Whoaah! Take a look at the wear in those atomic orbitals! I'm surprised the electrons are still attached to this baby...! Those protons look distinctly loose as well...

Yeah... looks like we're gonna have to strip the atom right back to the nucleus, overhaul the wavefunction, and rebuild from scratch. Might even need a new set of gluons. How long d'ya reckon all that'd take, Bill?...

Wellll....if we order The parts today and have them couriered across, and work at it around the clock, we're looking at three, maybe four weeks, at a total entropy cost to the Universe of about...

Quantum mechanics.
Ångström measured the wavelengths on the four visible lines of the hydrogen spectrum, obtained with a diffraction grating, whose dispersion is linear, and replaced Kirchhoff's arbitrary scale by the wavelengths, expressed in the metric system, using a small unit ($10^{-10}$ m) with which his name was to be associated.

<table>
<thead>
<tr>
<th>Line color</th>
<th>Wavelength</th>
</tr>
</thead>
<tbody>
<tr>
<td>red</td>
<td>6562.852 Å</td>
</tr>
<tr>
<td>blue-green</td>
<td>4861.33 Å</td>
</tr>
<tr>
<td>violet</td>
<td>4340.47 Å</td>
</tr>
<tr>
<td>violet</td>
<td>4101.74 Å</td>
</tr>
</tbody>
</table>
Balmer Series: 1885

Johann Balmer found an empirical equation that correctly predicted the four visible emission lines of hydrogen

\[ \lambda = B \left( \frac{m^2}{m^2 - n^2} \right) = B \left( \frac{m^2}{m^2 - 2^2} \right) \]

Rydberg constant

\[ R_H = 1.097373 \times 10^7 \text{ m}^{-1} \]

\[ n \] is an integer, \( n = 3, 4, 5, \ldots \)

The spectral lines correspond to different values of \( n \)

\( H_\alpha \) is red, \( \lambda = 656.3 \text{ nm} \)
\( H_\beta \) is green, \( \lambda = 486.1 \text{ nm} \)
\( H_\gamma \) is blue, \( \lambda = 434.1 \text{ nm} \)
\( H_\delta \) is violet, \( \lambda = 410.2 \text{ nm} \)
Joseph John Thomson
“Plum Pudding” Model 1904

• Received Nobel Prize in 1906
• Usually considered the discoverer of the electron
• Worked with the deflection of cathode rays in an electric field
• His model of the atom
  – A volume of positive charge
  – Electrons embedded throughout the volume
1911: Rutherford’s Planetary Model of the Atom

• A beam of positively charged alpha particles hit and are scattered from a thin foil target.

• Large deflections could not be explained by Thomson’s pudding model.

(Couldn’t explain the stability or spectra of atoms.)
1911: Rutherford’s Planetary Model of the Atom

- A beam of positively charged alpha particles hit and are scattered from a thin foil target.

- Large deflections could not be explained by Thomson’s model.

(Couldn’t explain the stability or spectra of atoms.)
Classical Physics at the Limit

WHY IS MATTER (ATOMS) STABLE?

FIGURE 38.23 The fate of a Rutherford atom.

According to classical physics, an electron would spiral into the nucleus while radiating energy as an electromagnetic wave.
Electrons exist in quantized orbitals with energies given by multiples of Planck’s constant. Light is emitted or absorbed when an electron makes a transition between energy levels. The energy of the photon is equal to the difference in the energy levels:

\[ E = n hf, \quad n = 0,1,2,3,... \]

\[ h = 6.626 \times 10^{-34} \text{ Js} \]

\[ E_\gamma = E_i - E_f = hf \]
Light Absorption & Emission

\[ E_\gamma = E_i - E_f = hf \]

Electron gains potential energy and moves farther from nucleus. A photon of light is absorbed.

Electron loses potential energy and moves closer to nucleus. A photon of light is emitted.

Electron

High potential energy

Low potential energy

Nucleus

Nucleus

n = 2

n = 3

(a) Absorption

(b) Emission

Frequency A

Frequency B

Frequency C

n = 1

n = 2

n = 3

A + B = C
Bohr’s Model 1913

1. Electrons in an atom can occupy only certain discrete quantized states or orbits. 

\[ E = n hf, \quad n = 0,1,2,3,... \]

2. Electrons are in stationary states: they don’t accelerate and they don’t radiate.

3. Electrons radiate only when making a transition from one orbital to another, either emitting or absorbing a photon.

Postulate: 

\[ E_\gamma = E_i - E_f = hf \]

The angular momentum of an electron is always quantized and cannot be zero:

\[ L = n \frac{h}{2\pi} \quad (n = 1, 2, 3,....) \]
Bohr’s Derivation of the Energy for Hydrogen:

Conservation of E:

\[ E = K + U = \frac{1}{2}m_e v^2 - \frac{kq_e^2}{r} \]

F is centripetal:

\[ \frac{kq_e^2}{r^2} = \frac{m_e v^2}{r} \quad \rightarrow \quad \frac{kq_e^2}{r} = m_e v^2. \quad (1) \]

Sub back into E:

\[ E = \frac{1}{2}m_e v^2 - \frac{kq_e^2}{r} = -\frac{1}{2}m_e v^2 \quad (2) \]

