CY121

Inorganic &

Physical Chemistry

Instructor:

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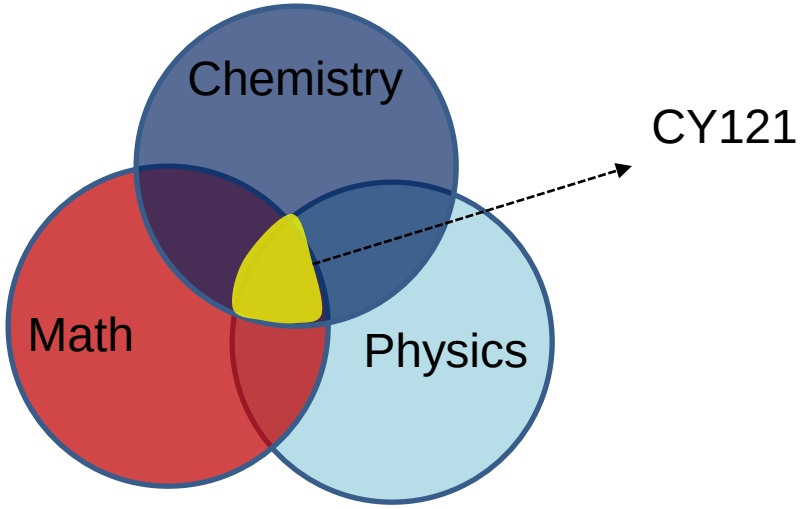
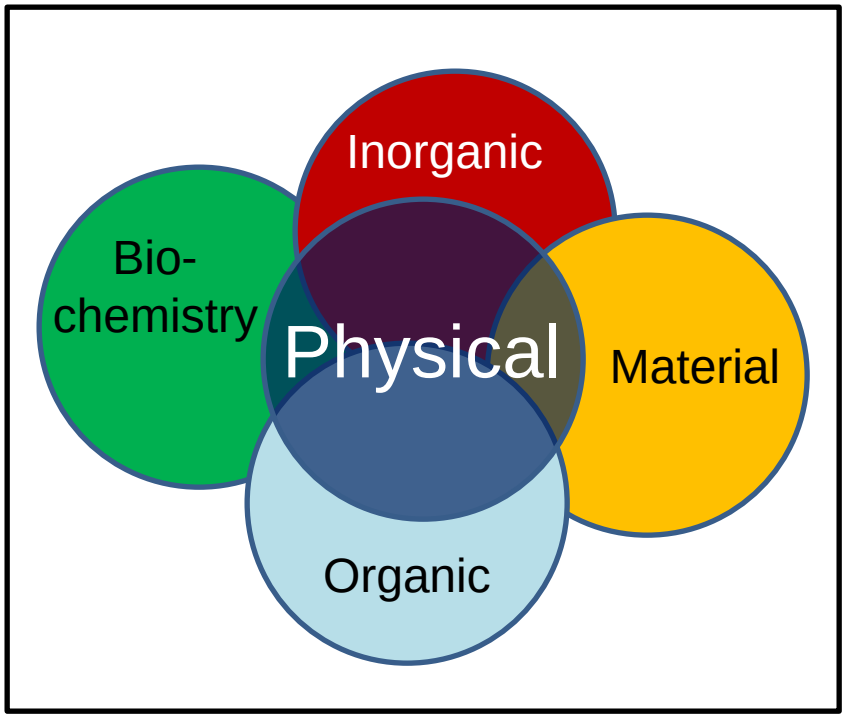
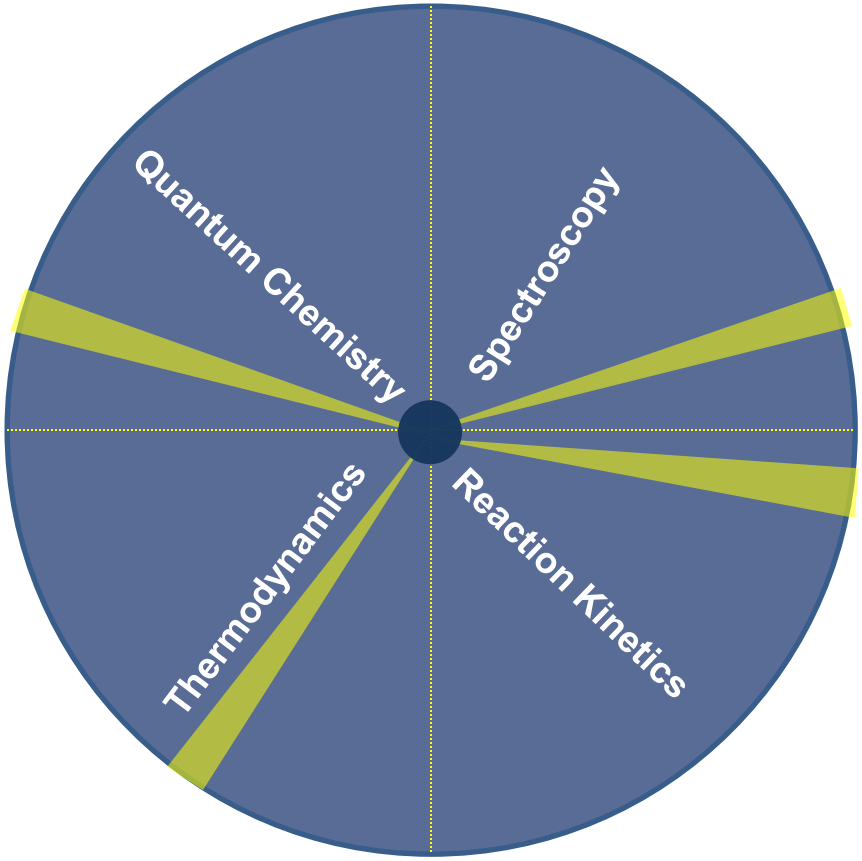


What are we going to cover ?





Is there anything "New" to learn ?

Unit IV.

- Wave functions, Probability density, Operator, Eigen function & Eigen Value
- Schrodinger equations,
- Particle in a Box/Ring problem,
- Hydrogen atom & Atomic orbitals

Quantum Chemistry

It describes atoms, molecules, their stability and the chemical transformations "ACCURATELY".

Reengineering chemistry to run on renewables *p. 1236*

Tomorrow's Earth *pp. 1249, 1263, & 1264*

Antibiotics in livestock *pp. 1251 & 1266*

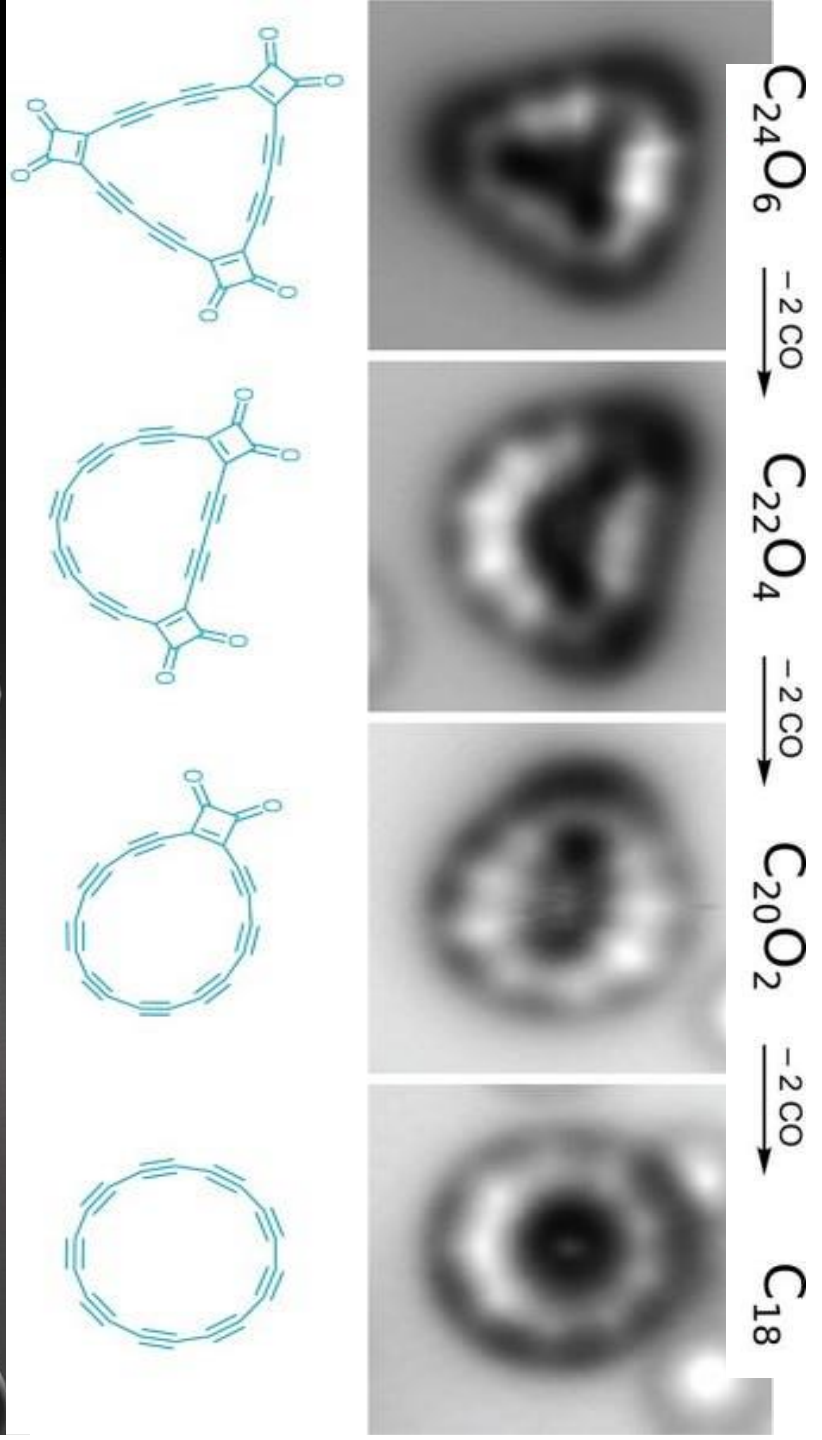
Science

$15
20 SEPTEMBER 2019
sciencemag.org

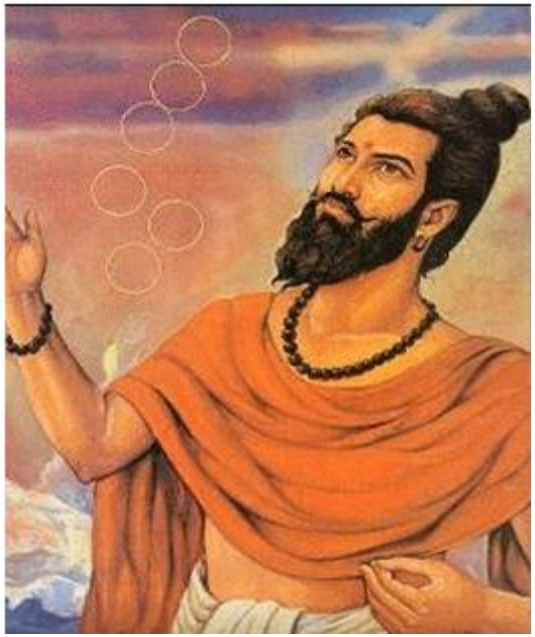
AAAS

CARBON RING

Microscope tip completes synthesis of cyclic allotrope *pp. 1245 & 1299*



History of Atomic Structures



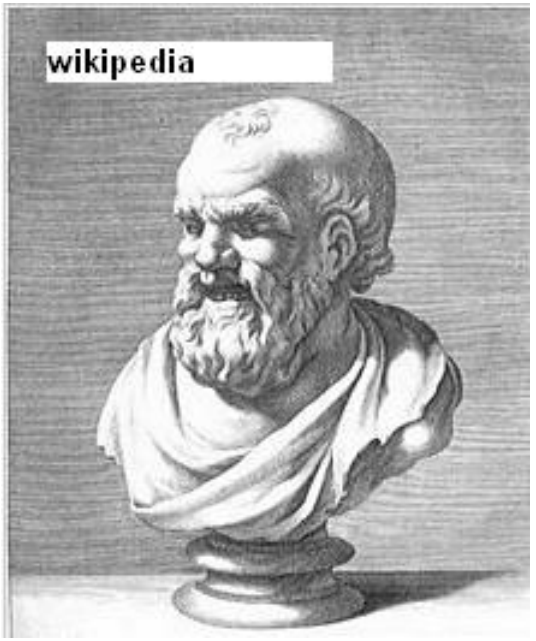
Acharya Kanad

~ 600 BC

Kan in Sanskrit means “smallest particle”

Real Name : Kashyap

"But in reality there are atoms and space."



