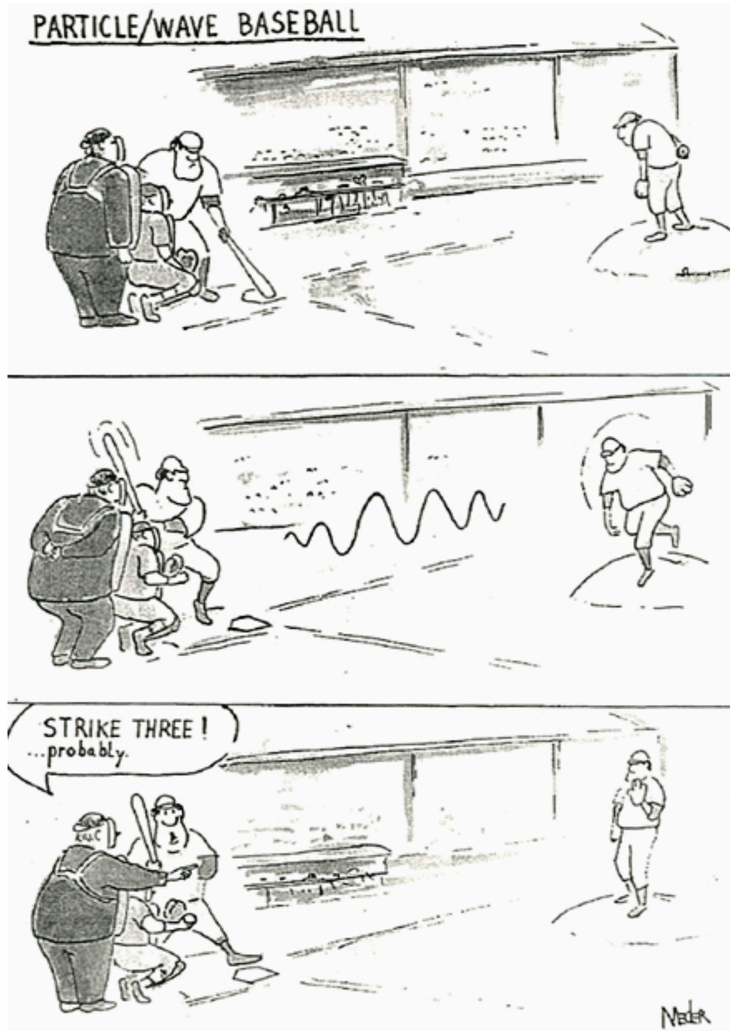

PARTICLE/WAVE BASEBALL
STRIKE THREE! ...probably.

Schrödinger's Wave Equation

Wave Mechanics --1926

An electron is described by a wave function $\Psi(x,t) = \psi(\mathrm{x})\phi(\mathrm{t})$

which satisfies Schrodinger's equation :

$$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t} \qquad (1)$$

where $\hbar$ is the reduced Planck constant, m is electron mass, and $V(x)$ is a potential function.

$\Psi(x,t)$ is positive - definite and single valued. Further, $\left|\Psi(x,t)\right|^2$ is a probability density function, hence

$$\int_{\mathrm{x}}^{\mathrm{x+dx}} \left|\psi(\mathrm{x})\right|^2 \mathrm{dx} = \text{the probability of finding the electron between x and x + dx}$$

Hence $\int_0^{\infty} \left|\psi(\mathrm{x})\right|^2 \mathrm{dx} = 1$.

Substituting $\Psi(x,t) = \psi(\mathrm{x})\phi(t)$ in (1) results in

$$\phi(t) = \mathrm{e}^{-i\frac{E}{\hbar}t} = \mathrm{e}^{-i\omega t}$$

hence $E = \hbar\omega$.

Schrödinger's Time Independent Wave Equation

$$\left[\frac{\partial^2}{\partial x^2} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\right]\psi(x) = 0$$

- Solve for free particle moving in +x

$$\left[\frac{\partial^2}{\partial x^2} + \frac{2mE}{\hbar^2}\right]\psi(x) = 0$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -k^2\psi(x), \text{ where } k^2 = \frac{2mE}{\hbar^2}.$$

Solution is:

$$\psi(x,t) = A\exp\left[i\left(kx - \omega t\right)\right]$$

with wave number $k = \dfrac{2\pi}{\lambda}$

where λ is the wavelength.