From Angular Momentum:

\[ r = \frac{n\hbar}{m_e v}. \quad \left[ \text{From:} \quad L = n\frac{\hbar}{2\pi} = mvr \quad (n = 1, 2, 3, \ldots) \right] \]

Sub r back into (1):

\[ kq_e^2 \frac{m_e v}{n\hbar} = m_e v^2 \]

\[ v = \frac{2\pi kq_e^2}{nh} = \frac{2\pi q_e^2}{4\pi\varepsilon_0 hn} = \frac{q_e^2}{2\varepsilon_0 hn} \]

Sub into (2):

\[ E_n = \frac{-m_e q_e^4}{8h^2\varepsilon_0^2 n^2} \frac{1}{n^2} \quad \rightarrow \quad E_n = (-13.6 \text{ eV}) \frac{1}{n^2} \]

Why is it negative?
Bohr Line Spectra of Hydrogen

Bohr’s Theory derived the spectra equations that Balmer, Lyman and Paschen had previously found experimentally!

\[ E_n = (-13.6 \text{ eV}) \frac{1}{n^2} \]

\[ \frac{1}{\lambda} = RZ^2 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \]

\[ R = 1.097 \times 10^7 \text{ m}^{-1} \]

Balmer: Visible
Lyman: UV
Paschen: IR
Bohr Orbital Binding Energy for The Hydrogen Atom

\[ E_n = -13.6\text{eV} \frac{1}{n^2} \]

Ground State: \( n = 1 \)
First Excited: \( n = 2 \)
2\textsuperscript{nd} Excited: \( n = 3 \)

1. -13.6eV is the energy of the H ground state.
2. Negative because it is the Binding Energy and work must be done on the atom (by a photon) to ionize it.
3. A 13.6eV photon must be absorbed to ionize the ground state
4. Bohr model only works for single electron atoms since it doesn’t take into account electron-electron interaction forces.
Bohr: Allowed Orbital Radii

\[ r_n = \frac{n^2 \hbar^2}{m_e k_e e^2} \quad n = 1, 2, 3, \ldots \]

\[ r_n = (5.9 \times 10^{-11} \text{ m}) n^2 \]

\[ r_n = a_0 n^2 \quad n = 1, 2, 3 \]

Bohr Radius (ground state): \( a_0 = 5.9 \times 10^{-11} \text{ m} \)
• The frequency of the photon emitted when the electron makes a transition from an outer orbit to an inner orbit is
\[ f = \frac{E_i - E_f}{h} = \frac{k_e e^2}{2a_0 h} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \]

• It is convenient to look at the wavelength instead

• The wavelengths are found by
\[ \frac{1}{\lambda} = \frac{f}{c} = \frac{k_e e^2}{2a_0 h c} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) = R_H \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \]
Problem

A hydrogen atom is in the third (n = 4) excited state. It can make a jump to a different state by transition A, B, or C as shown, and a photon is either emitted or absorbed.

a) Which transition, A, B, or C, emits a photon with the greatest energy? Calculate the wavelength in m and the energy in eV.

b) What is the energy of a photon needed to ionize the atom when the electron is initially in the third excited state? Calculate in eV.

\[ \frac{1}{\lambda} = RZ^2 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) = (1.097 \times 10^7 \text{ m}^{-1}) \frac{1}{1^2} \left( \frac{1}{4^2} \right) \]

\[ = 10284375 \text{ m}^{-1} \]

\[ \lambda = 9.72 \times 10^{-8} \text{ m} \]

\[ E_3 = -13.6 eV \frac{Z^2}{3^2} = -13.6 eV \frac{1^2}{3^2} \]

\[ \gamma = 1.51 eV \]
Spontaneous Emission: Random Transition Probabilities

*Fermi’s Golden Rule*

Transition probabilities correspond to the intensity of light emission.
IMPORTANT NOTE!!

Free electrons have continuous energy states! Only bound electrons have quantized energy states! This is because they are not forced to fit in a confined space like a wave in a box!!!
Problems with the Bohr's Model

1. Bohr model does not explain angular momentum postulate.
2. Bohr model does not explain splitting of spectral lines.
4. Bohr model does not explain ionization energies of elements.

\[ E_0 = Z^2 13.6eV \]
Problems with the Bohr's Model

1. Bohr model does not explain angular momentum postulate:

The angular momentum of an electron is always quantized and cannot be zero*: 

\[ L = n \frac{\hbar}{2\pi} = n\hbar \]

\( (n = 1, 2, 3, \ldots) \)

*If \( L=0 \) then the electron travels linearly and does not ‘orbit’....

But if it is orbiting then it should radiate and the atom would be unstable...eek gads!

WHAT A MESS!
If photons can be particles, then why can’t electrons be waves?

\[ p = \frac{E}{c} = \frac{hf}{c} = \frac{h}{\lambda} \]

deBroglie Wavelength:

\[ \lambda_e = \frac{h}{p} \]

Electrons are **STANDING WAVES** in atomic orbitals.

\[ h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s} \]
1924: de Broglie Waves

Explains Bohr’s postulate of angular momentum quantization:

\[2\pi r_n = n\lambda\]

\[2\pi r_n = n \frac{h}{p} = n \frac{h}{m_e v}\]

\[m_e v r_n = n \frac{h}{2\pi}\]

\[L = m_e v r_n = n\hbar\]

\((n = 1, 2, 3, \ldots)\)
1926: Schrödinger’s Equation

Rewrite the SE in spherical coordinates. Solutions to it give the possible states of the electron.