Democritus

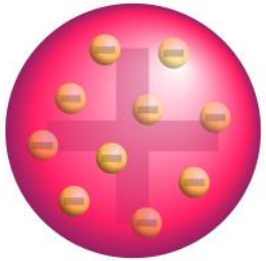
~ 400 BC

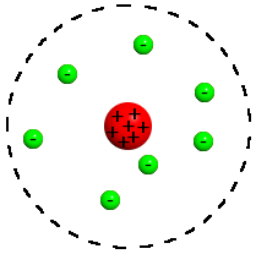
Debate

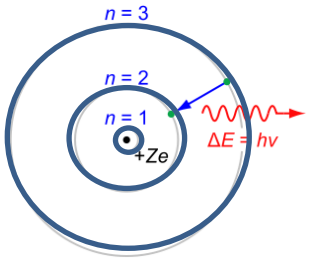
Speculation *vs.* *Authenticity*

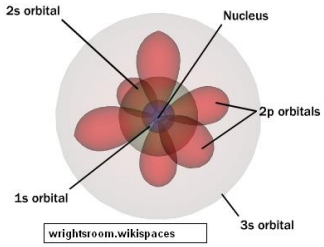
History of Atomic Structures

Atoms can be divided into smaller Particles

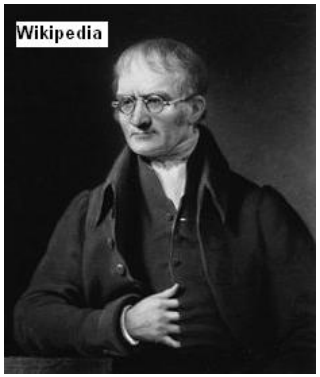








Dalton



Thomson

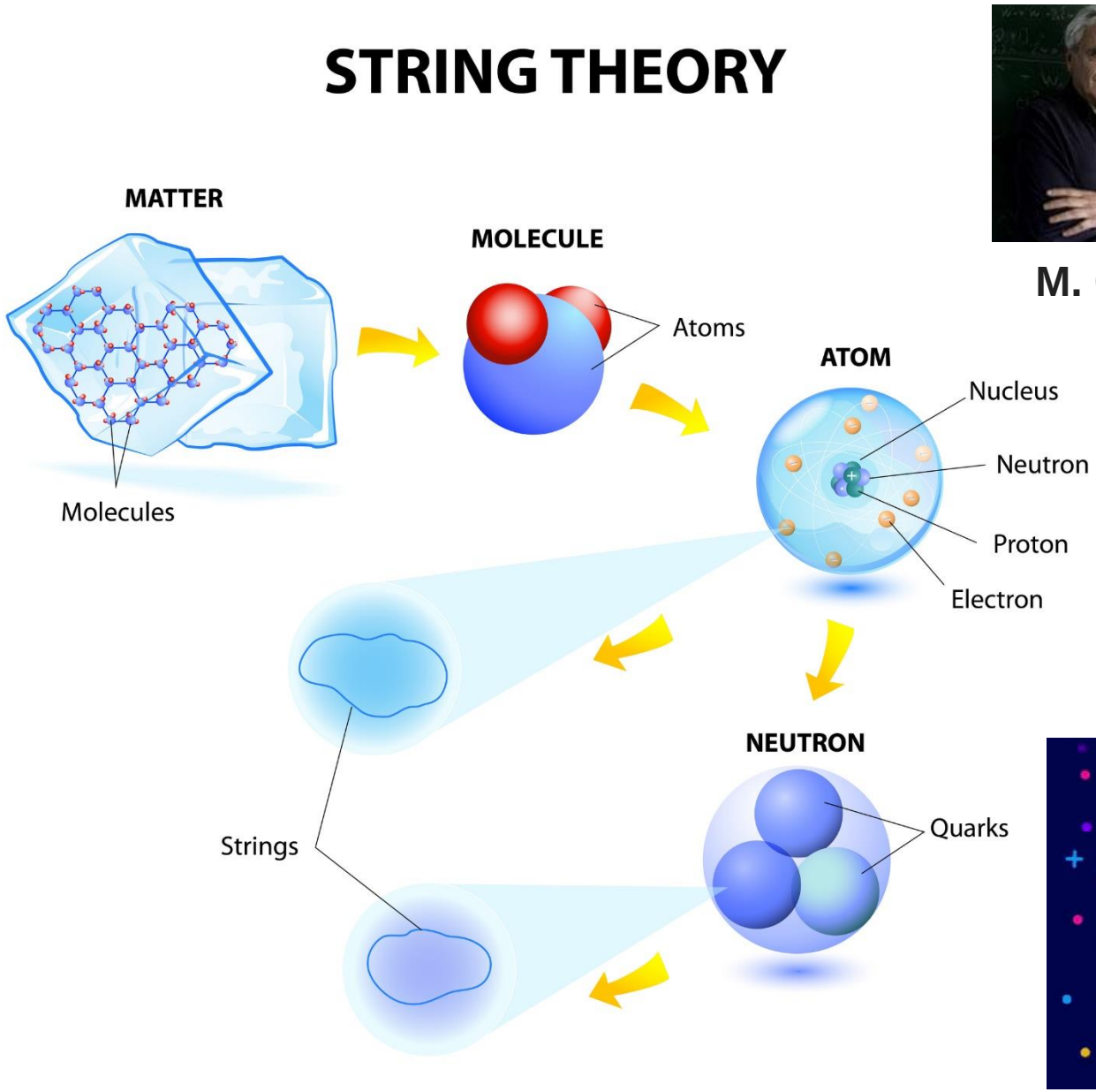
Rutherford

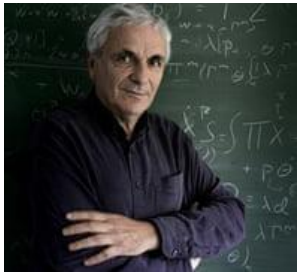
Niels Bohr

Schrodinger

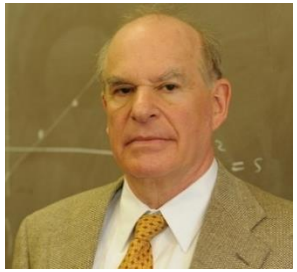
1803 — 1897 — 1911 — 1922 — 1930

Where we are now on Atomic Structure !!!





1984



M. Green

J. H. Schwarz

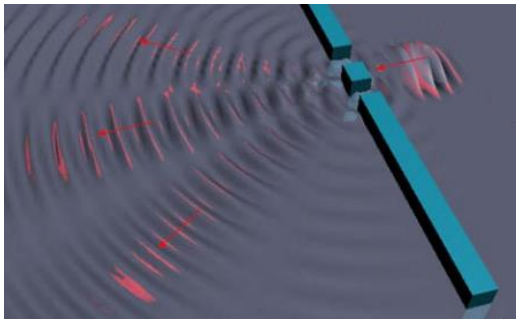
2003

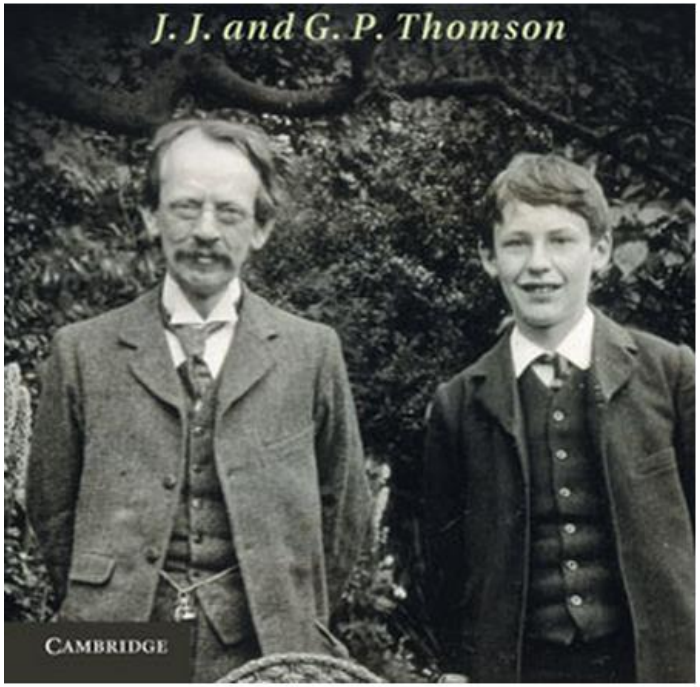
Michael R. Douglas

History of the Electron

Thompson:
Electrons are well known "particles" with a negative charge

Davisson and Germer Expts:
Electron show interference patterns



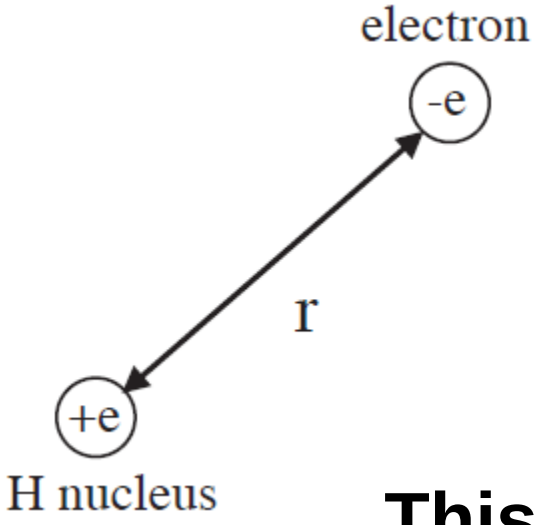


Their achievements have been summarized as JJ showing that the electron is a particle and GP showing that it is not, or rather that the electron can also behave as a wave.

FAILURE OF CLASSICAL MECHANICS

THE CLASSICAL DESCRIPTION OF AN ATOM

How is an e^- bound to the nucleus?



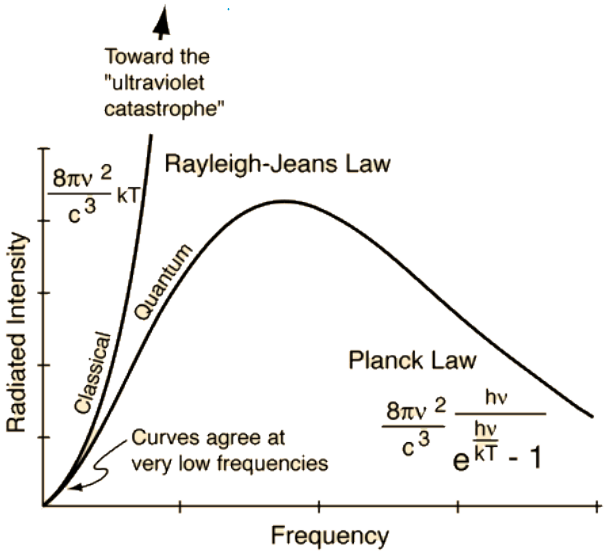
- Coulomb force $F(r) = \frac{-e^2}{4\pi\varepsilon_0 r^2}$

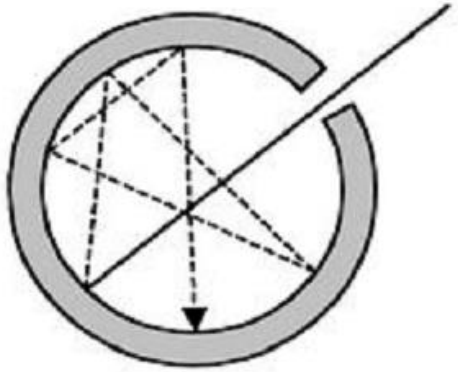
The closer the electron is to the nucleus, the larger the attractive force between the two charges.

This predicts that the electron should plummet into the nucleus.

FAILURES OF CLASSICAL MECHANICS

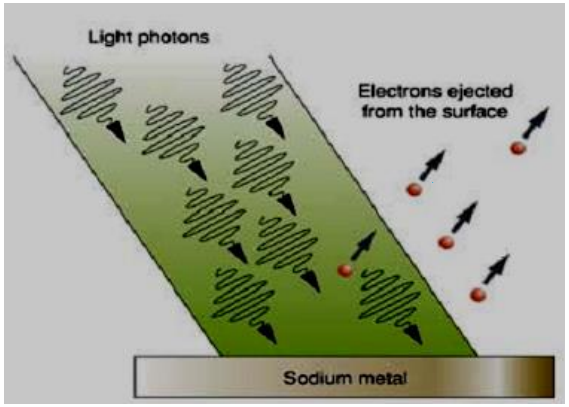
1. Black-Body Radiation





Sun, stars, Heated iron rods…

2. Photo-Electric effect



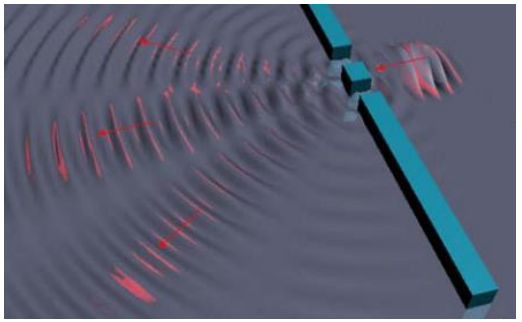
$$\underbrace{\frac{1}{2}m_e v_{\max}^2}_{\text{kinetic energy electron}} = \overbrace{\underbrace{h}_{\text{Planck constant}} \times \underbrace{\nu}_{\text{frequency photon}}}^{\text{energy photon}} - \underbrace{\phi}_{\text{work function}}$$

If this is larger than zero, i.e. > 0, then the electron flies off, or else it remains undisturbed.