$Note: \lambda = \dfrac{h}{p}$ where p is the momentum.

So, electron has wavelength $\lambda = \dfrac{h}{\sqrt{2mE}}$

known as deBroglie wavelngth.

So, electron is a plane wave with

$$\psi(x,t)\psi^*(x,t) = AA^*$$

A constant!.... (exists everywhere in space)

But this means that momentum is well defined

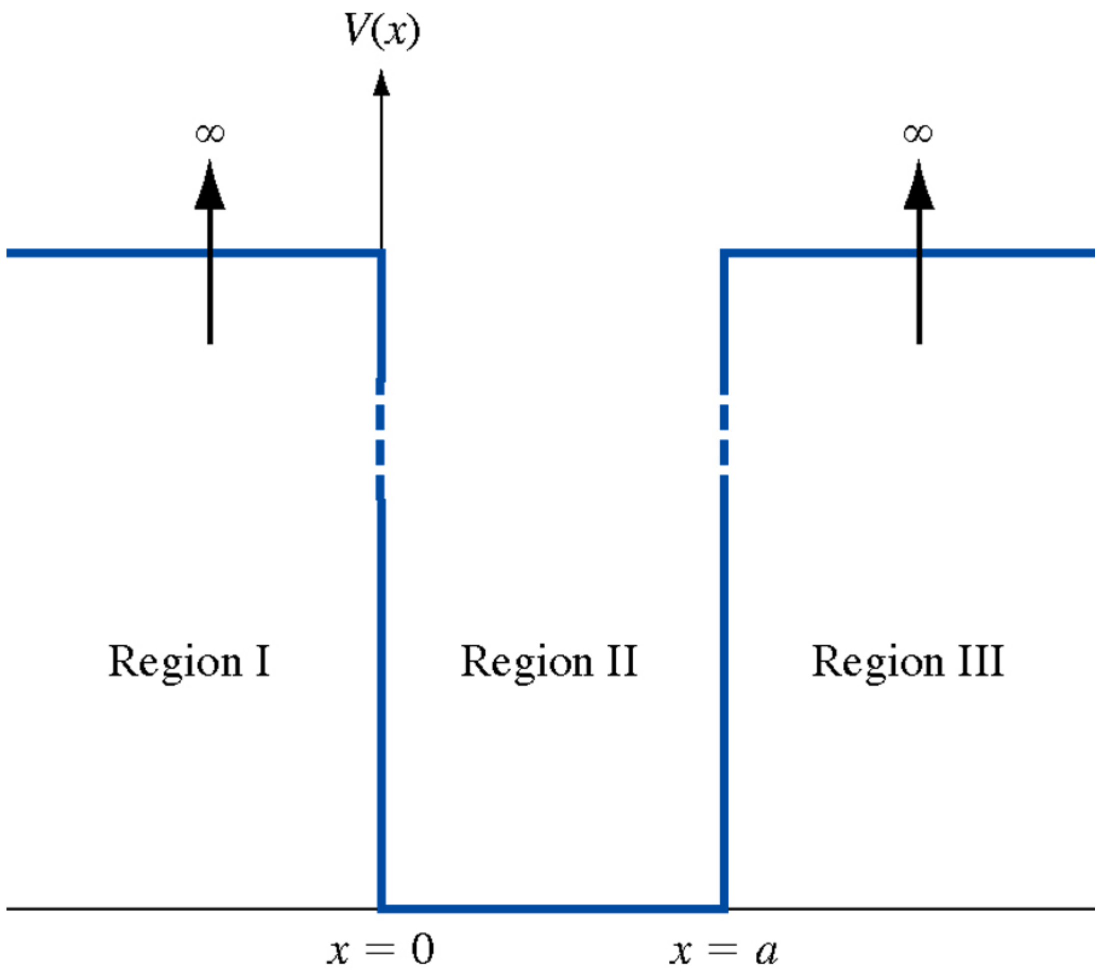
And this leads to the notion of a wave packet