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

\[-\frac{\hbar^2}{2\mu} \frac{1}{r^2 \sin \theta} \left[ \sin \theta \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2 \Psi}{\partial \phi^2} \right] \]

\[-U(r)\Psi(r,\theta,\phi) = E \Psi(r,\theta,\phi)\]

Solution is separable:

\[\Psi(r,\theta,\phi) = R(r)P(\theta)F(\phi)\]
Quantum Numbers and their quantization are derived purely from Mathematical Solutions of Schrodinger’s Equation (boundary conditions). However, they have a phenomenological basis!!

To be discussed later…

Solution:

\[ \Psi(r, \theta, \phi) = R(r)P(\theta)F(\phi) \]

- **R(r)**: Solution exists if and only if \( n = 1, 2, 3, \ldots \)
- **P(\theta)**: Solution exists if and only if \( \ell = 0, 1, 2, 3, \ldots, n-1 \)
- **F(\phi)**: Solution exists if and only if \( m_\ell = -\ell, -\ell + 1, \ldots, +\ell \)
Solutions to the Schrödinger equation for the hydrogen atom potential energy exist only if three conditions are satisfied:

1. The atom’s energy must be one of the values

\[
E_n = -\frac{1}{n^2} \left( \frac{1}{4\pi \varepsilon_0} \frac{e^2}{2a_B} \right) = -\frac{13.60 \text{ eV}}{n^2}, \quad n = 1, 2, 3, \ldots
\]

where \(a_B\) is the Bohr radius. The integer \(n\) is called the **principal quantum number**. These energies are the same as those in the Bohr hydrogen atom.
Stationary States of Hydrogen

2. The angular momentum $L$ of the electron’s orbit must be one of the values

$$L = \sqrt{l(l + 1)}\hbar \quad l = 0, 1, 2, 3, \ldots, n - 1$$

The integer $l$ is called the orbital quantum number.

3. The $z$-component of the angular momentum must be one of the values

$$L_z = m\hbar \quad m = -l, -l + 1, \ldots, 0, \ldots, l - 1, l$$

The integer $m$ is called the magnetic quantum number.

Each stationary state of the hydrogen atom is identified by a triplet of quantum numbers $(n, l, m)$.

**TABLE 42.1** Symbols used to represent quantum number $l$

<table>
<thead>
<tr>
<th>$l$</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$s$</td>
</tr>
<tr>
<td>1</td>
<td>$p$</td>
</tr>
<tr>
<td>2</td>
<td>$d$</td>
</tr>
<tr>
<td>3</td>
<td>$f$</td>
</tr>
</tbody>
</table>
Orbital Angular Momentum & its Z-component are Quantized

Angular momentum magnitude is quantized:

\[ L = \sqrt{l(l + 1)}\hbar \ (l = 0, 1, 2, \ldots n - 1) \]

Angular momentum direction is quantized:

\[ L_z = m_l \hbar \ (m_l = -l, \ldots -1, 0, 1, 2, \ldots l) \]

For each \( l \), there are \((2l+1)\) possible \( m_l \) states.

Note: for \( n = 1, \ l = 0 \). This means that the ground state angular momentum in hydrogen is zero, not \( \hbar/2\pi \), as Bohr assumed. What does it mean for \( L = 0 \) in this model??

Standing Wave

For each \( l \), there are \((2l+1)\) possible \( m_l \) states.
1896: Zeeman Effect

The Zeeman Effect is the splitting of spectral lines when a magnetic field is applied.
Lorentz Magnetic Force

A charged particle moving in an EXTERNAL magnetic field experiences a force that is perpendicular to both the velocity and field. Only the perpendicular components give rise to a force.

\[ \mathbf{F} = q \mathbf{v} \times \mathbf{B} \]

\[ F = q v B \sin \theta \]
Magnetic Dipole Moment

- The product $IA$ is defined as the **magnetic dipole moment**, $\mu$, of the loop
  - Often called the magnetic moment
- SI units: A $\cdot$ m$^2$
- Torque in terms of magnetic moment:
  \[
  \tau = \mu \times B
  \]
- Potential Energy of a magnetic moment in an external magnetic field:
  \[
  U = -\mu \cdot B
  \]
The Zeeman Effect is the splitting of spectral lines when a magnetic field is applied. This is due to the interaction between the external field and the B field produced by the orbital motion of the electron. Only certain angles are allowed between the orbital angular momentum and the external magnetic field resulting in the quantization of space!

\[ U = -\mu \cdot B \]

\[ L_z = m_l \hbar \quad (m_l = -l, -1, 0, 1, 2, \ldots l) \]
Particle in a Nonuniform Magnetic Field

• The motion is complex
• For example, the particles can oscillate back and forth between two positions
• This configuration is known as a *magnetic bottle*
Stern-Gerlach 1921

A beam of silver atoms sent through a non-uniform magnetic field was split into two discrete components. Classically, it should be spread out because the magnetic moment of the atom can have any orientation. QM says if it is due to orbital angular momentum, there should be an odd number of components, \((2l+1)\), but only two components are ever seen. This required an overhaul of QM to include Special Relativity. Then the electron magnetic ‘spin’ falls out naturally from the mathematics. The spin magnetic moment of the electron with two spin magnetic quantum number values:

\[
m_s = \pm \frac{1}{2}
\]
Intrinsic Spin is Quantized

Fine Line Splitting: B field due to intrinsic spin interacts with B field due to orbital motion and produces additional energy states.