Wave-Particle Duality: de Broglie Hypothesis

Thompson:
Electrons are well known "particles" with a negative charge

Davisson and Germer Expts:
Electron show interference patterns



de Broglie

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

Electron-wave moving @ 106 m/s

$$\lambda = \frac{h}{mv} = \frac{6.6\text{x}10^{-34}\ \text{J s}}{9.1\text{x}10^{-31}\ \text{Kg} \times\ 1\text{x}10^{6}\ \text{m/s}} = 7\times10^{-10}\,m$$

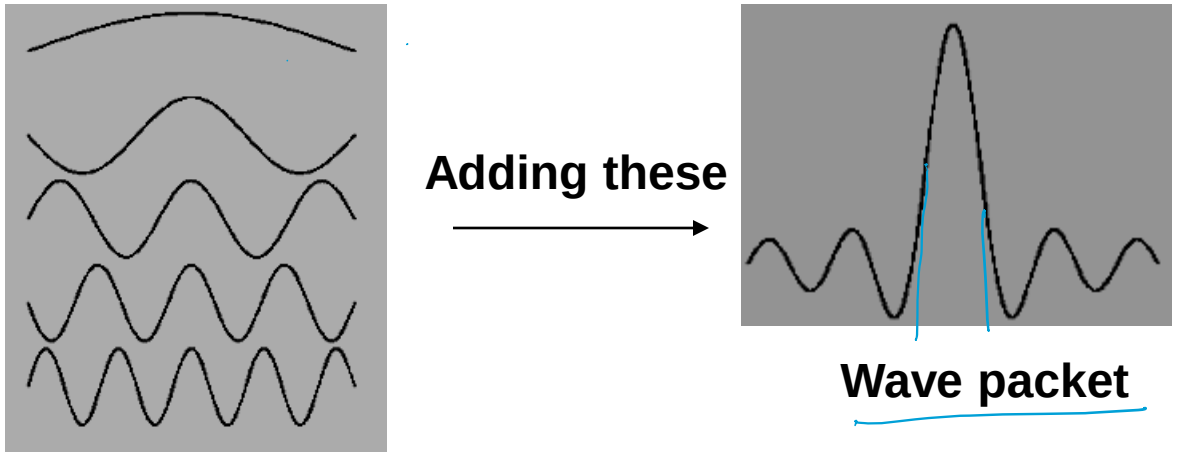
Heisenberg's Uncertainty Principle

If only one wave with known k (momentum), the position becomes completely uncertain, since 1 wave spreads indefinitely in space.

Specifying position accurately would require many waves, each having a fixed value of momentum (k),

→ P becomes completely uncertain.

$$\Delta x.\Delta p_x \geq \frac{h}{4\pi}$$

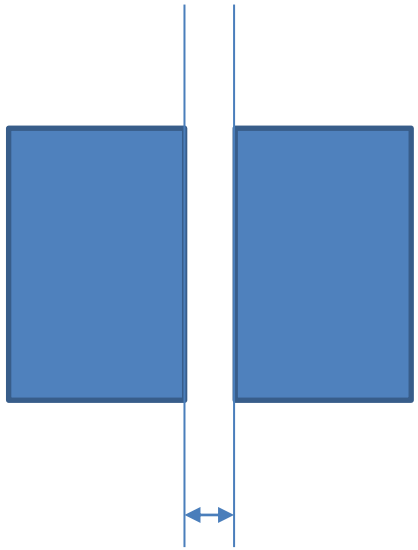


Can we rationalize Uncertainty Principle ?

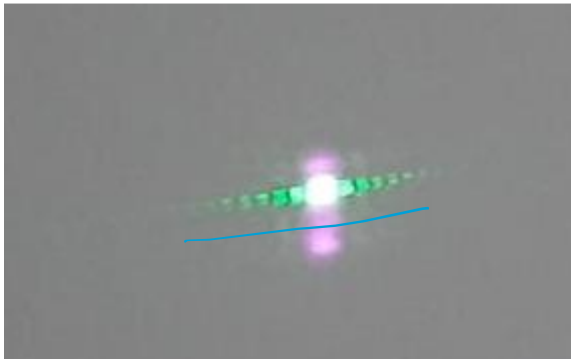
A Simple Experiment

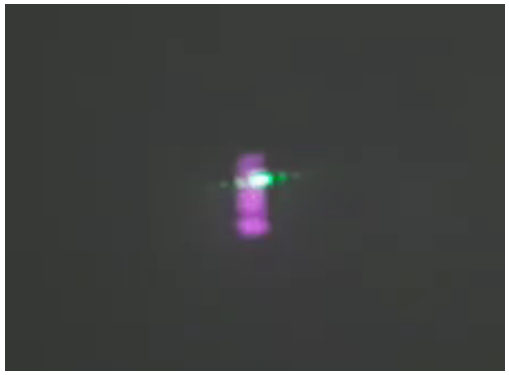
What do we need ?

1. Two Visiting Cards
2. One Laser Pointer (red/green)
3. Cello tape
4. Camera/Cellphone



0.02cm



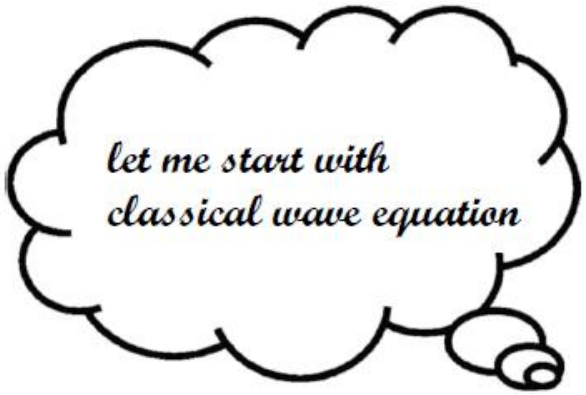


Schrodinger's Philosophy

Schrödinger

PARTICLES can be WAVES
& WAVES can be PARTICLES

Wave-like Equation for describing electrons, atoms or molecules.



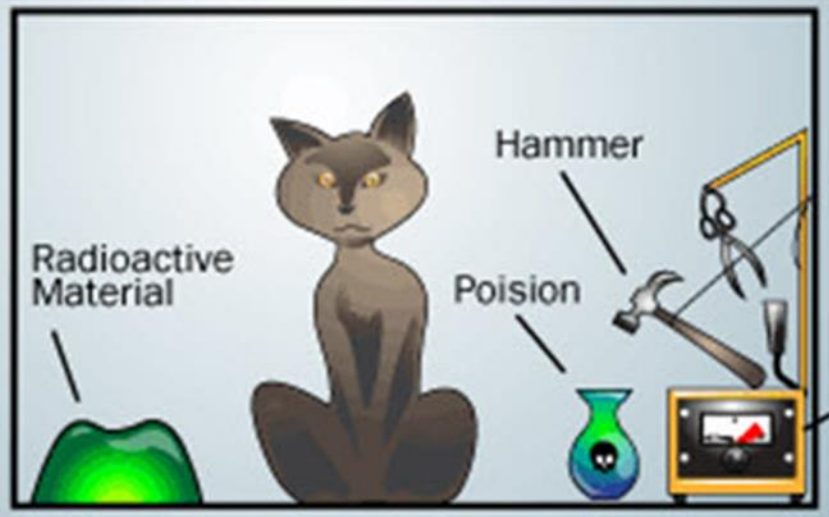
A concoction of

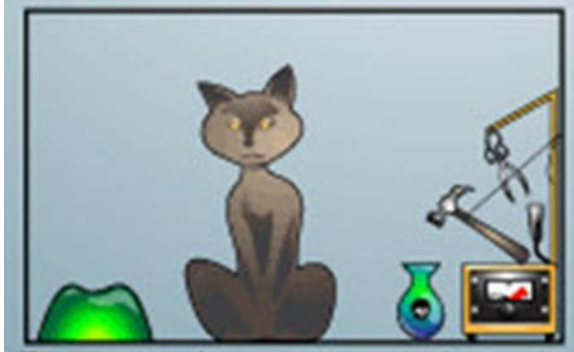
$$E = T + V = \frac{1}{2}mv^2 + V = \frac{p^2}{2m} + V$$

$E = h\nu = \hbar\omega$ Wave is Particle

$\lambda = \frac{h}{p} = \hbar k$ Particle is Wave

Schrödinger's Cat





The material does not decay; the cat lives.

The material has decayed; the cat has been killed by the poision.

According to the Copenhagen interpretation, the cat is both alive and dead. It exists in a state of "superposition."

Postulates of Quantum Mechanics

POSTULATE- 1

Any bound state of a dynamical system of n particles is described as completely as possible by an acceptable, square-integrable function $\Psi(q_1, q_2, \ldots q_{3n}, \omega_1, \omega_2, \ldots, \omega_n, t)$, *where the q's are spatial coordinates,* ω*'s are spin coordinates, and t is the time coordinate.* $\Psi^*\Psi\, d\tau$ *is the probability that the space-spin coordinates lie in the volume element* $d\tau (\equiv d\tau_1 d\tau_2 \cdots d\tau_n)$ *at time t, if* Ψ *is normalized.*

The state of a quantum mechanical system is completely specified by the function $\Psi(\mathbf{r}, t)$ that depends on the coordinates of the particle, $\mathbf{r}$ and the time, t. This function is called the wavefunction or state function and has the property that $\Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)d\tau$ is the probability that the particle lies in the volume element $d\tau$ located at $\mathbf{r}$ and time t.

This is the *probabalistic* interpretation of the wavefunction. As a result the wavefunction must satisfy the condition that finding the particle *somewhere* in space is 1 and this gives us the normalisation condition,

$$\int_{-\infty}^{+\infty} \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)d\tau = 1$$

The other conditions on the wavefunction that arise from the probabilistic interpretation are that it must be single-valued, continuous and finite. We normally write wavefunctions with a normalisation constant included.

Postulates of Quantum Mechanics

POSTULATE- **2**

To every observable dynamical variable M there can be assigned a linear hermitian operator $\widehat{\mathbf{M}}$ in quantum mechanics.

Observable	Classical Symbol	Quantum Operator	Operation
position	$\mathbf{r}$	$\hat{r}$	multiply by $\mathbf{r}$
momentum	$\mathbf{p}$	$\hat{p}$	$-i\hbar(\hat{i}\frac{\partial}{\partial x}+\hat{j}\frac{\partial}{\partial y}+\hat{k}\frac{\partial}{\partial z})$
kinetic energy	T	$\hat{T}$	$\frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})$
potential energy	$V(\mathbf{r})$	$\hat{V}(\mathbf{r})$	multiply by $V(\mathbf{r})$
total energy	E	$\mathcal{H}$	$\frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})+V(\mathbf{r})$
angular momentum	l_x	$\hat{l}_x$	$-i\hbar(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y})$
	l_y	$\hat{l}_y$	$-i\hbar(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z})$
	l_z	$\hat{l}_z$	$-i\hbar(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x})$

Hermitian Operators: A physical variable must have real expectation values (and eigenvalues).

Postulates of Quantum Mechanics

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	l_y	$\hat{l}_y$	$-i\hbar(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z})$
	l_z	$\hat{l}_z$	$-i\hbar(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x})$

Hermitian Operators: A physical variable must have real expectation values (and eigenvalues).

Postulates of Quantum Mechanics

POSTULATE- 3

In any measurement of the observable associated with operator $\hat{A}$, the only values that will ever be observed are the eigenvalues, a, that satisfy the eigenvalue equation,

$$\hat{A}\Psi = a\Psi$$

POSTULATE- 4

If a system is in a state described by the normalised wavefunction, Ψ, then the average value of the observable corresponding to $\hat{A}$ is given by

$$< \hat{A} >= \int_{-\infty}^{+\infty} \Psi^* \hat{A} \Psi d\tau$$

Eigen values

Operator operating on a function results in re-generating the same function multiplied by a number

$\hat{A} \cdot f(x) = a \cdot f(x)$ Eigen Value Equation

The function $f(x)$ is eigenfunction of operator $\hat{A}$ and a its eigenvalue

$f(x) = Sin(\alpha x)$

$\frac{d}{dx} f(x) = \alpha \cdot Cos(\alpha x)$

$Sin(\alpha x)$ is an eigenfunction of operator $\frac{d^2}{dx^2}$ and $-\alpha^2$ is its eigenvalue

$$\frac{d^2}{dx^2} f(x) = \frac{d}{dx}[\alpha . Cos(\alpha x)] = -\alpha^2 \cdot Sin(\alpha x) = -\alpha^2 \cdot f(x)$$

Operators

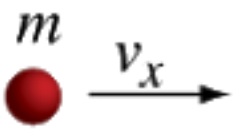
- A symbol that tells you to do something to whatever follows it
- Operators can be real or complex,
- Operators can also be represented as matrices

Classical Variable	QM Operator
Position, x	$\hat{x}$
Momentum, $p_x = mv$	$\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx} = -i\hbar\frac{d}{dx}$
Kinetic Energy, $T_x = \frac{p_x^2}{2m}$	$\hat{T}_x = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$
Kinetic Energy, $T = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$	$\hat{T} = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$
Potential Energy, $V(x)$	$\hat{V}(x)$

