Chapter II:
Quantum physics

Contents

Introduction (1)

- Quantum mechanics is a fundamental theory in physics → describes nature and explain properties of microscopic molecules, atoms and subatomic particles
- Small objects have characteristics of both particles and waves
- Work of Planck in 1900 (analyzing blackbody radiation) and Einstein in 1905 (analyzing the photoelectric effect) → light energy is delivered not smoothly and continuously as a wave but instead in concentrated bundles or « quanta »
- In 1924 de Broglie postulated that associated with a « particle » moving with momentum p is a « wave » of wavelength $\lambda = h/p$ (h = Planck's constant) → λ = de Broglie wavelength

Introduction (2)

- Probabilistic character of quantum mechanics → results of measurements are given as a collection of possibilities → each of them associated to a given probability
- The goal of quantum physics is to explain and foresee the evolution in time of a physical system (collection of particles)
- Principles of quantum mechanics are expressed in a series of postulates

- Remarks : in general cases → kinetic energy of particles is much smaller than rest energy → nonrelativistic quantum mechanics

Postulates (1)

First postulate:

At each instant the state of a physical system is represented by a ket $|\psi>$ in the space of states

Comments:

- The space of states is a vector space
- The space of states includes the concept of inner product → the inner product associates a complex number to any two states →

$$(|\psi\rangle\,,|\phi\rangle) \equiv \langle\psi|\phi\rangle = \int dx \psi^*(x)\phi(x)$$

- A function *f*(*x*) can be evaluated in the $|\psi>$ system → expectation value of *f* →

$$\langle\psi|f|\psi\rangle = \int dx \psi^*(x) f(x) \psi(x)$$

Postulates (2)

Second postulate:

Every observable attribute of a physical system is described by an operator that acts on the kets that describe the system

Comments:

- By convention an operator *A* acting on a ket $|\psi>$ is denoted by left multiplication →

$$A : |\psi\rangle \to |\psi'\rangle = A\,|\psi\rangle$$

- In the context of wave-mechanics → state is replaced by wavefunction ψ(x) → example of momentum operator (1D) $p = -i\hbar d/dx$ →

$$p\,|\psi\rangle = p\psi(x) = -i\hbar\frac{d\psi(x)}{dx}$$

Postulates (3)

Third postulate:

The only possible result of the measurement of an observable A is one of the eigenvalues of the corresponding operator A

Comments:

- Origin of the word « quantum »
- For every operator → there are special states that are not changed by the action of an operator (except for being multiplied by a constant) → they are the eigenstates and the constant numbers are the eigenvalues of the operator:

$$A\,|\psi_a\rangle = a\,|\psi_a\rangle$$

Postulates (4)

Fourth postulate:

When a measurement of an observable *A* is made on a state $|\psi>$ the probability of obtaining an eigenvalue a_n is given by the square of the inner product of $|\psi>$ with the eigenstate $|a_n>$

$\rightarrow |<a_n|\psi>|^2$

Comments:

- The states are (normally) assumed to be normalized to unity $\rightarrow$ $|<\psi|\psi>|$ = 1 and $|<a_j|a_k>| = \delta_{jk}$
- The complex number $|<a_n|\psi>|$ is known as the « probability amplitude » or « amplitude » to measure a_n as the value for *A* in the state $|\psi>$

Postulates (5)

Fifth postulate:

Immediately after the measurement of an observable A has yielded a value a_n, the state of the system is the normalized eigenstate $|a_n>$

Comments:

- This is known as the « collapse of the wavepacket »

Postulates (6)

Sixth postulate:

The state $|\psi(t)>$ of each non-relativistic quantum system is a solution of the Schrödinger equation depending on the time →

$$i\hbar\frac{d}{dt}\left|\psi(t,\boldsymbol{r})\right\rangle = H\left|\psi(t,\boldsymbol{r})\right\rangle$$

Comments:

– *H* is the Hamiltonian operator → it represents the total energy of the particle of mass *m* in the potential field *V* → time-independent or stationary Schrödinger equation →

$$H\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}) \quad \text{with}$$

$$H = -\frac{\hbar^2}{2m}\Delta\Psi + V(\boldsymbol{r})$$

Problems in one dimension: Free particle (1)

- No forces → *V*(*x*) = 0 →

$$H\psi(x) = E\psi(x)$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

$$\Rightarrow \psi(x) = Ae^{ikx} + Be^{-ikx} \Leftrightarrow \psi(x) = C\sin kx + D\cos kx$$

$$k^2 = \frac{2mE}{\hbar^2}$$

A, *B*, *C* and *D* are constants

- First term exp → wave travelling in the positive *x* direction
- Second term exp → wave travelling in the negative *x* direction

Problems in one dimension: Free particle (2)

- Intensities of the waves are given by $|A|^2$ and $|B|^2$

- No boundary conditions → no restrictions on the energy E → all values of E give solutions to the equation

- No convergence at $+\infty$ or $-\infty$ → normalization condition cannot be applied in this case

- Different normalization system → source such as an accelerator located at $x = -\infty$ emitting particles at a rate I (particles s^{-1}) with momentum $p = \hbar k$ in the positive x direction → particles traveling in the positive x direction → $B = 0$ → particle current $j = (\hbar k/m)|A|^2$

Problems in one dimension: Step potential $E > V_0$ (1)

$$\begin{aligned} V(x) &= 0 \quad x < 0, \text{ region } 1 \\ &= V_0 \quad x > 0, \text{ region } 2 \end{aligned}$$

with $V_0 > 0$

- For $x < 0$ → as free particle with $k = k_1 = (2mE/\hbar)^{1/2}$
- For $x > 0$ →

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \qquad k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$$

- Boundary conditions give → $A+B = C+D$ and $k_1(A-B) = k_2(C-D)$
- Particle comes from source at $x = -\infty$ → A term represents the incident wave / B term is the reflected wave / C term is the transmitted wave / $D = 0$ (no possibility of reflection after the step)

Problems in one dimension: Step potential $E > V_0$ (2)

- Reflection coefficient or probability →

$$R = \frac{|B|^2}{|A|^2} = \left(\frac{1 - k_2/k_1}{1 + k_2/k_1}\right)^2$$

- Transmission coefficient

$$T = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2} = \frac{4k_2/k_1}{(1 + k_2/k_1)^2}$$

- Application in nucleon-nucleon scattering problems

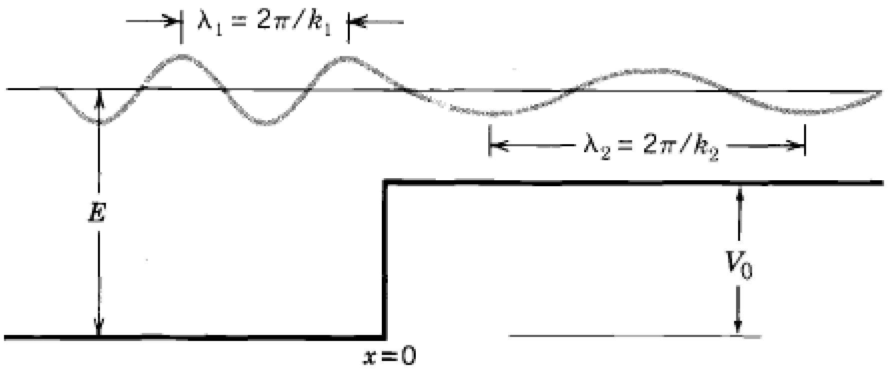


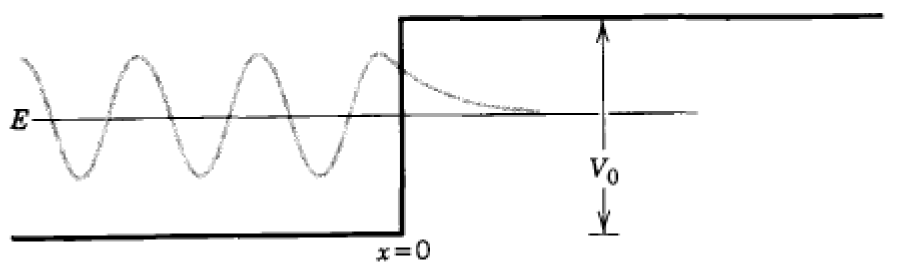
Image taken from: K.S. Krane, *Introductory Nuclear Physics*, Wiley, Oboken, 1988