Wave Packet

$$\Psi(z,t) = \int_{-\infty}^{+\infty} a(k - k_0) e^{z - z_0} e^{-i\omega(k)t} dk$$

Describes a particle near z_0 with momentum near hk

2. Infinite Well



Schrödinger's Wave Equation

ψ = 0 outside the well (regions I, III)

ψ and its derivative are continuous

$$\left[\frac{\partial^2}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - V(x)\right)\right]\psi(x) = 0$$

For the infinite well, solution is

$$\psi(x) = A_1 \cos(kx) + A_2 \sin(kx)$$

$$where \quad k = \sqrt{2m_0 E/\hbar^2}$$

Use boundary conditions @ x = *0*, and *a*

$$\text{at x} = 0,\ A_1 \cos(0) + A_2 \sin(0) = 0 \Rightarrow A_1 = 0$$

$$\text{at x} = \text{a},\ A_2 \sin(ka) = 0 \Rightarrow ka = n\pi$$

$$hence \quad k = k_n = n\frac{\pi}{a} = \sqrt{2m_0 E_n/\hbar^2};\ and$$

$$E_n = n^2 \frac{\pi^2\hbar^2}{2m_0 a^2}$$

Energy and momentum are both quantized

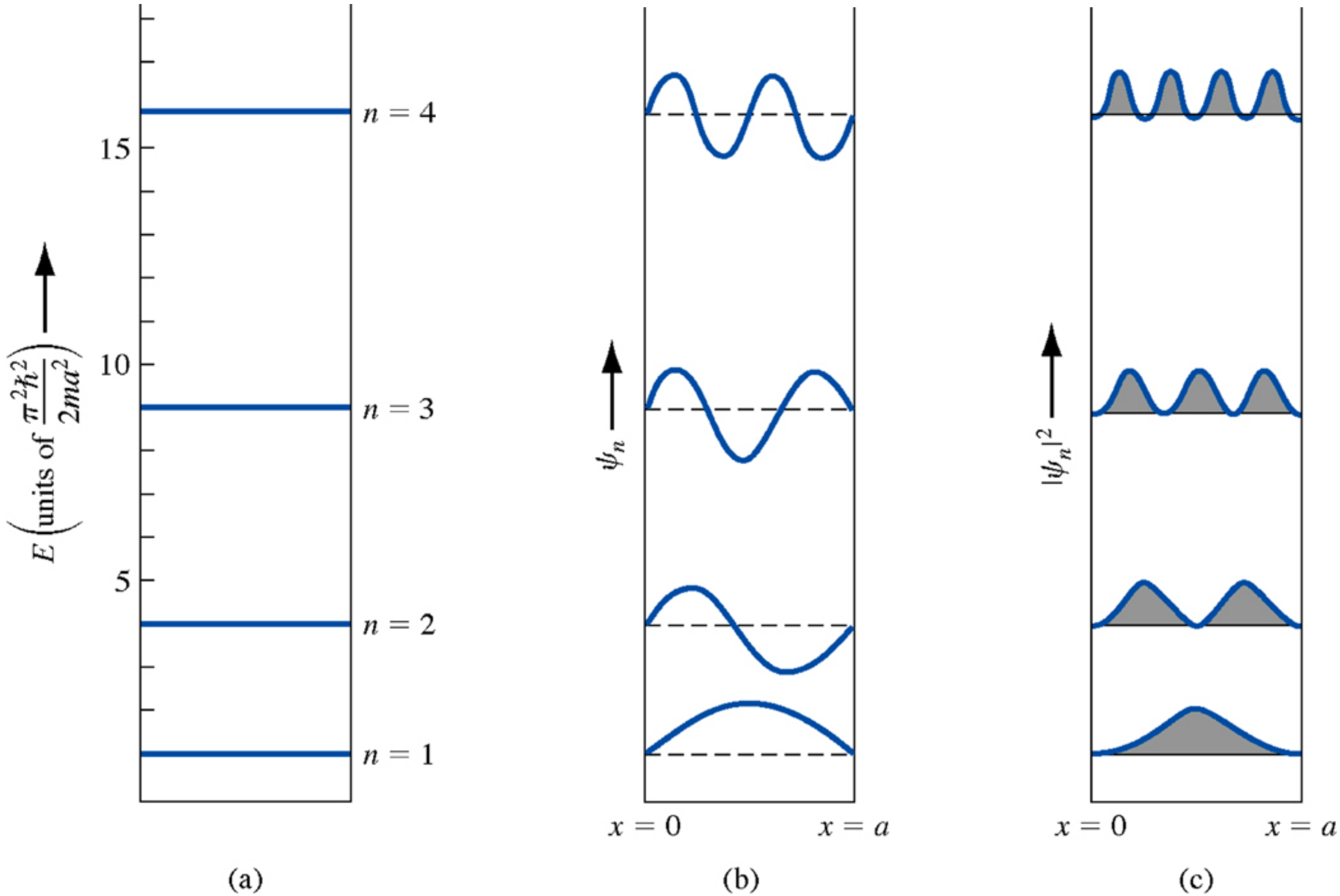
Normalize to get A_1

$$\int_0^\infty |\psi(x)|^2 = \int_0^\infty \psi^*(x)\psi(x)dx = 1$$

$$\int_0^a A_2^2 \sin^2(k_n x)dx = \frac{A_2^2}{2}\int_0^a \left(1 - \cos\left(2k_n x\right)\right)dx = 1$$