Operators

Linear momentum

$$p_x = mv_x$$

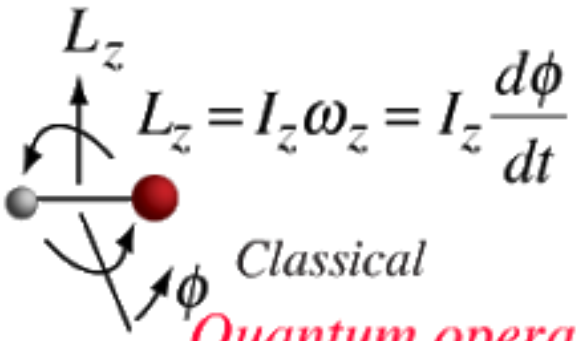


Classical

Quantum operator

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

Angular momentum



Classical

Quantum operator

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial \phi}$$

Rationalizing the Momentum Operator

$$\Psi(x,t) = e^{ikx}e^{i\omega t}$$

$$\Psi(x) = Ae^{ikx}$$

$$\frac{\partial \Psi}{\partial x} = ik\Psi = i\frac{p}{\hbar}\Psi$$

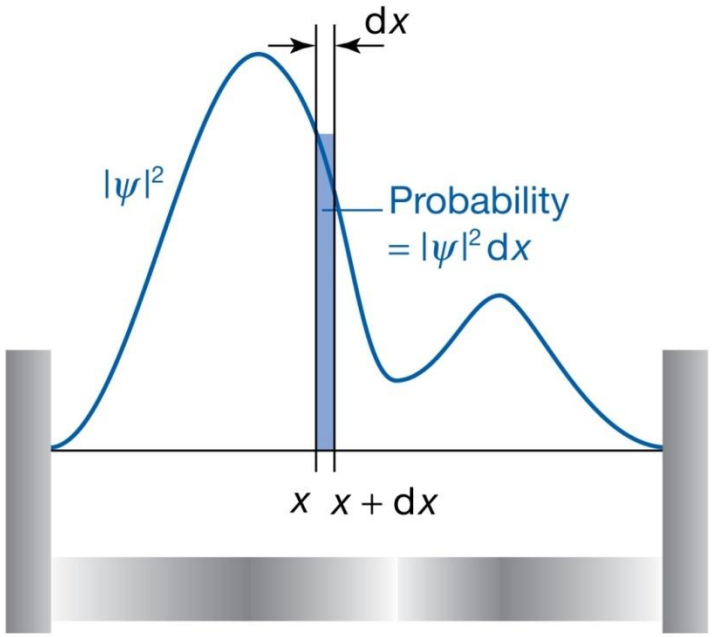
$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = \frac{p}{\hbar}$$

$$\frac{\hbar}{i}\frac{\partial \Psi}{\partial x} = p\Psi$$

$$\hat{p} \equiv \frac{\hbar}{i}\frac{\partial}{\partial x}$$

Wave function (Ψ)

For every dynamical system, there exists a wave function Ψ, from which all possible predictions about the physical properties of the system can be obtained.



If the wavefunction of a particle has the value ψ at some point x, then the probability of finding the particle between x and $x + dx$ is proportional to $|\psi|^2 dx$.

Wave function

A wave function consists of all information about the given quantum mechanical system.

Conditions for an Acceptable Wave function:

1) The wave function must be continuous. All its partial derivatives must also be continuous.

2) It must be quadratically integrable.

3) It must be single valued.

4) The wave function must satisfy the boundary conditions of the quantum mechanical system it represents.

Born Interpretation : Probability density

The state of a quantum mechanical system is completely specified by a wavefunction $\Psi(x,t)$,which can be complex

All possible information can be derived from $\Psi(x,t)$

From the analogy of classical wave equation, Intensity is replaced by Probability. The probability is proportional to the square of the of the wavefunction $|\Psi(x,t)|^2$, known as probability density $P(x)$

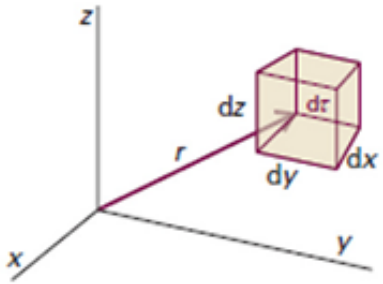
Born Interpretation

Probability density

$$P(x) = \left|\Psi(x,t)\right|^2 = \Psi^*(x,t)\cdot\Psi(x,t)$$

Probability

$$P(x_a \le x \le x_a + dx) = \left|\Psi(x,t)\right|^2 dx = \Psi^*(x_a,t)\cdot\Psi(x_a,t)dx$$



Probability in 3-dimensions

$$\begin{aligned} &\mathrm{P}(x_a \le x \le x_a + dx, y_a \le y \le y_a + dy, z_a \le z \le z_a + dz) \\ &\quad = \Psi^*(x_a, y_a, z_a, t').\Psi(x_a, y_a, z_a, t')dxdydz \\ &\quad = \left|\Psi(x_a, y_a, z_a, t')\right|^2 d\tau \end{aligned}$$

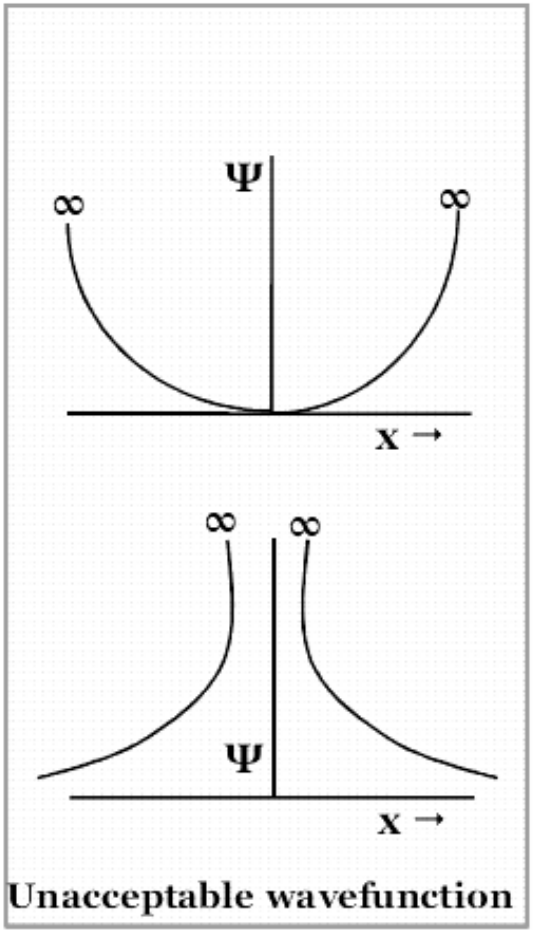
Normalization of Wave function

Since $\Psi^*\Psi d\tau$ is the probability, the total probability of finding the particle somewhere in space has to be unity

$$\iiint_{all\ space} \Psi^*(x,y,z).\Psi(x,y,z)dxdydz$$

$$= \int_{all\ space} \Psi^*\Psi d\tau = \langle \Psi | \Psi \rangle = 1$$

If integration diverges, i.e. $\rightarrow \infty$: Ψ can not be normalized, and therefore is NOT an acceptable wave function. However, a constant value $C \neq 1$ is perfectly acceptable.



Unacceptable wavefunction

Ψ must vanish at $\pm\infty$, or more appropriately at the boundaries and Ψ must be finite

Laws of Quantum Mechanics: Average Value

The mathematical description of quantum mechanics is built upon the concept of an operator

The values which come up as result of an experiment are the eigenvalues of the self-adjoint linear operator.

The average value of the observable corresponding to operator $\hat{A}$ is

$$\langle a \rangle = \int \Psi^* \hat{A} \Psi d\upsilon$$

The state of a system is completely specified by the wavefunction $\boldsymbol{\Psi(x,y,z,t)}$ which evolves according to time-dependent Schrodinger equation

Time-Independent Schrödinger equation

TIME-DEPENDENT Schrödinger equation :

$$\hat{H}\cdot\Psi(x,y,z,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,y,z,t)$$

$$\Psi(x,y,z,t)=\psi(x,y,z)\cdot\phi(t)$$

$$\hat{H}=\frac{-\hbar^2}{2m}\nabla^2+V(x,y,z)$$

$$\hat{H}(\psi\cdot\phi)=i\hbar\frac{\partial}{\partial t}(\psi\cdot\phi)$$

$\hat{H}$ operates only on ψ and $\frac{\partial}{\partial t}$ operates only on ϕ

$$\phi\cdot\hat{H}\psi=\psi\left(i\hbar\frac{\partial}{\partial t}\phi\right)\quad\Rightarrow\quad\frac{\hat{H}\psi}{\psi}=\frac{1}{\phi}\left(i\hbar\frac{\partial}{\partial t}\phi\right)$$

Time-Independent Schrödinger equation

In classical mechanics $\hat{H}$ represents total energy
We can therefore write

$\hat{H}\psi = W\psi$ as $\hat{H}\psi = E\psi$

$$\hat{H}\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\cdot\psi(x)$$

Schrodinger equation is an eigen-value equation

There can be many solutions $\boldsymbol{\psi_n(x)}$ each corresponding to different energy $\boldsymbol{E_n}$

Time-Independent Schrödinger equation

In 3-dimensions the Schrodinger equation is

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x,y,z)\right]\psi(x,y,z)=E\cdot\psi(x,y,z)$$

For 'n' particle system the Schrodinger equation in 3-dimensions is

$$\sum_{i=1}^{n}\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}\right)+V(x,y,z)\right]\psi=E\cdot\psi$$

$$\psi \Leftarrow \psi(x_1,x_2,x_3,\ldots x_{n-1},x_n,y_1,y_2,y_3,\ldots y_{n-1},y_n,z_1,z_2,z_3,\ldots z_{n-1},z_n)$$

Exactly Solvable QM System: Free Particle

Time-independent Schrodinger equation

$$\hat{H}\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi(x) = E\cdot\psi(x)$$

For a free particle $V(x)$=0
There are no external forces acting

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\cdot\psi(x)$$

Free Particle

Let us assume

$\psi(x) = A\sin kx + B\cos kx$ Trial Solution

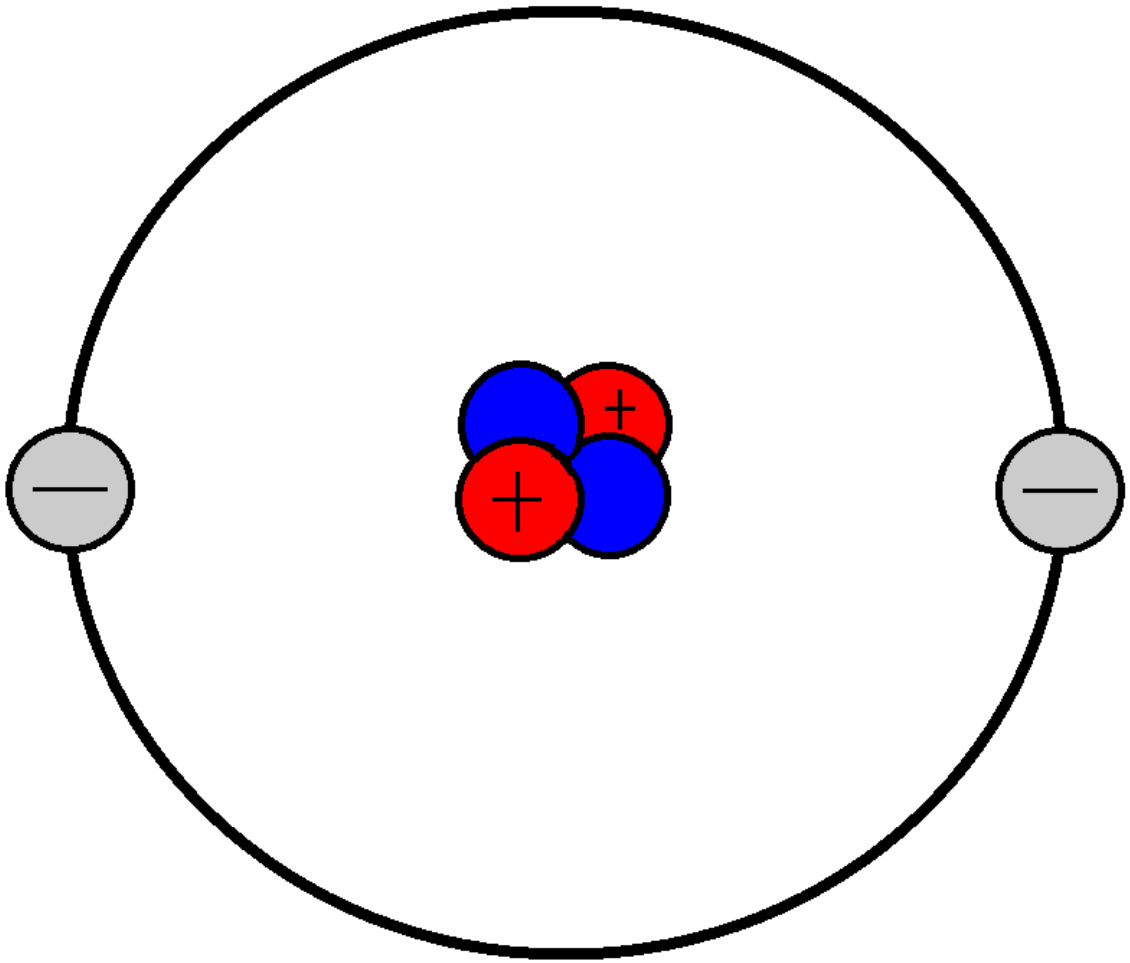
$$\psi(x) = A\sin kx + B\cos kx$$

$$\frac{\partial}{dx}\psi(x) = \frac{\partial}{dx}\left(A\sin kx + B\cos kx\right) = k\left(A\cos kx - B\sin kx\right)$$

$$\frac{\partial^2}{dx^2}\psi(x) = -k^2\left(A\sin kx + B\cos kx\right) = -k^2\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\cdot\psi(x)$$

$$\frac{\hbar^2}{2m}k^2\psi(x) = E\cdot\psi(x) \quad \Rightarrow \quad E = \frac{\hbar^2k^2}{2m} \quad \Rightarrow \quad k = \pm\frac{\sqrt{2mE}}{\hbar}$$