Problems in one dimension: Step potential $E < V_0$

- In region 2 →

$$\psi_2(x) = Ce^{k_2 x} + De^{-k_2 x} \qquad k_2^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

- As first term $\rightarrow\ \infty$ for $x \rightarrow \infty$ → $C = 0$
- Important difference compared to classical mechanics → All classical particles are reflected at the boundary ↔ the quantum mechanical wave packet can penetrate a short distance into the forbidden region



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Problems in one dimension: Barrier potential $E > V_0$ (1)

$$\begin{aligned} V(x) &= 0 \quad x < 0, \text{ region 1} \\ &= V_0 \quad 0 \geq x \geq a, \text{ region 2} \\ &= 0 \quad x > a, \text{ region 3} \end{aligned}$$

Solutions in regions 1, 2 and 3 →

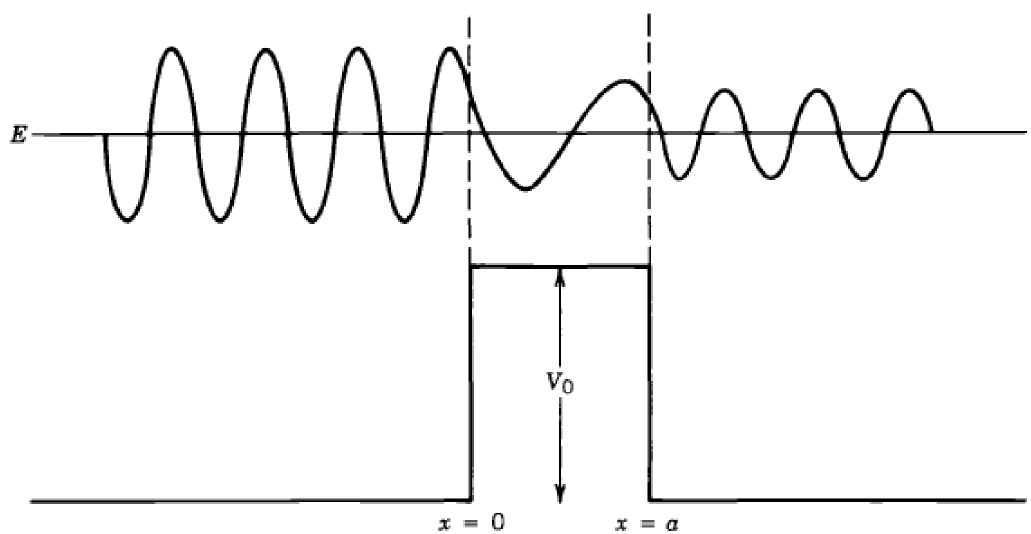
$$\begin{aligned} \psi_1(x) &= Ae^{ik_1 x} + Be^{-ik_1 x} \\ \psi_2(x) &= Ce^{ik_2 x} + De^{-ik_2 x} \\ \psi_3(x) &= Fe^{ik_3 x} + Ge^{-ik_3 x} \end{aligned}$$

$$k_1^2 = k_3^2 = \frac{2mE}{\hbar^2} \qquad k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$$

Problems in one dimension: Barrier potential $E > V_0$ (2)

- We use continuity conditions at $x = 0$ and at $x = a$
- We assume particles coming from $x = -\infty \rightarrow G = 0$
- After calculations → transmission coefficient becomes

$$T = \left(1 + \frac{1}{4}\frac{V_0^2}{E(E-V_0)}\sin^2 k_2 a\right)^{-1}$$



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Problems in one dimension: Barrier potential $E < V_0$ (1)