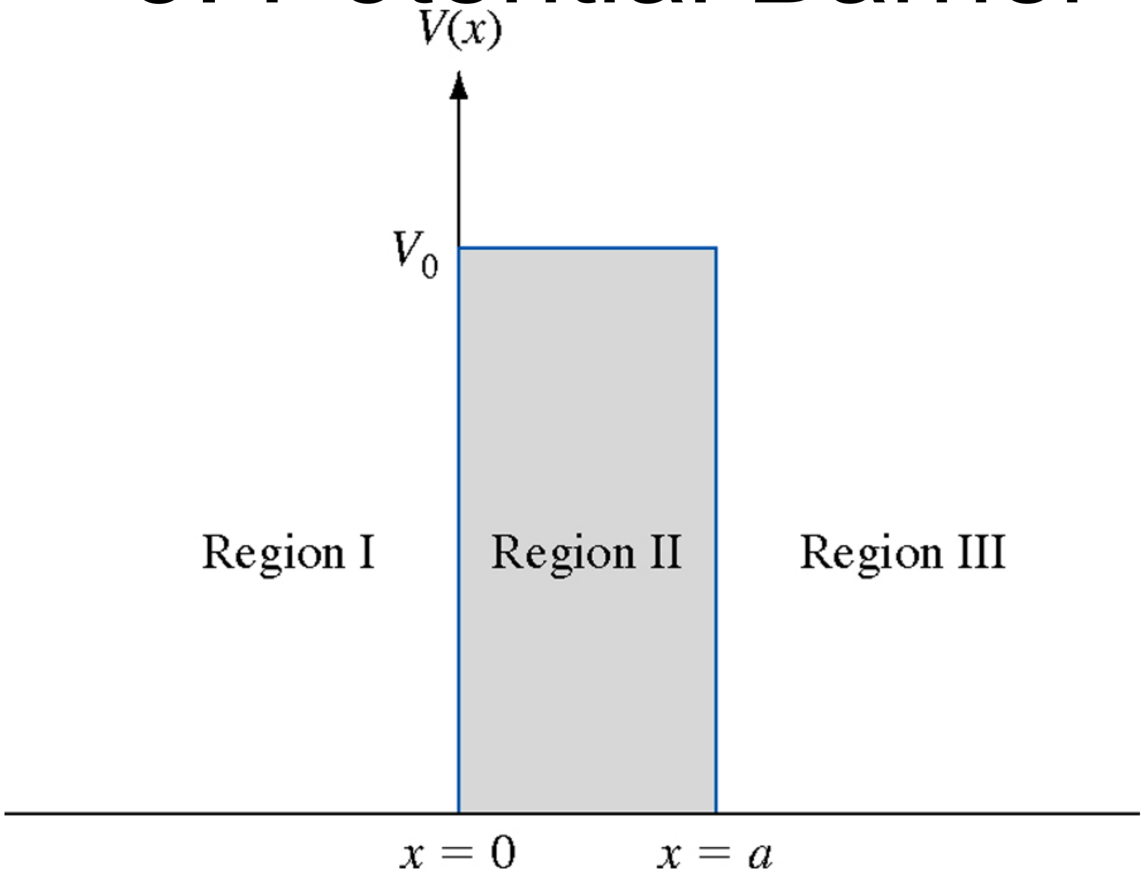
Resulting in

$$\psi(x) = \sqrt{\frac{2}{a}}\sin(k_n x)$$

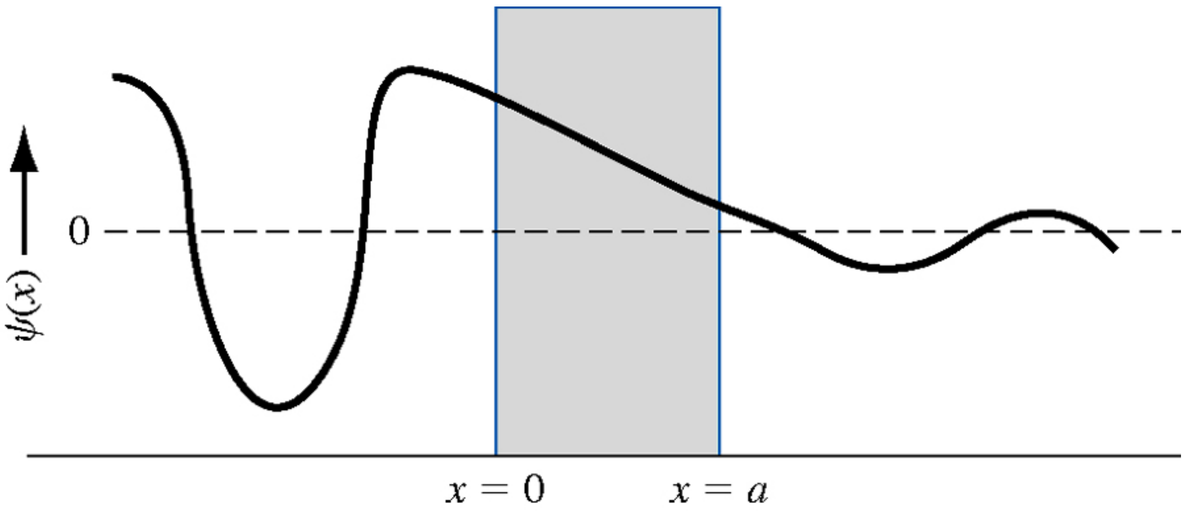


$E\left(\text{units of } \frac{\pi^2\hbar^2}{2ma^2}\right)$
15
10
5
$n = 4$
$n = 3$
$n = 2$
$n = 1$
ψ_n
$|\psi_n|^2$
$x = 0$
$x = a$
$x = 0$
$x = a$
(a)
(b)
(c)

3. Potential Barrier



Electron Wave Function