Spin magnitude is quantized and fixed:

\[ S = \sqrt{s(s+1)} \frac{h}{2\pi} = \frac{\sqrt{3}}{2} \frac{h}{2\pi} \]

Spin direction is quantized:

\[ S_z = m_s \frac{h}{2\pi} \quad (m_s = +\frac{1}{2}, -\frac{1}{2}) \]

\[ \mu_{\text{spin}} = -\frac{e}{m} S \]
Quantum Numbers

Once the principal quantum number is known, the values of the other quantum numbers can be found. The possible states of a system are given by combinations of quantum numbers!

Quantum Rules

\[ n = 1, 2, 3, 4, \ldots \]
\[ l = 0, 1, 2, \ldots n - 1 \]
\[ m_l = -l, -l + 1, \ldots, 0, 1, \ldots l - 1, l \]
\[ m_s = -1/2, +1/2 \]

<table>
<thead>
<tr>
<th>( l )</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( s )</td>
</tr>
<tr>
<td>1</td>
<td>( p )</td>
</tr>
<tr>
<td>2</td>
<td>( d )</td>
</tr>
<tr>
<td>3</td>
<td>( f )</td>
</tr>
</tbody>
</table>

\[ \Psi(r, \theta, \phi) = R(r)P(\theta)F(\phi) \]

\( n \) : principal quantum number
\( \ell \) : orbital quantum number
\( m_\ell \) : magnetic quantum number

\( n = 2, \ell = 1, m_\ell = \pm 1 \)
\( (2, 1, \pm 1) \)
Shells and Subshells

Shells are determined by the principle quantum number, \( n \). Subshells are named after the type of line they produce in the emission spectrum and are determined by the \( l \) quantum number.

- **s**: Sharp line \((l = 0)\)
- **p**: Very bright principle line \((l = 1)\)
- **d**: Diffuse line \((l = 2)\)
- **f**: Fundamental (hydrogen like) \((l = 3)\)

<table>
<thead>
<tr>
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<tr>
<td>0</td>
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<td>( d )</td>
</tr>
<tr>
<td>3</td>
<td>( f )</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
1s & : n = 1, \ell = m_\ell = 0 \\
2s & : n = 2, \ell = 0, m_\ell = 0 \\
2p & : n = 2, \ell = 1, m_\ell = \pm 1
\end{align*}
\]
Wave Functions given by Quantum Numbers!!

The probability of finding an electron within a shell of radius \( r \) and thickness \( \delta r \) around a proton is

\[
\text{Prob(in } \delta r \text{ at } r) = |R_{nl}(r)|^2 \delta V = 4\pi r^2 |R_{nl}(r)|^2 \delta r = P_r(r) \delta r
\]

\[
P_r(r) = 4\pi r^2 |R_{nl}(r)|^2
\]

where the first three radial wave functions of the electron in a neutral hydrogen atom are

\[
R_{1s}(r) = \frac{1}{\sqrt{\pi a_B^3}} e^{-r/a_B}
\]

\[
R_{2s}(r) = \frac{1}{\sqrt{8\pi a_B^3}} \left(1 - \frac{r}{2a_B}\right) e^{-r/2a_B}
\]

\[
R_{2p}(r) = \frac{1}{\sqrt{24\pi a_B^3}} \left(\frac{r}{2a_B}\right) e^{-r/2a_B}
\]
Wave Functions for Hydrogen

• The simplest wave function for hydrogen is the one that describes the 1s (ground) state and is designated $\psi_{1s}(r)$

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_o^3}} e^{-r/a_o}$$

• As $\psi_{1s}(r)$ approaches zero, $r$ approaches $\infty$ and is normalized as presented

• $\psi_{1s}(r)$ is also *spherically symmetric*
  – This symmetry exists for all $s$ states
Radial Probability Density

The radial probability density function $P(r)$ is the probability per unit radial length of finding the electron in a spherical shell of radius $r$ and thickness $dr$

- A spherical shell of radius $r$ and thickness $dr$ has a volume of $4\pi r^2 \, dr$
- The radial probability density function is
  $$P(r) = 4\pi r^2 \, |\psi|^2$$

where
  $$|\psi_{1s}|^2 = \left(\frac{1}{\pi a_o^3}\right) e^{-2r/a_o} \quad \rightarrow \quad P_{1s}(r) = \left(\frac{4r^2}{a_o^3}\right) e^{-2r/a_o}$$

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_o^3}} e^{-r/a_o}$$
$P(r)$ for $1s$ State of Hydrogen

- The radial probability density function for the hydrogen atom in its ground state is

$$P_{1s}(r) = \left( \frac{4r^2}{a_o^3} \right) e^{-2r/a_o}$$

- The peak indicates the most probable location, the Bohr radius.
- The average value of $r$ for the ground state of hydrogen is $3/2 \ a_o$
- The graph shows asymmetry, with much more area to the right of the peak
Electron Clouds

• The charge of the electron is extended throughout a diffuse region of space, commonly called an *electron cloud*.

• This shows the probability density as a function of position in the $xy$ plane.