Free Particle

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

There are no restrictions on k

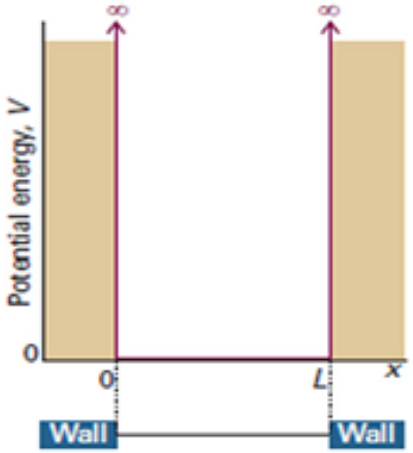
E can have any value

Energies of free particles are continuous

$$\psi(x) = A\sin\frac{\sqrt{2mE}}{\hbar}x + B\cos\frac{\sqrt{2mE}}{\hbar}x$$

No Quantization **All energies are allowed**

Particle in one-dimensional Box



$$V(x)=\begin{cases}\infty & x<0\\ 0 & 0\le x\le L\\ \infty & x>L\end{cases}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+V(x)\psi(x)=E\cdot\psi(x)$$

For regions in the space $x<0$ and $x>\mathrm{L}\Rightarrow V=\infty$

$$\frac{\partial^2}{\partial x^2}\psi(x)=\frac{2m}{\hbar^2}(V-E)\cdot\psi(x)=\infty\cdot\psi(x)$$

Particle in one-dimensional Box

Boundary Condition $x = 0 \Rightarrow \psi(x) = 0$

$$\psi(x) = A\sin kx + B\cos kx \Rightarrow \psi(x) = A\sin kx$$

Boundary Condition $x = L \Rightarrow \psi(L) = 0$

$$\sin kL = 0 \Rightarrow kL = n\pi \quad \text{n=1,2,3,4...}$$

$$E = \frac{\hbar^2 k^2}{2m} \text{ and } k = \frac{n\pi}{L}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2} \quad \text{n=1,2,3,4...}$$

what is energy of a particle in 1D box

The energy of a particle in a one-dimensional box (also known as a "particle in a box") is quantized, meaning that it can only take on certain specific values. The allowed energy levels are given by the equation E_n = (n^2 * h^2) / (8 * m * L^2), where n is an integer (1, 2, 3, ...), h is Planck's constant, m is the mass of the particle, and L is the length of the box. The lowest energy level (n = 1) is called the ground state, and the higher energy levels (n = 2, 3, ...) are called excited states.

DE

Explain quantum chemistry in simple terms

Quantum chemistry is a branch of chemistry that uses quantum mechanics to study the behavior of atoms and molecules. It helps to explain how chemical reactions happen and predict the properties of new molecules. It is based on the principles of wave-particle duality and the idea that energy is quantized, meaning it can only exist in certain specific amounts. This allows scientists to understand and predict the behavior of very small particles, such as atoms and molecules, that cannot be directly observed. In simple terms, quantum chemistry is a way of understanding how the tiny building blocks of matter interact and behave.

DE write a poem on particle in a 1D box

Trapped in a box, a particle so small,
No room to move, no space at all.
A prison of length, with no way to escape,
A fate it must bear, with no hope to shape.

It bounces and bounces, in its tiny cell,
With energy high, and a tale to tell.
A wave of probability, in the confined space,
A quantum dance, with a steady pace.

It cannot be seen, but it's always there,
A prisoner of the box, with no room to spare.
But its energy states, they form a range,
A spectrum of light, with a hidden change.

So let us not pity, the particle's plight,
For it is a marvel, in the world of quantum light.
It may be confined, but it's still alive,
A spark in the darkness, that will always thrive.

DE write a poem on RGIPT Jais Amethi

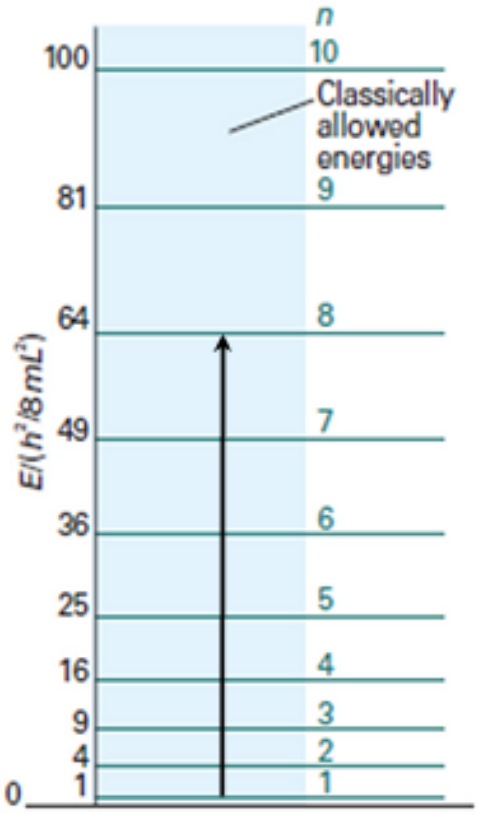
In the land of Amethi, so green and fair,
RGIPT stands tall, a beacon of care.
Where knowledge and technology meet,
Its halls are bustling with students so sweet.

With a faculty of great renown,
RGIPT's reputation will never drown.
Research and innovation lead the way,
As students learn and grow each day.

In Jais, a town of peace and pride,
RGIPT's future shines bright and wide.
With a vision to excel and reach new heights,
RGIPT's story will be one of great lights.

So let us sing of RGIPT's glory,
In Amethi's land, so fair and hoary.
May its name be known far and wide,
A leader in education, forever abide.

Particle in one-dimensional Box



The lowest allowed energy level is for $n=1$

$E_1 = \dfrac{\pi^2\hbar^2}{2mL^2}$ has a non zero value $\Rightarrow$ Zero Point Energy

$$h\nu = \Delta E = E_f - E_i = \frac{n_f^2 h^2}{8mL^2} - \frac{n_i^2 h^2}{8mL^2} = \left(n_f^2 - n_i^2\right)\frac{h^2}{8mL^2}$$

Wavefunction $\psi(x) = A\sin kx = A\sin\dfrac{n\pi}{L}x$

Normalization $\displaystyle\int_0^L \psi^*(x)\cdot\psi(x)\cdot dx = A^2\int_0^L \sin^2\frac{n\pi}{L}x\cdot dx = 1$

$$A = \sqrt{\frac{2}{L}} \qquad \psi(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x$$

Particle in one-dimensional Box

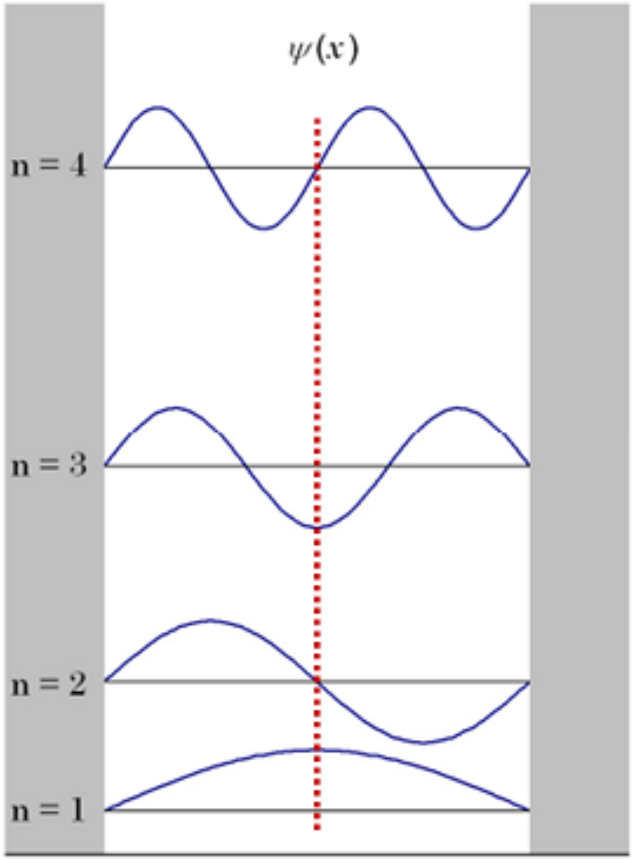
Wavefunction $\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$

n=1,3.. (odd)
Symmetric
(even function)

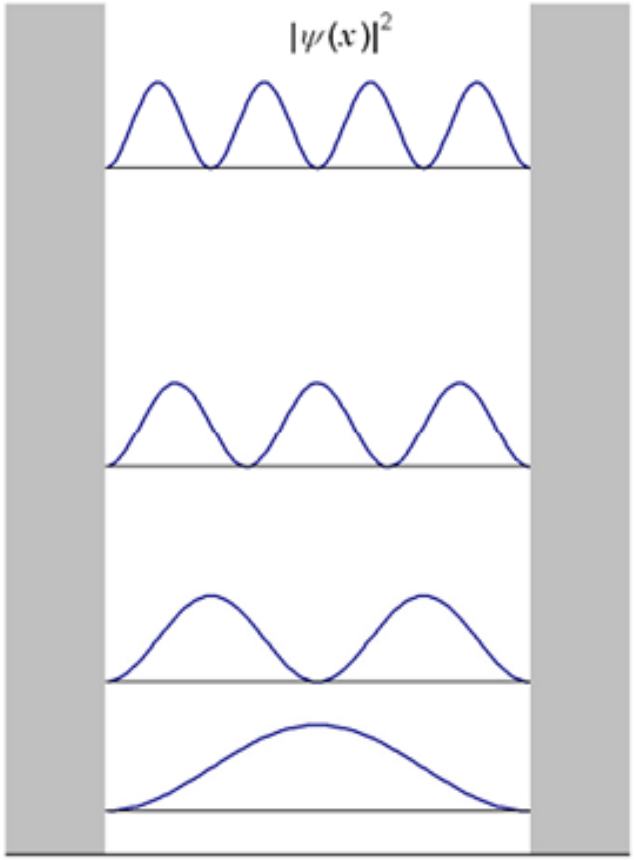
n=2,4.. (even)
Anti-Symmetric
(odd function)

Number of Nodes
(zero crossings) = n-1

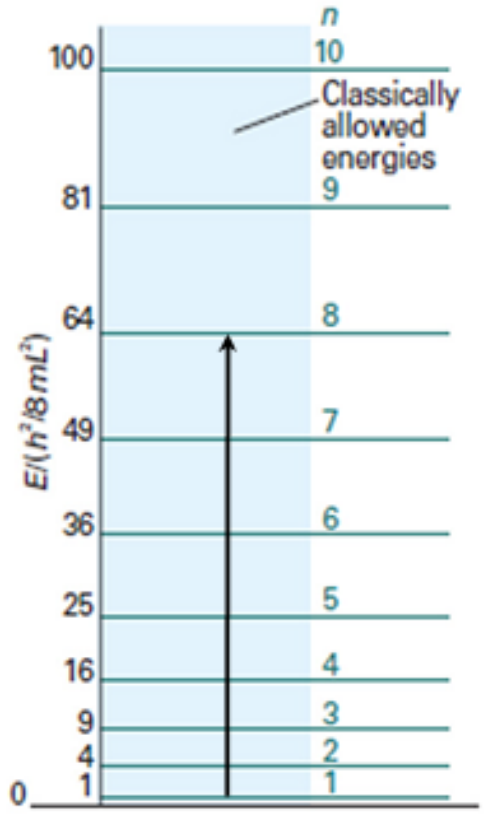
Wave function



Probability density



Particle in one-dimensional Box



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Normalization $\int_0^L \psi^*(x)\cdot\psi(x)\cdot dx = A^2\int_0^L \sin^2\dfrac{n\pi}{L}x\cdot dx = 1$

$A = \sqrt{\dfrac{2}{L}}$ $\psi(x) = \sqrt{\dfrac{2}{L}}\sin\dfrac{n\pi}{L}x$

Particle in one-dimensional Box

Expectation Value for position

$$\langle x \rangle = \int \psi^* \cdot x \cdot \psi \cdot dx$$

$$= \int_0^L \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \cdot x \cdot \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \cdot dx$$

$$= \frac{2}{L} \int_0^L x \cdot \sin^2 \frac{n\pi}{L} x \cdot dx$$

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

Expectation Value for momentum

$$\langle p_x \rangle = \int \psi^* \cdot \left(-i\hbar \frac{\partial}{\partial x} \right) \cdot \psi \cdot dx$$

$$= -i\hbar \int_0^L \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \cdot \frac{\partial}{\partial x} \cdot \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \cdot dx$$

$$= \frac{-2i\hbar n\pi}{L^2} \int_0^L \sin \frac{n\pi}{L} x \cdot \cos \frac{n\pi}{L} x \cdot dx$$

$$= 0$$

Building Up the Periodic Table: The Basis

1. **Various quantum numbers**

2. **Hund's Rule:**

When more than one orbital has the same energy (e.g. px, py, pz), electron occupy separate orbitals and do so
with parallel spins.

3. **Pauli (Exclusion) Principle**

No more than two electrons shall occupy a single orbital and, if two do occupy a single orbital, then their spins must be paired. or
"no two electrons can have the same four quantum numbers"

4. **The order of orbitals for a given quantum number depends on**

Shielding Effects (Z*)
Penetration of orbitals

Electronic Configuration

H	$1s^1$
He	$1s^2$
Li	$1s^2 2s^1$
.....	
F	$1s^2 2s^2 2p^5$
Ne	$1s^2 2s^2 2p^6$

3s < 3p < 3d

Four Quantum Numbers

The principal quantum number, n = 1, 2, ...,

determines the energy *E* of the electron in the atom.