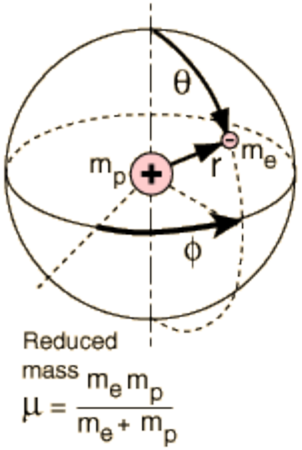
$$\text{Transmission Coefficient } T \approx 16\left(\frac{E}{V_0}\right)\left(1-\frac{E}{V_0}\right)\exp(-2k_2 a)$$

4. Hydrogen Atom

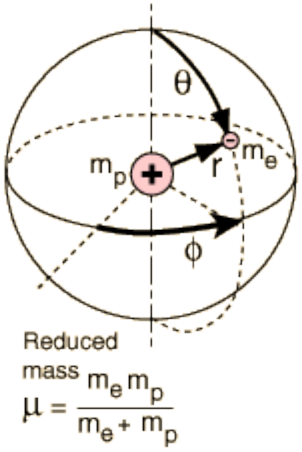
- The electron in the hydrogen atom sees a spherically symmetric potential, so it is logical to use spherical polar coordinates to develop the Schrodinger equation.