- Expressions in region 1 and 3 are identical and in region 2 →

$$\psi_2(x) = Ce^{k_2 x} + De^{-k_2 x} \qquad k_2^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

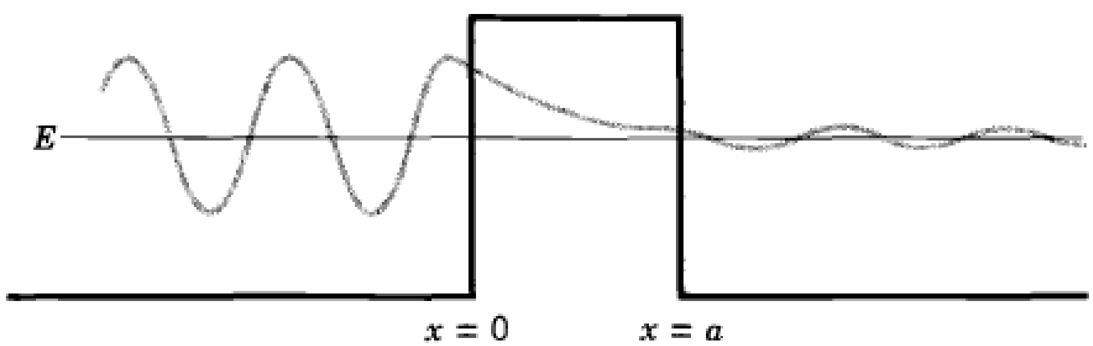
- As x varies between 0 and a in region 2 → C and $D \neq 0$
- After calculations → transmission coefficient becomes

$$T = \left(1 + \frac{1}{4}\frac{V_0^2}{E(V_0 - E)}\sinh^2 k_2 a\right)^{-1}$$

- Classically $T = 0$ → the particle is not permitted to enter the forbidden region (negative kinetic energy) ↔ the quantum wave can penetrate the barrier → nonzero probability to find the particle beyond the barrier.

Problems in one dimension: Barrier potential $E > V_0$ (2)

- This phenomenon is called barrier penetration or quantum mechanical tunneling or tunnel effect
- Important applications in nuclear physics → α decay and fission



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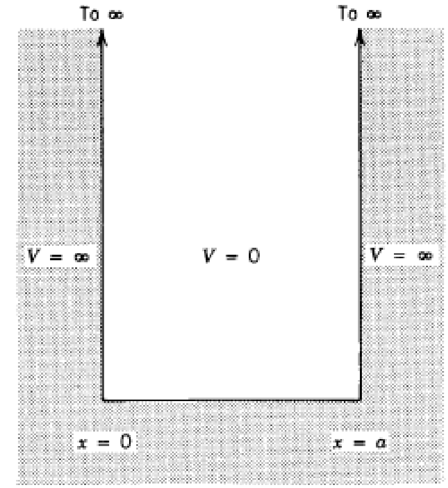
1D problem: Infinite well (1)

$$V(x) = \infty \quad x < 0,\, x > a$$
$$ = 0 \quad 0 \leq x \leq a$$



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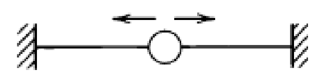


- The walls are absolutely impenetrable → particle is trapped between *x* = 0 and *x* = *a*
- Inside the solution of the Schrödinger equation is →
$$\psi(x) = A \sin kx + B \cos kx$$
- Continuity condition at *x* = 0 → ψ(0) = 0 → true only for *B* = 0
- At *x* = *a* → the continuity condition gives →

