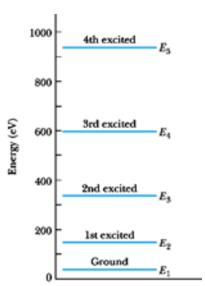
1. Particle in a trap.
2. Potential Well.
3. Hydrogen Atom

Quantum States 1. Particle in a trap.

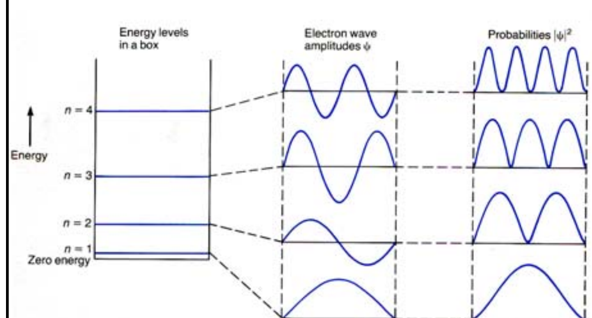


$$\lambda = \frac{2L}{n}$$

$$E = n^2 E_0$$



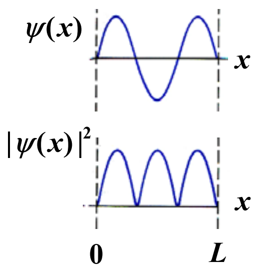
Energies, Wavefunctions, and Probabilities



Q.39-1

An electron moves along the x axis, bouncing back and forth between walls at $x=0$ and $x=L$. It is in its state of lowest energy (ground state) and its energy is 10 eV.

Now this electron is given some extra energy, so that it goes into an excited state. Its wavefunction and position probability distribution in the excited state are shown in the figure.



What is the electron's energy in this excited state?

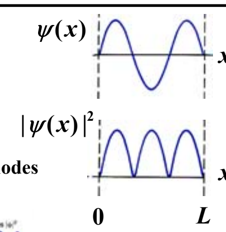
(1) 20 eV (2) 30 eV (3) 40 eV (4) 80 eV (5) 90 eV

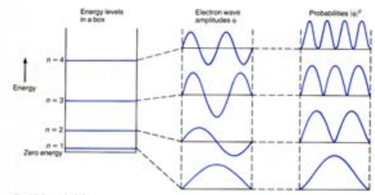
Q.39-1

The ground state energy is 10 eV.
What's the energy in this excited state?

$$E = n^2 E_0$$

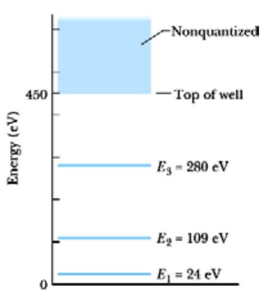
Quantum number n = number of antinodes = number of maxima in ψ^2 = 3.

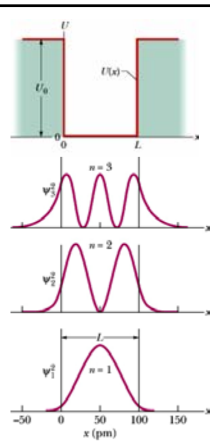




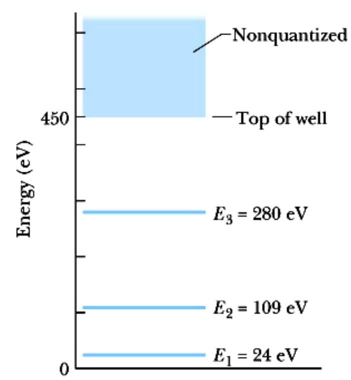
(1) 20 eV (2) 30 eV (3) 40 eV (4) 80 eV (5) 90 eV

Quantum States 2. Potential Well.





Bound and Unbound States



Any $E > U_0$ is allowed.

Note ground state has kinetic energy. "Zero point energy."

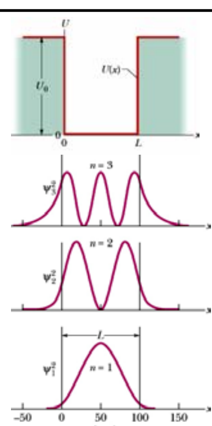
Potential Well

Ground state and first two excited states. Note penetration into classically forbidden region outside the well.

$$L = 100\ pm$$

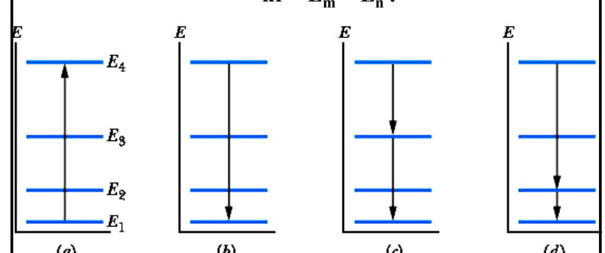
$$U_0 = 450\ eV$$

But what if $E > U_0$?