• The darkest area, $r = a_0$, corresponds to the most probable region.
FIGURE 42.5 The probability densities of the electron in the 1s, 2s, and 2p states of hydrogen.

An electron in the 1s state is most likely to be found at the origin. An electron in a 2s state is likely to be found either at the origin or in a surrounding shell. The p electrons are more likely to be found in some directions than in others.

1s
m = 0

2s
m = 0

2p
m = 0

2p
m = ±1
Hydrogen 1s Radial Probability
Sample Problem

19. The ground-state wave function for the electron in a hydrogen atom is

\[ \psi(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \]

where \( r \) is the radial coordinate of the electron and \( a_0 \) is the Bohr radius. (a) Show that the wave function as given is normalized. (b) Find the probability of locating the electron between \( r_1 = a_0/2 \) and \( r_2 = 3a_0/2 \).
Quantum H Atom

• 1s Wave Function: \[ \psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \]

• Radial Probability Density: \[ P(r) = 4\pi r^2 |\psi|^2 \]

• Most Probable value: \[ \text{solve} \quad \frac{dP}{dr} = 0 \]

• Average value: \[ r_{ave} = \langle r \rangle = \int_0^\infty rP(r)dr \]

• Probability in (0-r): \[ P = \int_0^r P(r)dr \]
Sample Problem

(a) \[ \int |\psi|^2 \, dV = 4\pi \int_0^\infty |\psi|^2 \, r^2 \, dr = 4\pi \left(\frac{1}{\pi \, a_0^3}\right) \int_0^\infty r^2 \, e^{-2r/a_0} \, dr \]

Using integral tables,

\[ \int |\psi|^2 \, dV = -\frac{2}{a_0^2} \left[ e^{-2r/a_0} \left( r^2 + a_0 \, r + \frac{a_0^2}{2} \right) \right]_0^\infty = \left( -\frac{2}{a_0^2} \right) \left( -\frac{a_0^2}{2} \right) = 1 \]

so the wave function as given is normalized.

(b) \[ P_{a_0/2 \to 3a_0/2} = 4\pi \int_{a_0/2}^{3a_0/2} |\psi|^2 \, r^2 \, dr = 4\pi \left(\frac{1}{\pi \, a_0^3}\right) \int_{a_0/2}^{3a_0/2} r^2 \, e^{-2r/a_0} \, dr \]

Again, using integral tables,

\[ P_{a_0/2 \to 3a_0/2} = -\frac{2}{a_0^2} \left[ e^{-2r/a_0} \left( r^2 + a_0 \, r + \frac{a_0^2}{2} \right) \right]_{a_0/2}^{3a_0/2} = -\frac{2}{a_0^2} \left[ e^{-3} \left( \frac{17a_0^2}{4} \right) - e^{-1} \left( \frac{5a_0^2}{4} \right) \right] = 0.497 \]
Wave Function of the $2s$ state

• The next-simplest wave function for the hydrogen atom is for the $2s$ state
  \[ n = 2; \ell = 0 \]

• The wave function is

\[
\psi_{2s}(r) = \frac{1}{4\sqrt{2\pi}} \left( \frac{1}{a_o} \right)^{3/2} \left( 2 - \frac{r}{a_o} \right) e^{-r/2a_o}
\]

\[ \psi_{2s} \] depends only on $r$ and is spherically symmetric
Hydrogen 2s Radial Probability

Quantum numbers:
- $n = 2$
- $\ell = 0$
- $m_\ell = 0$
- $m_s = \pm \frac{1}{2}$

Maximum 2 Electrons

Radial probability $4\pi r^2 R^2_{n\ell}$. The graph shows the radial probability distribution for the 2s state of hydrogen, with peaks at 5a₀, 10a₀, 15a₀, and 20a₀ respectively.
Comparison of 1s and 2s States

- The plot of the radial probability density for the 2s state has two peaks.
- The highest value of $P$ corresponds to the most probable value.
  - In this case, $r \approx 5a_0$. 

![Graph showing the radial probability density for 1s and 2s states.](image)
Hydrogen 1s Radial Probability
Hydrogen 2s Radial Probability

Quantum numbers:
- $n = 2$
- $\ell = 0$
- $m_\ell = 0$
- $m_s = \pm \frac{1}{2}$

Maximum 2 Electrons
Hydrogen 2p Radial Probability

Quantum numbers:

- $n = 2$
- $\ell = 1$
- $m_\ell = -1, 0, 1$
- $m_s = \pm \frac{1}{2}$

Maximum 6 Electrons

$m_\ell = \pm 1$
$m_\ell = 0$
Hydrogen 3s Radial Probability
Hydrogen 3p Radial Probability
Hydrogen 3d Radial Probability

Quantum numbers:

- $n = 3$
- $\ell = 2$
- $m_\ell = \pm 2, \pm 1, 0$
- $m_s = \pm \frac{1}{2}$

Maximum 10 Electrons

$m_\ell = \pm 2$
$m_\ell = \pm 1$
$m_\ell = 0$
Multielectron Atoms

• For multielectron atoms, the positive nuclear charge $Ze$ is largely shielded by the negative charge of the inner shell electrons
  – The outer electrons interact with a net charge that is smaller than the nuclear charge

• Allowed energies are

$$E_n = -\frac{13.6 \ Z_{\text{eff}}^2}{n^2} \ \text{eV}$$

  – $Z_{\text{eff}}$ depends on $n$ and $\ell$
Pauli Exclusion Principle

No two electrons can have the same set of quantum numbers. That is, no two electrons can be in the same quantum state.