The potential energy is simply that of a point charge:

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



- **Hydrogen Schrödinger Equation**
- Coordinate System:



- The expanded form of the Schrödinger equation is:

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

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

- Solving it involves separating the variables into the form

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

$$\Psi(r,\theta,\phi) = R_n(r)P_l(\theta)F_{m_l}(\phi)$$

n	**l**	$\mathbf{m_l}$
Principal Quantum Number	Orbital Quantum Number	Magnetic Quantum Number

Electron Energy is derived as

$$E_n = -\frac{m_0 e^4}{(4\pi\varepsilon_0)^2 2\hbar^2 n^2}$$

The 3 quantum numbers are:

$n = 1, 2, 3, \ldots$

$l = n-1, n-2, n-3, \ldots, 0$

$|m| = l, l-1, \ldots, 0$

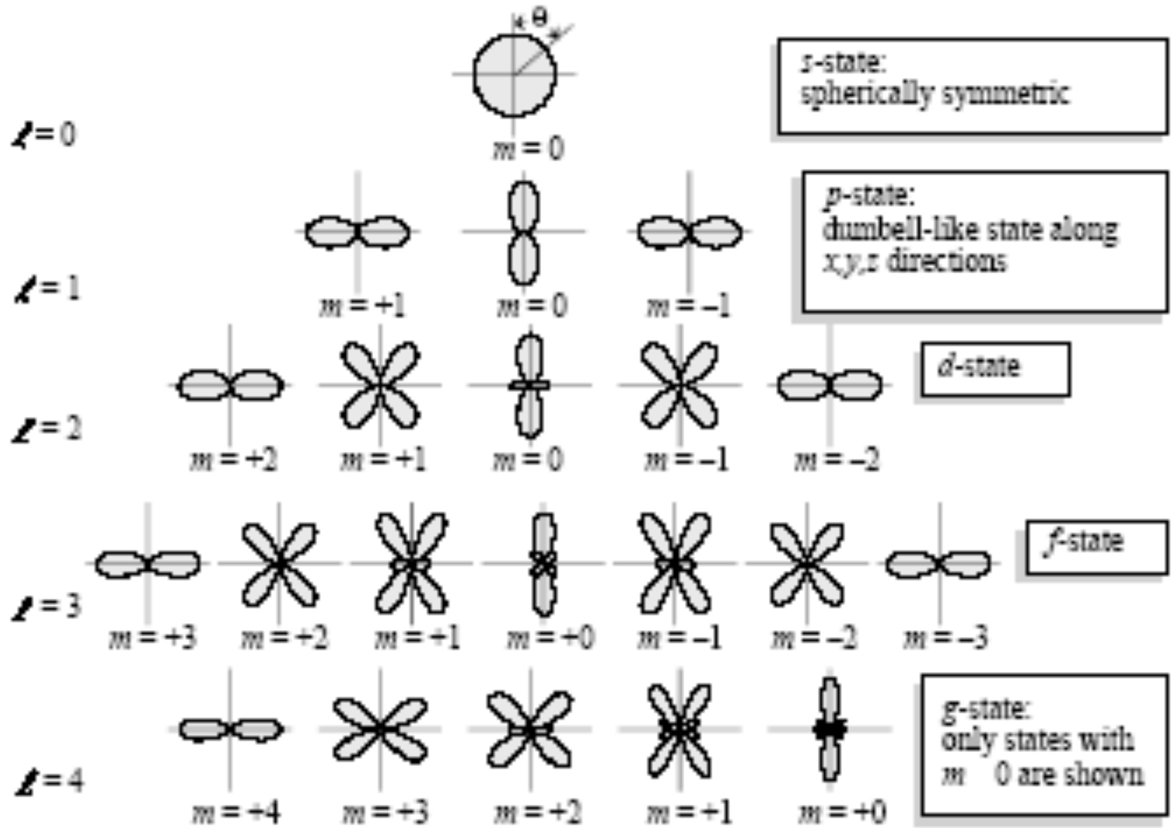
Spin is the 4th quantum number.