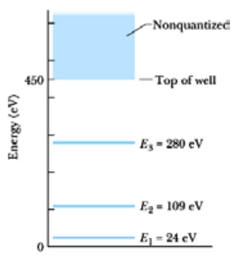
Quantum jumps

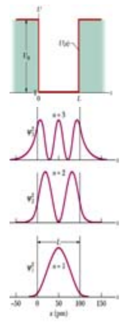
System can gain or lose only specific quanta of energy. For example, absorb or emit a photon of energy $hf = E_m - E_n$.



Example

If the electron in this potential well jumps from state E3 to state E2, what wavelength photon could be emitted?





$$hf = E_3 - E_2 = 280 - 109 = 171\ eV$$

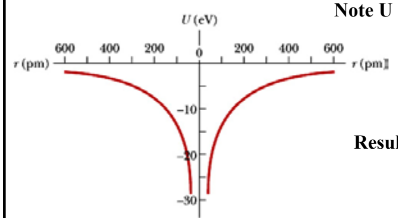
$$\lambda = \frac{hc}{hf} = \frac{1240\ eV \cdot nm}{171\ eV} = \underline{7.25\ nm}$$

(This is far UV, λ << 400 nm.)

Quantum States 3. <u>Hydrogen Atom.</u>

General idea: Electron trap in 3 dimensions. Allowed states are labeled with 3 quantum numbers, described by energy levels and wave functions. The trap is provided by the Coulomb potential.

Note U → 0 at large distance.

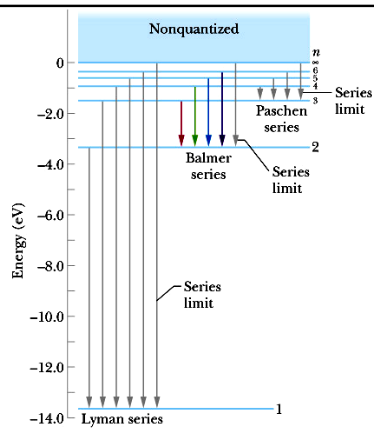


Results:

$$E = -E_0 / n^2$$
$$n = 1, 2, 3, \cdots$$
$$E_0 = 13.6\ eV$$

Energy levels of hydrogen

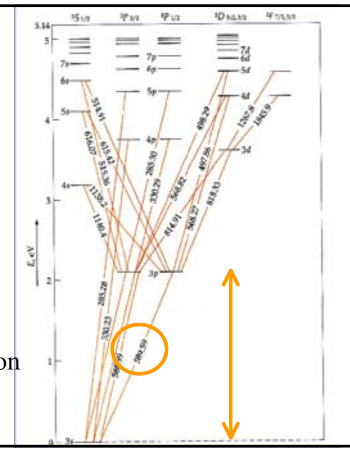
Arrows show some of the observed quantum jumps. These give rise to photon emission and absorption.



Energy Level Diagram for the Sodium Atom

Energies in eV.
Wavelengths in nm.

Note strong yellow line at 590 nm, photon energy 2.1 eV.



Q.39-2

In sodium atoms we find that a transition with energy about 2 eV gives yellow light of wavelength about 600 nm.

What kind of emission do we expect from an atomic transition of energy <u>6 eV</u>?

(1) An Xray of wavelength 0.6 nm.
(2) Ultraviolet radiation of wavelength 200 nm.
(3) Infrared radiation of wavelength 1200 nm.

Q.39-2

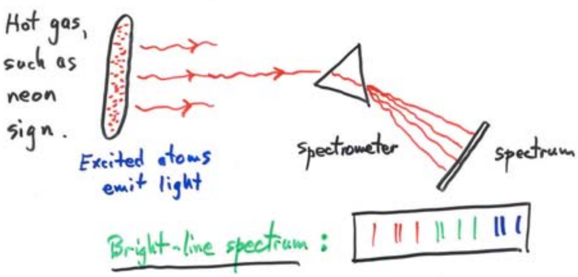
What kind of emission do we get from an atomic transition of energy 6 eV?