From the exclusion principle, it can be seen that only two electrons can be present in any orbital: One electron will have spin up and one spin down.

Maximum number of electrons in a shell is: $# = 2n^2$
Maximum number of electrons in a subshell is: $# = 2(2l+1)$

You must obey Pauli to figure out how to fill orbitals, shells and subshells.
(This is not true of photons or other force carrying particles such as gravitons or gluons (bosons))
How many electrons in n=3 Shell?

Quantum Rules

\[ n = 1, 2, 3, 4, \ldots \]
\[ l = 0, 1, 2, \ldots, n - 1 \]
\[ m_l = -l, -l + 1, \ldots, 0, 1, \ldots, l - 1, l \]
\[ m_s = -1/2, +1/2 \]

\[ n = 3 \]
\[ l = 0, 1, 2 \]
\[ m_l = -2, -1, 0, 1, 2 \]
\[ m_s = -1/2, +1/2 \]

\[ 2(2l + 1) = 2e \quad 6e \quad 10e \quad = 18e = 2n^2 \]
Hund’s Rule

• Hund’s Rule states that when an atom has orbitals of equal energy, the order in which they are filled by electrons is such that a maximum number of electrons have unpaired spins
  – Some exceptions to the rule occur in elements having subshells that are close to being filled or half-filled
The filling of electronic states must obey both the Pauli Exclusion Principle and Hund’s Rule.
**FIGURE 42.23** Summary of the order in which subshells are filled in the periodic table.

<table>
<thead>
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<th>1s</th>
<th>2s</th>
<th>3s</th>
<th>4s</th>
<th>3d</th>
<th>4d</th>
<th>5s</th>
<th>4p</th>
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<th>6p</th>
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<td></td>
</tr>
</tbody>
</table>

* 6s
† 7s

* 4f
† 5f
FIGURE 42.20 The modern periodic table of the elements, showing the atomic number $Z$ of each.
Ionization Energy

The ionization energy or ionization potential is the energy necessary to remove an electron from the neutral atom. It is a minimum for the alkali metals which have a single electron outside a closed shell. It generally increases across a row on the periodic maximum for the noble gases which have closed shells.
QM for Molecules (Chapter 43)
Multi-Atoms: Change Potential Energy Function in SE Equation

• The potential energy for a system of two atoms can be expressed in the form

$$U(r) = -\frac{A}{r^n} + \frac{B}{r^m}$$

– $r$ is the internuclear separation distance
– $m$ and $n$ are small integers
– $A$ is associated with the attractive force
– $B$ is associated with the repulsive force
Wave Function – Two Atoms Far Apart

• Each atom has a wave function
  \[ \psi_{1s}(r) = \frac{1}{\sqrt{\pi a_o^3}} e^{-r/a_o} \]

• There is little overlap between the wave functions of the two atoms when they are far away from each other
Wave Function – Molecule

- The two atoms are brought close together
- The wave functions overlap and form the compound wave shown
- The probability amplitude is larger between the atoms than on either side
Excited States and Spectra

An atom can jump from one stationary state, of energy $E_1$, to a higher-energy state $E_2$ by absorbing a photon of frequency

$$f = \frac{\Delta E_{\text{atom}}}{h} = \frac{E_2 - E_1}{h}$$

In terms of the wavelength:

$$\lambda = \frac{c}{f} = \frac{hc}{\Delta E_{\text{atom}}} = \frac{1240 \text{ eV nm}}{\Delta E (\text{in eV})}$$

Note that a transition from a state in which the valence electron has orbital quantum number $l_1$ to another with orbital quantum number $l_2$ is allowed only if

$$\Delta l = |l_2 - l_1| = 1$$

(selection rule for emission and absorption)
Spontaneous Emission: Random Transition Probabilities

*Fermi’s Golden Rule*

Transition probabilities correspond to the intensity of light emission.
Hydrogen Energy Level Diagram

Selection Rules

- The selection rules for allowed transitions are
  - $\Delta \ell = \pm 1$
  - $\Delta m_\ell = 0, \pm 1$

- Transitions in which $\ell$ does not change are very unlikely to occur and are called *forbidden transitions*
  - Such transitions actually can occur, but their probability is very low compared to allowed transitions
Continuous

Visible light

Infrared  Red  Orange  Yellow  Green  Blue  Violet  Ultraviolet

800  700  600  500  400  300  λ (nm)

Discrete

Emission Ionization

Lyman series  Balmer series  Paschen series

0 eV  10.19 eV  12.07 eV  12.73 eV  13.6 eV

Absorption
Lifetimes of Excited States

Consider an experiment in which $N_0$ excited atoms are created at time $t = 0$. The number of excited atoms remaining at time $t$ is described by the exponential function

$$N_{\text{exc}} = N_0 e^{-t/\tau}$$

where

$$\tau = \frac{1}{r} = \text{the lifetime of the excited state}$$
EXAMPLE 42.8 The lifetime of an excited state in mercury

QUESTIONS:

The mercury atom has two valence electrons. One is always in the 6s state, the other is in a state with quantum numbers \( n \) and \( l \). One of the excited states in mercury is the state designated 6s6p. The decay rate of this state is \( 7.7 \times 10^8 \) s\(^{-1}\).

a. What is the lifetime of this state?

b. If \( 1.0 \times 10^{10} \) mercury atoms are created in the 6s6p state at \( t = 0 \), how many photons will be emitted during the first 1.0 ns?
EXAMPLE 42.8 The lifetime of an excited state in mercury

SOLVE

a. The lifetime is

\[ \tau = \frac{1}{r} = \frac{1}{7.7 \times 10^8 \text{ s}^{-1}} = 1.3 \times 10^{-9} \text{ s} = 1.3 \text{ ns} \]

b. If there are \( N_0 = 10^{10} \) excited atoms at \( t = 0 \), the number still remaining at \( t = 1.0 \text{ ns} \) is

\[ N_{\text{exc}} = N_0 e^{-t/\tau} = (1.0 \times 10^{10}) e^{- (1.0 \text{ ns})/(1.3 \text{ ns})} = 4.63 \times 10^9 \]

This result implies that \( 5.37 \times 10^9 \) atoms undergo quantum jumps during the first 1.0 ns. Each of these atoms emits one photon, so the number of photons emitted during the first 1.0 ns is \( 5.37 \times 10^9 \).
Lasers

Light Amplification by Stimulated Emission of Radiation

"A splendid light has dawned on me about the absorption and emission of radiation..."

Albert Einstein, 1916
"When you come right down to it, there is really no such thing as truly spontaneous emission; its all stimulated emission. The only distinction to be made is whether the field that does the stimulating is one that you put there or one that God put there..."

David Griffiths, *Introduction to Quantum Mechanics*
FIGURE 42.34 Stimulated emission creates a chain reaction of photon production in a population of excited atoms.
Stimulated Emission

- Transition from ground state to first metastable state
- From first metastable to second state
- From second to third state
- Spontaneous emission
- Stimulated emission

Totally silvered mirror
Partially silvered mirror
Sample Problem

What average wavelength of visible light can pump neodymium into levels above its metastable state?

From the figure it takes 2.1 eV to pump neodymium into levels above its metastable state. Thus,

\[
\lambda = \frac{hc}{E} = \frac{1.24 \times 10^{-6} \text{ eV} \cdot \text{m}}{2.10 \text{ eV}} = 5.90 \times 10^{-7} \text{ m} = 590 \text{ nm}
\]
Laser Applications
Phaser?
Fluorescence

UV in, vibrant color out.
BTW: Iridescence: Diffraction

[Images of iridescent patterns and butterflies]
We know that the electron in an atom is allowed to exist ONLY in the discrete energy states. So where is it when it transitions between $n=5$ and $n=1$?

It is in a superposition of all the possible states! It exists in “Potentia” not in Reality!
NOTE: A Quantum Jump
Is not necessarily a LARGE Jump!
It can be quite a small jump.
The weirdness of the Quantum Jump is that it goes from one place (state) to another without traveling in between!!!
Super Simplified Quantum Theory:

The wave function is a superposition of all possible positions. Each position is “weighted” based on how likely it is for the electron to be there. This weighting factor is called a “probability amplitude” and is given by $a_n$.

$$\Psi(x) = a_1 x_1 + a_2 x_2 + a_3 x_3 + \cdots$$

Before a measurement is made, the electron is in a superposition of all positions! The total probability for all positions equals 1 which is 100% probability.

Total Probability $= \Psi^2(x) = 1$

When a measurement is made the wave function “collapses” into a single position.

Warning! This is a GROSS mathematical oversimplification BUT it is the basic idea of the ‘mechanics’ of quantum.
Super Simplified Quantum Theory: Spectra

The intensity of each spectral line of hydrogen is related to the rate and/or probability of that transition to occur. Again, each transition is ‘weighted’ and given a probability amplitude. The Red transition happens most often and is thus weighted more and so on. For example:

\[ a_{\text{red}} = .591, \quad a_{\text{cyan}} = .566, \quad a_{\text{violet}_1} = .48, \quad a_{\text{violet}_2} = .316 \]

The wave function is in a superposition or sum of all these possibilities:

\[ \Psi = .591 \text{red} + .566 \text{cyan} + .48 \text{violet}_1 + .316 \text{violet}_2 \]

The total probability of some transition happening is given the square of the entire wave function added up over all the possible transitions. This sum equals 1 which is 100% probability.

\[ \Psi^2 = .35 + .32 + .23 + .1 = 1 \]

Warning! This is a GROSS mathematical oversimplification BUT is the basic idea of the ‘mechanics’ of quantum.
The Quantum Jump: Where is the electron when it jumps between allowed states?

It is in a superposition of all the possible states!
It exists in “Potentia” not in Reality!

\[ \Psi = 0.591 \text{red} + 0.566 \text{cyan} + 0.48 \text{violet 1} + 0.316 \text{violet 2} \]

Only when a measurement is made (red light is detected) does the electron exist in a defined state. We say that the wave function “Collapsed” from a superposition of states to a definite state.
Wave Function Collapse

The system stays in a superposition of states until it is observed. This is the “Collapse” of the wave function.
The observation causes the wave function to collapse. The wave function represents our knowledge about the phenomena we are studying, not the phenomena itself.
Schrödinger's Cat Paradox

*Is the cat dead or alive?*

The cat is in a superposition of dead and live states until we open the box and make a measurement (observation), collapsing the wave function!