There is one electron state for each set of 4 quantum numbers

Nature of atomic functions:

These are important, since the cell periodic part of Block states is often made up of atomic-like states

- $\ell=0$: angular momentum is zero; called *s*-state
- $\ell=1$: angular momentum is one ($\hbar$); called *p*-state



A plot of the probability density function of electronic states in an atom as a function of the angle θ for the
s, p, d, f, g electrons.

IV Semiconductors

C $1s^2\underbrace{2s^2 2p^2}$

Si $1s^2 2s^2 2p^6 \underbrace{3s^2 3p^2}$

Ge $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} \underbrace{4s^2 4p^2}$

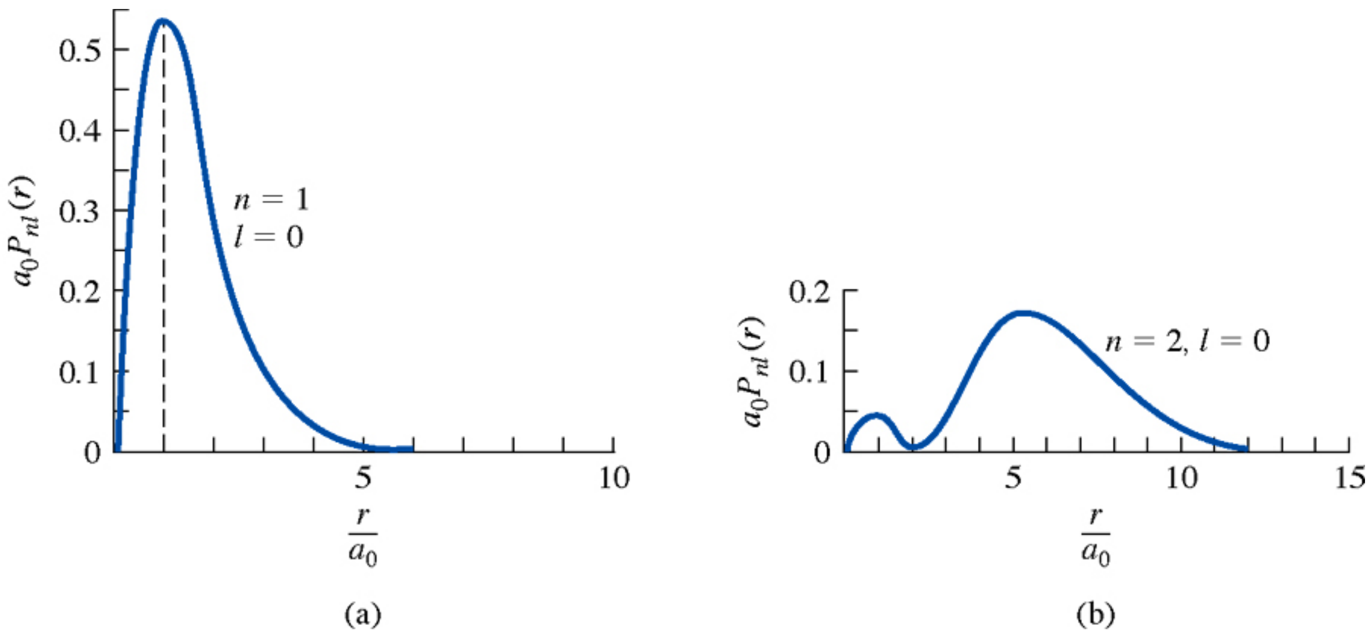
III-V Semiconductors

Ga $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} \underbrace{4s^2 4p^1}$

As $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} \underbrace{4s^2 4p^3}$

Outermost atomic levels are either s-type or p-type.

Radial Probability Density Function for a hydrogen atom



$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_0e^2} = 0.529\,\dot{A}$$