E = hf and f = c/λ

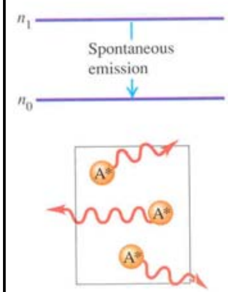
So λ ∝ 1/E so λ = 600/3 = 200 nm.

(1) An Xray of wavelength 0.6 nm.
(2) Ultraviolet radiation of wavelength 200 nm.
(3) Infrared radiation of wavelength 1200 nm.

Emission Lines



Emission Spectrum



An ***excited*** atom makes a ***downward*** quantum jump. Photon of energy E_γ is emitted, with

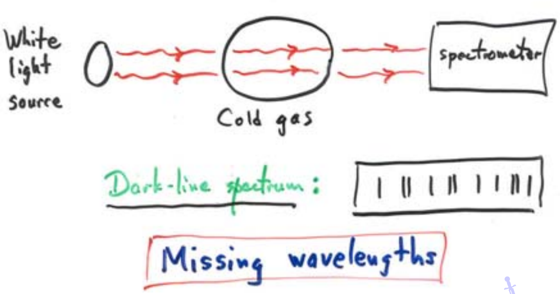
$$E_\gamma = hf = E_1 - E_0$$

So light of wavelength

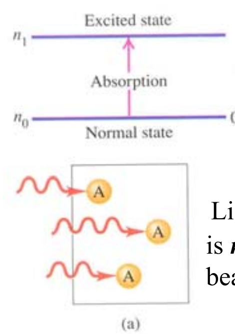
$$\lambda = hc / E_\gamma$$

is ***emitted*** by the hot gas, giving a ***bright*** spectrum line.

Absorption Lines



Absorption Spectrum



Photon of energy E_γ is ***absorbed***. Absorbing atom makes an ***upward*** quantum jump. Cannot happen unless energy is conserved:

$$E_\gamma = hf = E_1 - E_0$$

Light of wavelength $\lambda = hc / E_\gamma$ is ***removed*** from the incident beam, giving a ***dark*** spectrum line.

Hydrogen wave functions and quantum numbers

$n = 1,2,3,\cdots$ $\qquad E = -E_0 / n^2$

$l = 0,1,\cdots(n-1)$ $\qquad L = \sqrt{l(l+1)}\,\hbar$

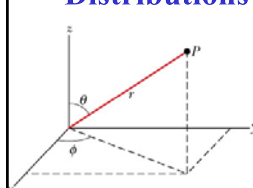
$m = -l,(-l+1),\cdots,l$ $\qquad L_z = m\hbar$

For example in the n=3 shell there are 3 subshells:

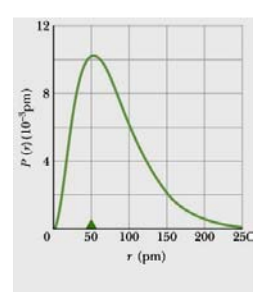
s → l=0
p → l=1
d → l=2
etc.

3s (1 function)
3p (3 functions)
3d (5 functions)

Distributions in polar coordinates



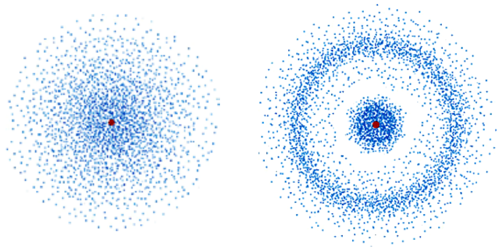
Ground state (n=1, l=0) radial probability distribution P(r):



$$\psi = \psi_0 R_{nl}(r) Y_{lm}(\theta,\phi)$$

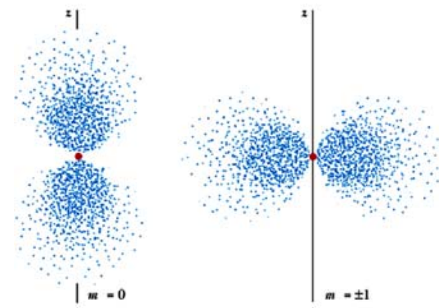
Dependence on angle is determined by l,m. If l=0, ψ is round.

Electron probability distributions in hydrogen



Probability distributions for hydrogen 1s and 2s.

Hydrogen probability distributions



Probability distributions for 2p (m=0, m=±1).