The angular momentum quantum number, ℓ = 0, 1, 2, ..., n-1,

determines the orbital angular momentum of the electron.

ℓ =0	s	"sharp"
ℓ =1	p	"principal"
ℓ =2	d	"diffuse"
ℓ =3	f	"fundamental or fine"

The magnetic quantum number, m = 0, ±1, ..., ± ℓ

determines the amount of angular momentum of the electron around a particular axis.

The Spin quantum number, s = ± 1/2

Orbit *and* Orbital

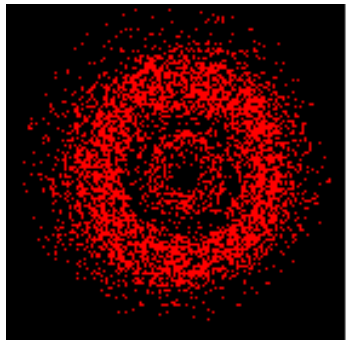
An **Orbit** is the path of an electron around the nucleus of an atom.

When a planet moves around the sun, you can plot a definite path for it which is called an orbit.

The impossibility of drawing orbits for electrons

The ***Heisenberg Uncertainty Principle*** says - that you can't know with certainty both where an electron is and where it's going next.

An **Orbital** is the three dimensional space where the probability of finding an electron around the nucleus is maximum. In other words, 'Orbital' refers to an electron's probable location.



Schrodinger equation for Hydrogen-like Atom

$$\left[-\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{\hbar^2}{2mr^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)+V(r)\right]\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi)$$

$$\psi(r,\theta,\phi) = R(r)\cdot P(\theta)\cdot F(\phi)$$

$Y_{l,m_l}(\theta,\phi)$ ← Angular part

Radial part

$R(r)$ → **Solution exists iff** → ***n= 1, 2, 3, …..***

$P(\theta)$ → **Solution exists iff** → ***ℓ = 0, 1, 2,….., n-1***

$F(\phi)$ → **Solution exists iff** → ***m_l= -ℓ, -ℓ +1, ….., + ℓ***

In three dimensions the Schrodinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$$

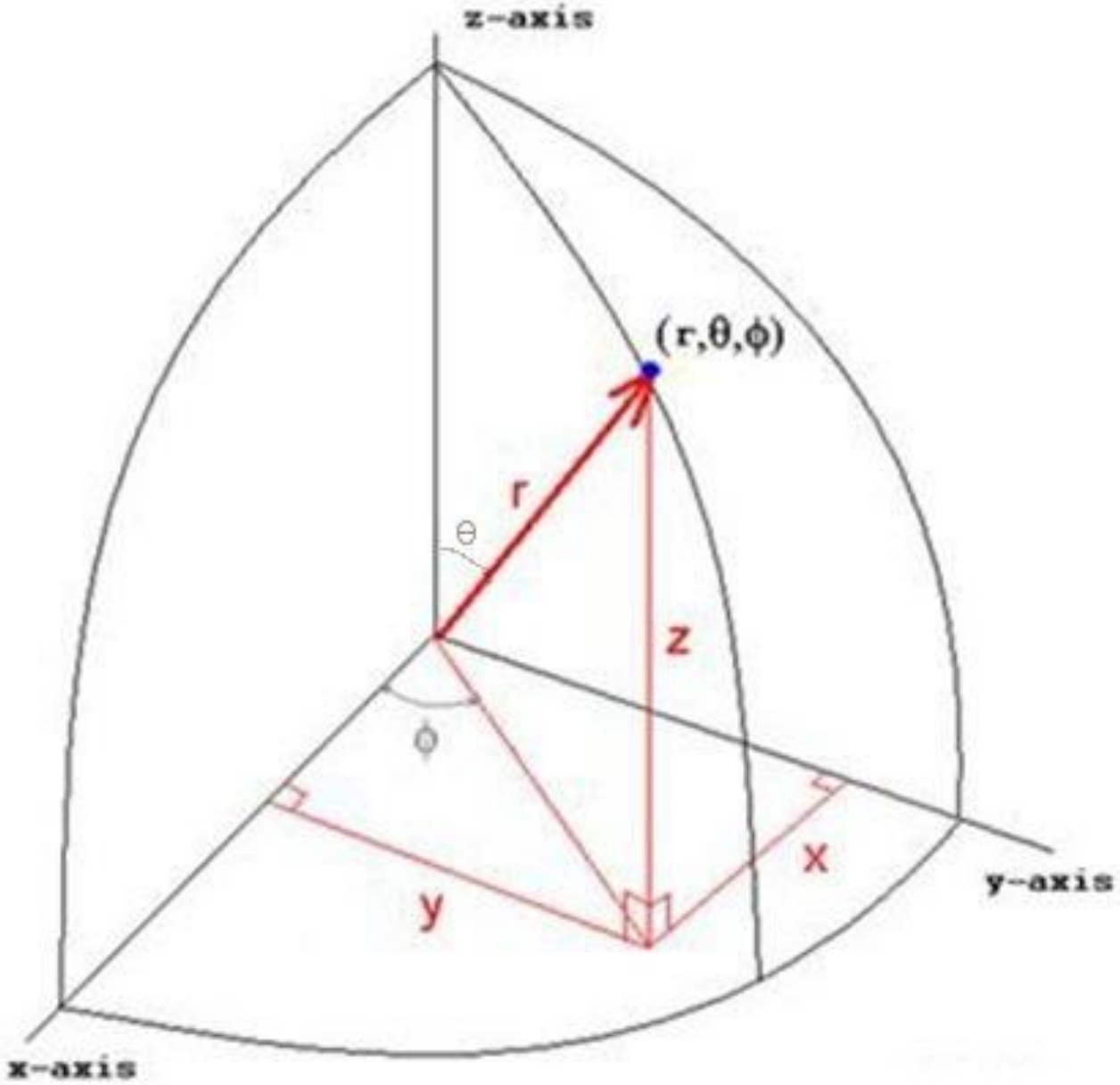
where ∇^2 is the Laplacian operator

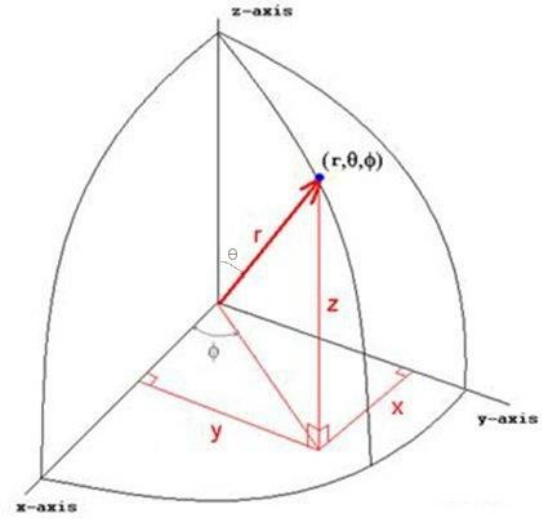
Laplacian in spherical coordinates

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right)$$

Using the Laplacian in spherical coordinates, the Schrodinger equation becomes

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right]\psi + V(r)\psi = E\psi$$


z-axis
(r,θ,ϕ)
r
θ
z
ϕ
x
y
y-axis
x-axis



$$z = r\ \cos\theta$$

$$r_{projection} = r\ \sin\theta$$

$$x = r_{projection}\cos\varphi = r\cos\varphi\sin\theta$$

$$y = r_{projection}\sin\varphi = r\sin\varphi\sin\theta$$

Seperation of Variables: Solution to SE equation of the form

$$\psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi)$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r)\,Y(\theta,\phi) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)R(r)\,Y(\theta,\phi)$$

$$+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}R(r)\,Y(\theta,\phi) - \frac{2m}{\hbar^2}\Big[V(r)-E\Big]R(r)\,Y(\theta,\phi) = 0$$

$$Y(\theta,\phi)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r) + R(r)\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi)$$

$$+R(r)\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi) - \frac{2m}{\hbar^2}\Big[V(r)-E\Big]R(r)\,Y(\theta,\phi) = 0.$$

$$Y(\theta,\phi)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r)+R(r)\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi)$$

$$+R(r)\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi)-\frac{2m}{\hbar^2}\Big[V(r)-E\Big]R(r)\,Y(\theta,\phi)=0.$$

Dividing the equation by R(r) Y (θ, φ), multiplying by r^2 , and rearranging

$$\left\{\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r)-\frac{2mr^2}{\hbar^2}\Big[V(r)-E\Big]\right\}$$

$$+\left[\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi)+\frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi)\right]=0.$$

$$\left\{\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r)-\frac{2mr^2}{\hbar^2}\Big[V(r)-E\Big]\right\}$$

$$+\left[\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi)+\frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi)\right]=0.$$

The only way the sum of the groups can be zero, **if each group is equal to the same constant.** The constant chosen is known as the separation constant **(K).**

Some of the physicists and mathematicians of the previous 300 years predicted the separation constant,

the enlightened choice of $\ell(\ell+1)$ as the separation constant (K).

The radial equation

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) - \frac{2mr^2}{\hbar^2}\Big[V(r) - E\Big] = l(l+1)$$

The angular equation

$$\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi) + \frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi) = -l(l+1)$$

The signs on the right side are opposite so they do, in fact, sum to zero.

The angular equation

$$\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi)+\frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi)=-l(l+1)$$

The spherical harmonics are also separable

$$Y(\theta,\phi)=f(\theta)\,g(\phi)$$

$$\frac{1}{f(\theta)\,g(\phi)\,\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta)\,g(\phi)+\frac{1}{f(\theta)\,g(\phi)\,\sin^2\theta}\frac{\partial^2}{\partial\phi^2}f(\theta)\,g(\phi)=-l(l+1)$$

$$\Rightarrow\quad\frac{1}{f(\theta)\,\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta)+\frac{1}{g(\phi)\,\sin^2\theta}\frac{\partial^2}{\partial\phi^2}g(\phi)=-l(l+1).$$

$$\frac{1}{f(\theta)\,\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta)+\frac{1}{g(\phi)\,\sin^2\theta}\frac{\partial^2}{\partial\phi^2}g(\phi)=-l(l+1).$$

Multiplying the equation by $\sin^2\theta$ and rearranging

$$\frac{\sin\theta}{f(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta)+l(l+1)\,\sin^2\theta+\frac{1}{g(\phi)}\frac{\partial^2}{\partial\phi^2}g(\phi)=0.$$

$$\frac{\sin\theta}{f(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta)+l(l+1)\,\sin^2\theta+\frac{1}{g(\phi)}\frac{\partial^2}{\partial\phi^2}g(\phi)=0.$$

Again, the only non–trivial solution such that the sum is zero is if the groups of terms each dependent on a single variable is equal to the same constant. Again using an enlightened choice, we pick m^2 as the separation constant

$$\frac{\sin\theta}{f(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)f(\theta)+l(l+1)\,\sin^2\theta=m^2$$

$$\frac{1}{g(\phi)}\frac{d^2}{d\phi^2}g(\phi)=-m^2$$

that is how the magnetic moment quantum number is introduced

The radial equation

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) - \frac{2mr^2}{\hbar^2}\Big[V(r) - E\Big] = l(l+1)$$

The Polar Angle Equation

$$\frac{\sin\theta}{f(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)f(\theta) + l(l+1)\,\sin^2\theta = m^2$$

The azimuthal angle equation

$$\frac{1}{g(\phi)}\frac{d^2}{d\phi^2}g(\phi) = -m^2$$

The solution to the azimuthal angle equation

$$\frac{1}{g(\phi)}\frac{d^2}{d\phi^2}g(\phi) = -m^2$$

$$g(\phi) = e^{im\phi}$$

$$\Rightarrow \quad g_m(\phi) = e^{im\phi}$$

there are as many solutions as there are allowed values of m

Hint

$$\frac{d^2}{d\phi^2}g_m(\phi) = \frac{d^2}{d\phi^2}e^{im\phi} = \frac{d}{d\phi}(im)e^{im\phi} = (im)^2 e^{im\phi} = -m^2 g_m(\phi).$$

$$\frac{1}{g(\phi)}\frac{d^2}{d\phi^2}g(\phi) = -m^2$$

The solution to the Polar Angle Equation

$$\frac{\sin\theta}{f(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)f(\theta)+l(l+1)\,\sin^2\theta=m^2.$$

$$\sin\theta\,\frac{d}{d\theta}\left(\sin\theta\,\frac{d}{d\theta}\right)f(\theta)+l(l+1)\,\sin^2\theta\,f(\theta)-m^2\,f(\theta)=0.$$

$$\begin{aligned}\sin\theta\,\frac{d}{d\theta}\left(\sin\theta\,\frac{d}{d\theta}\right)f(\theta) &= \sin\theta\,\frac{d}{d\theta}\left(\sin\theta\,\frac{df(\theta)}{d\theta}\right)\\ &= \sin\theta\left(\cos\theta\,\frac{df(\theta)}{d\theta}+\sin\theta\,\frac{d^2f(\theta)}{d\theta^2}\right)\\ &= \sin^2\theta\,\frac{d^2f(\theta)}{d\theta^2}+\sin\theta\,\cos\theta\,\frac{df(\theta)}{d\theta}.\end{aligned}$$

$$\sin^2\theta\,\frac{d^2f(\theta)}{d\theta^2}+\sin\theta\,\cos\theta\,\frac{df(\theta)}{d\theta}+l(l+1)\,\sin^2\theta\,f(\theta)-m^2\,f(\theta)=0.$$

$$\sin^2\theta \frac{d^2 f(\theta)}{d\theta^2} + \sin\theta\cos\theta \frac{d f(\theta)}{d\theta} + l(l+1)\sin^2\theta f(\theta) - m^2 f(\theta) = 0.$$

This is a kind of the associated Legendre equation

The solutions to the associated Legendre equation are the associated Legendre polynomials

$$P_{l,m}(x) = (-1)^m \sqrt{(1-x^2)^m} \frac{d^m}{dx^m} P_l(x)$$

$$P_l(x) = \frac{(-1)^l}{2^l l!} \frac{d^l}{dx^l}(1-x^2)^l.$$

The solutions to the polar angle equation are the associated Legendre polynomials, which are different for each choice of orbital angular momentum and magnetic moment quantum number.