$\Psi_{total} = \Psi_{Dead} + \Psi_{Alive}$

This paradox shows the limits of quantum superposition applied to macroscopic systems. Or does it?
Many Worlds Hypothesis

Hugh Everett

under the many-worlds hypothesis, each quantum event splits the Universe into $U_1$ and $U_2$.

No collapse is necessary!

and each Universe follows its own path into the future.

all the possible Universe's exist, but none can communicate with another.
Many Worlds Leads to Parallel Universes and a *Multiverse*

"You’re in the right place and this is the right time, but I’m afraid you’re in the wrong alternate universe."
The hidden variables hypothesis assumes that far below the quantum level lies deterministic parameters, unseen to the observer, that control the observed quantum numbers.
God does not play dice with the Universe!

Why doesn’t Einstein like Quantum?
• Reality should be deterministic and not based on probabilities.
• Reality should be objective and not dependent on an observer!
Einstein, Podolsky & Rosen
EPR Paradox

Measurement of Correlations between Components of Nuclear Spin
EPR Paradox
Quantum Non-Localilty

• Two particles are ‘entangled’ quantum mechanically – that is, they are described by one wave function.
• Suppose they have total zero spin.
• Then they are separated. If the spin of one is flipped in flight to the detector, the other one flips *instantaneously*, *faster than light*.
• This violates the speed limit of light.
• OR, somehow the particles are connected across space – they are *NONLOCAL*. This is a big no-no to Einstein and his Quantum Pals.
EPR Particles: Entanglement

EPR particles are particles that are ‘entangled’ that is, there is a single wavefunction that describes both particles. Until a measurement is made, the particles remain in an entangled state. While entangled, the particles are connected in a ‘nonlocal’ way so that even if they are separated over great distances they can communicate faster than light.
I don’t like this spooky action at a distance!
At the heart of the realm of quantum computation is the qubit. The quantum bit, by analogy with the binary digit, the bit, used by everyday computers, the qubit is the quantum computer's unit of currency. Instead of being in a 1 or zero state, a qubit can be in a superposition of both states.
Physicist Eugene Wigner's representation of quantum superposition state (the two lumps) showing interference fringes in the center. Image also corresponds to a qubit in a superposition state of 0 and 1.
Quantum Teleportation

Entangled photons are used to teleport other photons.
Quantum Teleportation??

Quantum Uncertainty will make it very difficult to teleport a complex organism since there is always uncertainty in the position of its atoms!
Quantum Consciousness

Why are we not zombies?

What Causes our Subjective Experience of Inner Being?

Each caged electron is a qubit in a nanoscale quantum dot. We have a billion billion of them enslaved by coherent near electromagnetic brain fields of low frequency. This forms a mind-brain hologram. There is direct back-reaction of the coherent phased array of single electron dipoles on their mental pilot landscape field. This generates our inner conscious experience.

- Jack Sarfatti
THE PROBLEM
Coherence & De-Coherence

In order for particles to be entangled in a non-local way they must be in a coherent superposition. Observing the system collapses the wavefunction into a localized state. The problem is that it is very difficult to maintain coherent superpositions because the environment can collapse the wavefunction. In order for quantum phenomena to function in the biological realm, coherence must be maintained for at least a millisecond. This is not currently achievable and perhaps not even theoretically possible. Coherence is also the problem with quantum computers. It is also the problem with any claim of macrocosmic entanglement and quantum nonlocal effects - maintaining coherence is very difficult in any environment!!!
Quantum Quackery?
SPACE-TIME AND BEYOND

Consciousness is the origin of all space-time.

Energy and space are all the same thing.

We are intimately connected to every part of the universes.

There is life in everything.

The interpretation of the universes has begun.

Bob Tovin

In conversation with physicists Jack Sarfatti and Fred Wolf
For each of us, an indefinite number of universes exists simultaneously.

Each universe has its own time sequence.

Each universe may be a slight variation of the next one or may be entirely unrelated.

Many Worlds Hypothesis
ALL THINGS ARE POSSIBLE!

THERE IS AN INDEFINITE NUMBER OF HARMONIES
CONSTRUCTING AN INDEFINITE NUMBER OF POSSIBILITIES

WE EXIST IN ALL THE UNIVERSE LAYERS SIMULTANEOUSLY

ONE OF AN INDEFINITE NUMBER OF REALITIES

ANOTHER OF THE INDEFINITE NUMBER OF REALITIES
WE CONSTRUCT OUR OWN INDIVIDUAL REALITIES

ALL WE CAN THINK OR PERCEIVING IS BROUGHT INTO AWARENESS WITH OUR INDIVIDUAL THOUGHTS

Collapsing Wave Function

QUANTUM HEALING
EXPLORING THE FRONTIERS OF MIND/BODY MEDICINE

DEEPAK CHOPRA, M.D.
Entanglement

Healing with the Hands

Healer mentally constructs a union with the oneness of all.

Biogravitons mix with gravitons forming a solid bridge or connection allowing phase harmony entrainment.

A link is established between the patient and the harmony of the universe, which contains the knowledge, or "vibrations," to reestablish a normal state of health.
I think I can safely say that nobody understands quantum mechanics.

Richard Feynman