Angular Wave Functions

$$Y_{l,m}(\theta,\phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_{l,m}(\cos\theta)\, e^{im\phi} \qquad m \geq 0$$

$$Y_{l,-m}(\theta,\phi) = Y^*_{l,m}(\theta,\phi), \qquad m < 0$$

the $P_{l,m}(\cos\theta)$ are associated Legendre polynomials

The solution to the Angular Equation

$$l = 0 \qquad Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$l = 1 \qquad Y_{1,\pm 1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\varphi}$$

$$l = 2 \qquad Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\varphi}$$

$$l = 3 \qquad Y_{3,\pm 3} = \sqrt{\frac{35}{64\pi}} \sin^3\theta e^{\pm 3i\varphi}$$

The solution to the Radial Equation

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) - \frac{2mr^2}{\hbar^2}\Big[V(r) - E\Big] = l(l+1)$$

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) - \frac{2\mu r^2}{\hbar^2}\Big[-\frac{e^2}{r} - E\Big] - l(l+1) = 0$$

$$\Rightarrow \quad \frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) - \frac{2\mu r^2}{\hbar^2}\Big[-\frac{e^2}{r} - E\Big]R(r) - l(l+1)\,R(r) = 0$$

$$\Rightarrow \quad \frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) + \Big[\frac{2\mu r^2}{\hbar^2}\frac{e^2}{r} + \frac{2\mu r^2}{\hbar^2}E - l(l+1)\Big]R(r) = 0.$$

The solution to the Radial Equation

$$y_j^k(x) = e^{-x/2} x^{(k+1)/2} L_j^k(x)$$

k = 2l + 1,
(k + 1)/2 = l + 1,
j + l + 1 = n

Radial Wave Functions

$$R_{n,l}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}} e^{-r/na_0} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)$$

The solution to the Radial Equation

$$
\begin{aligned}
R_{10} &= 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0} \\
R_{21} &= \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0} \\
R_{20} &= 2\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(1-\frac{Zr}{2a_0}\right) e^{-Zr/2a_0} \\
R_{32} &= \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0} \\
R_{31} &= \frac{4\sqrt{2}}{3}\left(\frac{Z}{3a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right)\left(1-\frac{Zr}{6a_0}\right) e^{-Zr/3a_0} \\
R_{30} &= 2\left(\frac{Z}{3a_0}\right)^{\frac{3}{2}}\left(1-\frac{2Zr}{3a_0}+\frac{2(Zr)^2}{27a_0^2}\right) e^{-Zr/3a_0}
\end{aligned}
$$

The First Seven Laguerre Polynomials

Laguerre polynomials are solutions to the Laguerre equation

$$
\begin{aligned}
L_0(x) &= 1 \\
L_1(x) &= -x + 1 \\
L_2(x) &= x^2 - 4x + 2 \\
L_3(x) &= -x^3 + 9x^2 - 18x + 6 \\
L_4(x) &= x^4 - 16x^3 + 72x^2 - 96x + 24 \\
L_5(x) &= -x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120 \\
L_6(x) &= x^6 - 36x^5 + 450x^4 - 2400x^3 + 5400x^2 - 4320x + 720
\end{aligned}
$$

Associated Laguerre polynomials can be calculated from Laguerre polynomials using the generating function

$$L_j^k(x) = (-1)^k \frac{d^k}{dx^k} L_{j+k}(x)$$

Some Associated Laguerre Polynomials.

Associated Laguerre polynomials can be calculated from Laguerre polynomials using the generating function

$$L_j^k(x) = (-1)^k \frac{d^k}{dx^k} L_{j+k}(x)$$

$$L_0^0(x) = L_0(x)$$
$$L_1^0(x) = L_1(x)$$
$$L_1^1(x) = -2x + 4$$
$$L_0^1(x) = 1$$
$$L_2^0(x) = L_2(x)$$
$$L_2^1(x) = 3x^2 - 18x + 18$$
$$L_2^2(x) = 12x^2 - 96x + 144$$
$$L_1^2(x) = -6x + 18$$

$$L_0^2(x) = 2$$
$$L_3^0(x) = L_3(x)$$
$$L_3^1(x) = -4x^3 + 48x^2 - 144x + 96$$
$$L_2^3(x) = 60x^2 - 600x + 1200$$
$$L_3^3(x) = -120x^3 + 2160x^2 - 10800x + 14400$$
$$L_3^2(x) = -20x^3 + 300x^2 - 1200x + 1200$$
$$L_1^3(x) = -24x + 96$$
$$L_0^3(x) = 6$$

Schrodinger equation for Hydrogen-like Atom

n	ℓ	m_ℓ	$F(\phi)$	$P(\theta)$	$R(r)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}\, a_0^{3/2}}\left[2 - \frac{r}{a_0}\right] e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$
2	1	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$

Schrodinger equation for Hydrogen-like Atom

n	ℓ	m_ℓ		$\psi_{n\,\ell\,m_\ell}(r, \theta, \phi)$
1	0	0	1s	$\frac{1}{\sqrt{\pi}\, a_0^{3/2}} e^{-r/a_0}$
2	0	0	2s	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}} \left[2 - \frac{r}{a_0}\right] e^{-r/2a_0}$
2	1	0	2p	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta$
2	1	±1	2p	$\frac{1}{8\sqrt{\pi}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \sin\theta\, e^{\pm i\phi}$

$$a_0 = \frac{\hbar^2}{me^2} = .0529 \text{ nm} = \text{first Bohr radius}$$

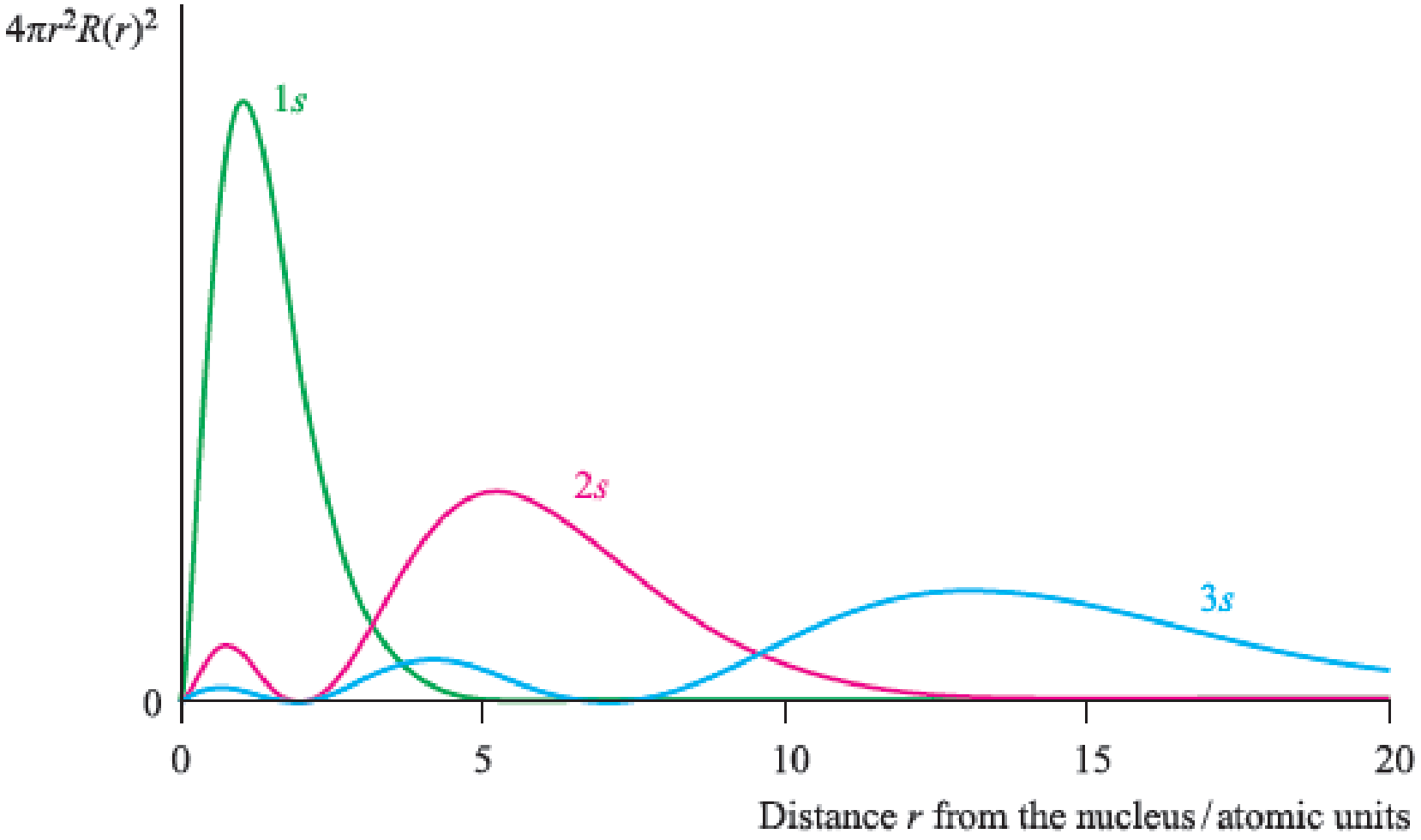
Schrodinger equation for Hydrogen-like Atom

n	ℓ	m_ℓ	$F(\phi)$	$P(\theta)$	$R(r)$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}\,a_0^{3/2}}\left[27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right]e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{4}{81\sqrt{6}\,a_0^{3/2}}\left[6 - \frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/3a_0}$
3	1	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{4}{81\sqrt{6}\,a_0^{3/2}}\left[6 - \frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/3a_0}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4}(3\cos^2\theta - 1)$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$
3	2	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{15}}{2}\sin\theta\cos\theta$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$
3	2	±2	$\frac{1}{\sqrt{2\pi}}e^{\pm i2\phi}$	$\frac{\sqrt{15}}{4}\sin^2\theta$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$

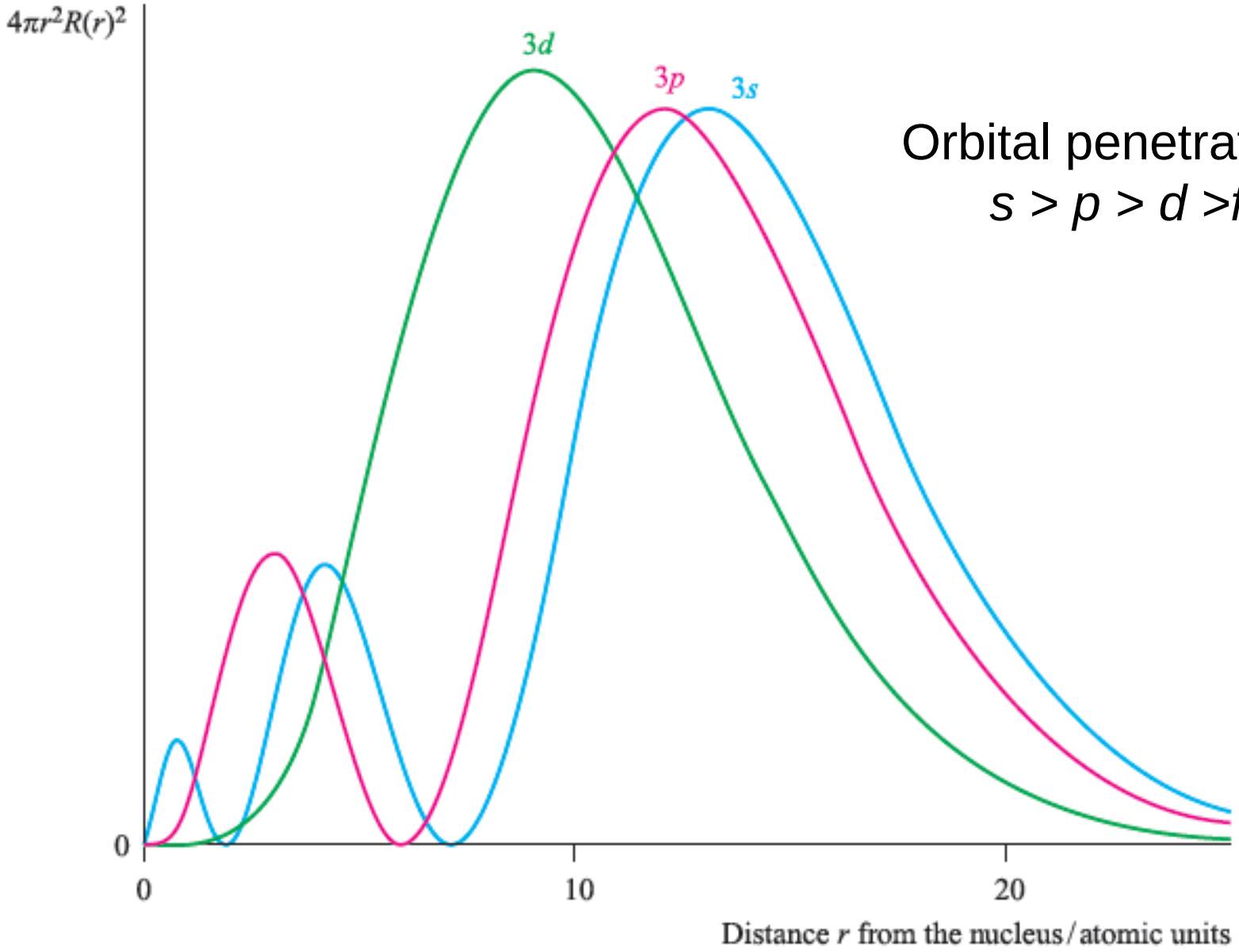
Schrodinger equation for Hydrogen-like Atom

n	ℓ	m_ℓ		$\psi_{n\,\ell\,m_\ell}(r, \theta, \phi)$
3	0	0	3s	$\frac{1}{81\sqrt{3\pi}\,a_0^{3/2}}\left[27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right]e^{-r/3a_0}$
3	1	0	3p	$\frac{\sqrt{2}}{81\sqrt{\pi}\,a_0^{3/2}}\left[6 - \frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/3a_0}\cos\theta$
3	1	±1	3p	$\frac{\sqrt{2}}{81\sqrt{\pi}\,a_0^{3/2}}\left[6 - \frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/3a_0}\sin\theta\, e^{\pm i\phi}$
3	2	0	3d	$\frac{1}{81\sqrt{6\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}(3\cos^2\theta - 1)$
3	2	±1	3d	$\frac{1}{81\sqrt{\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin\theta\cos\theta\, e^{\pm i\phi}$
3	2	±2	3d	$\frac{1}{162\sqrt{\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin^2\theta\, e^{\pm i2\phi}$

Distribution of Radial Probability density



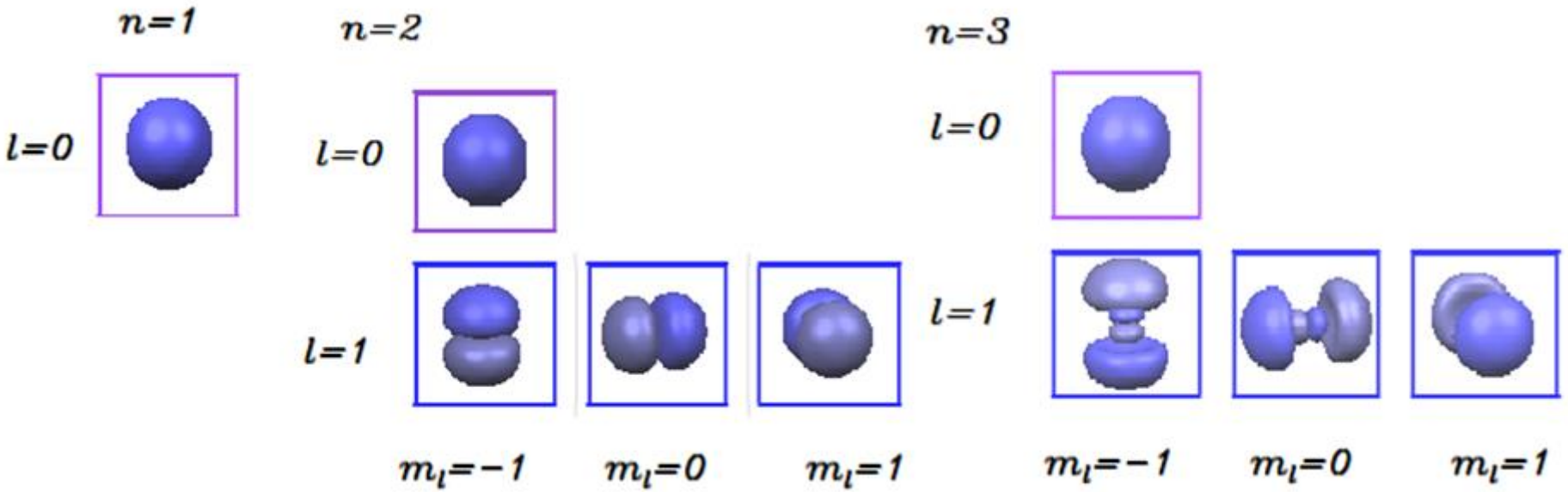
Distribution of Radial Probability density



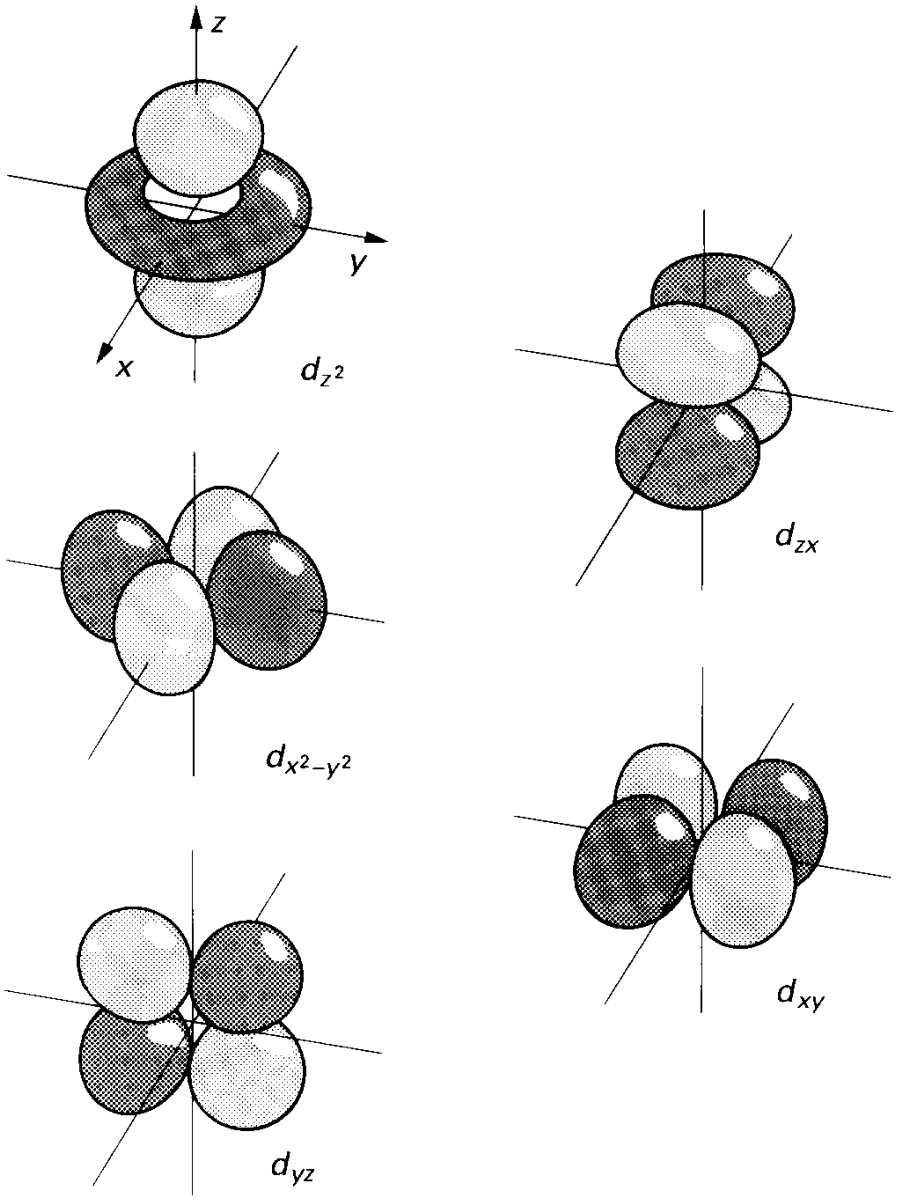
Orbital penetration:

s > *p* > *d* >*f*

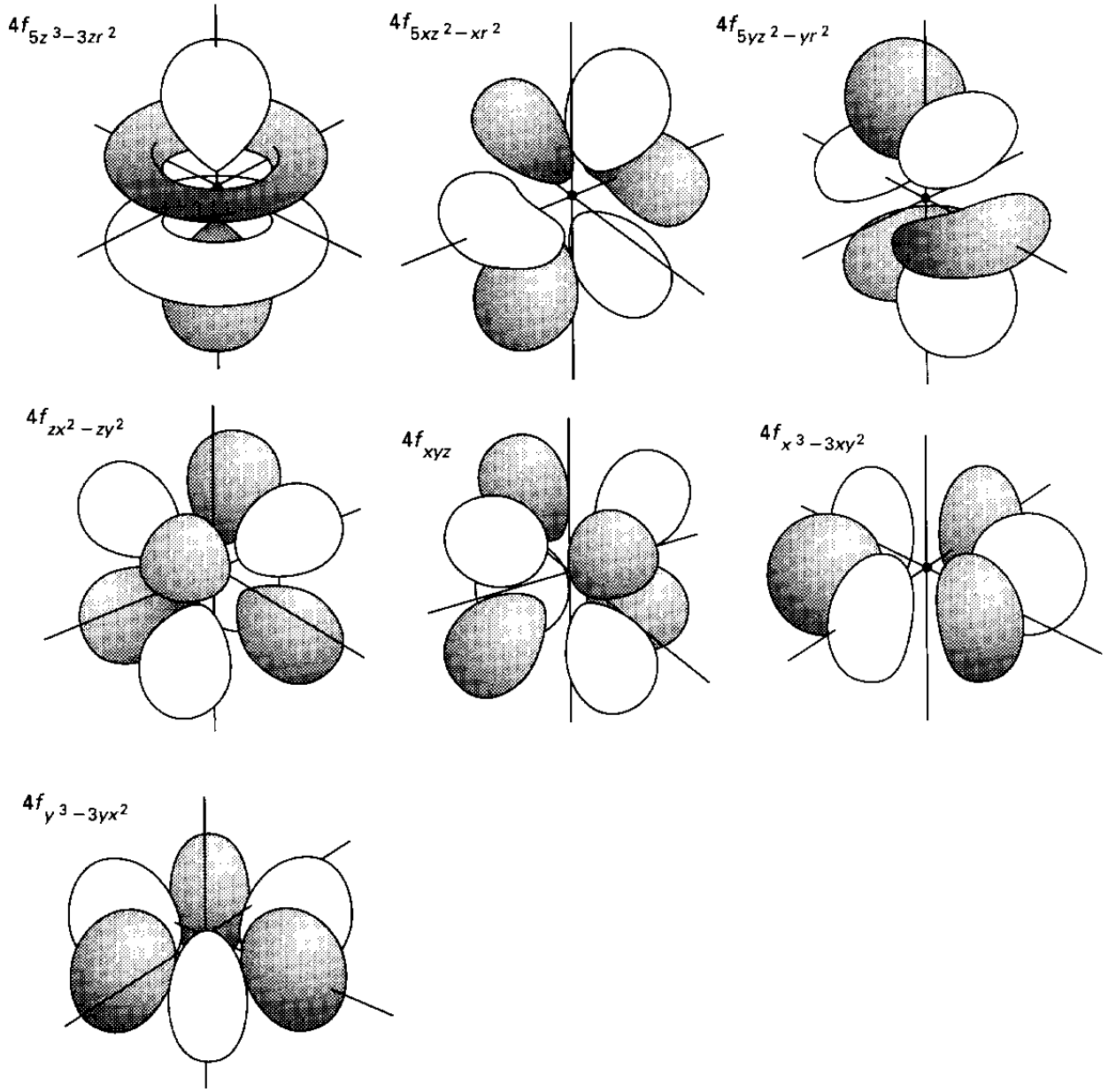
s & p-type Orbitals



d -type Orbitals



f -type Orbitals



Electronics Engineering

1. What are the conditions for which a wave function will be acceptable ?
2. Using Planck distribution of energy spectral density for blackbody radiation, show that at room temperature the proportion of blue light (λ = 450 nm) in comparison to red light (λ = 700 nm) is insignificant.

$$\rho(\lambda, T) = \frac{8\pi hc}{\lambda^5 (e^{hc/\lambda kT} - 1)}$$

3. Evaluate the kinetic energy of the particle with wavefunction, where χ (chi) is a parameter.

$$\psi = (cos\chi)e^{ikx} + (sin\chi)e^{-ikx}$$

4. Determine the probability of finding particle in an 1D box from 0.25L to 0.5L for n=2 , L= 710 pm. Predict the probability from Classical Physics Standpoint.

Information Technology

1. State the postulates of quantum chemistry.
2. Calculate the wavelength of a neutron with a translational kinetic energy equal to kT at 300 K.
3. What is the uncertainty in position of a projectile (1.0 g) moving with a speed 1 μms^{-1}.
4. Write down the Hamiltonian operator of He_2 molecule.
5. Calculate kinetic energy for a particle in an 2D box for n_x=n_y= 1, L_x = L_y = 288 pm. Draw the wavefunction for the particle confined in this square well (2D box).