$$A \sin kx = 0$$

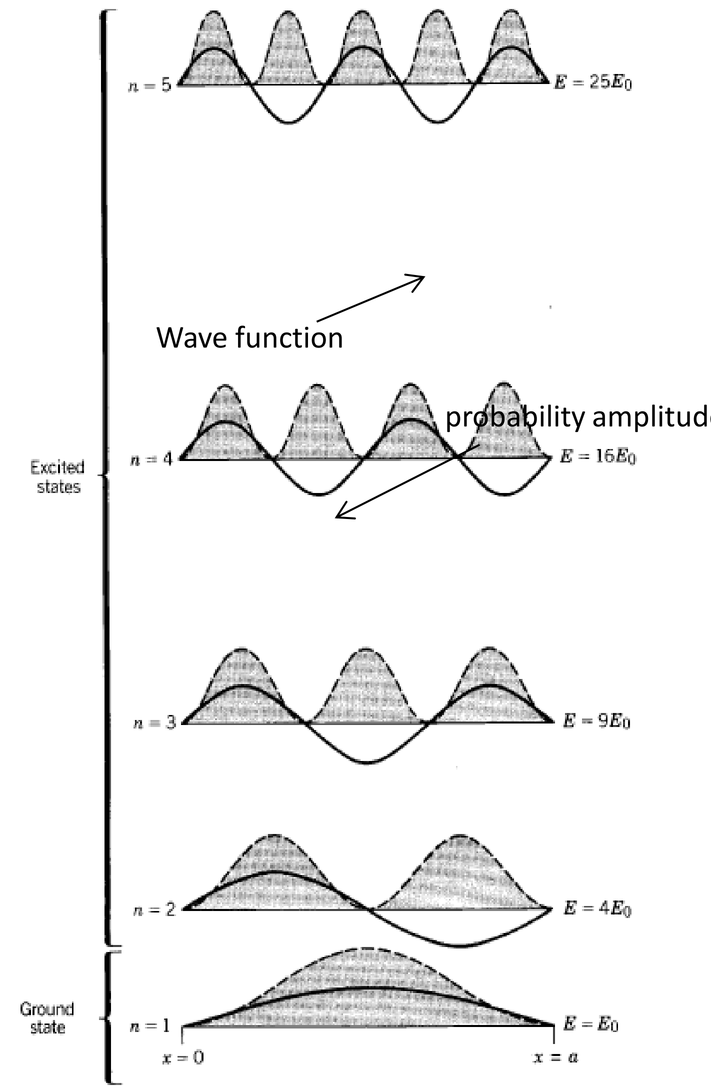
1D problem: Infinite well (2)

- As $A = 0$ is not acceptable → $\sin ka = 0$ → $ka = n\pi$ for $n = 1,2,3,\ldots$
- Quantification condition on energy →

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$

- Corresponding states ψ are bound states (potential confines particle in a certain region of space) →

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$



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1D problem: Finite well (1)

$$\begin{aligned} V(x) &= V_0 \quad |x| > a/2 \\ &= 0 \quad |x| < a/2 \end{aligned}$$

- Bound-state solutions (with $E < V_0$) are

$$\begin{aligned} \psi_1(x) &= Ae^{k_1 x} + Be^{-k_1 x} && \text{for } x < -a/2 \\ \psi_2(x) &= Ce^{ik_2 x} + De^{-ik_2 x} && \text{for } -a/2 \leq x \leq a/2 \\ \psi_3(x) &= Fe^{k_1 x} + Ge^{-k_1 x} && \text{for } x > a/2 \end{aligned}$$

$$k_1^2 = \frac{2m(V_0 - E)}{\hbar^2} \qquad k_2^2 = \frac{2mE}{\hbar^2}$$

1D problem: Finite well (2)

- Wave function has to be finite in region 1 → for $x = -\infty$ → $B = 0$
- Wave function has to be finite in region 3 → for $x = \infty$ → $F = 0$
- Due to continuity at $x = \pm a/2$ →

$$k_2 \tan \frac{k_2 a}{2} = k_1 \quad \Longleftrightarrow \quad -k_2 \cot \frac{k_2 a}{2} = k_1$$

- Eq. cannot be resolved directly → numerical or graphical methods → graphical solutions easiest with eq. in the form →

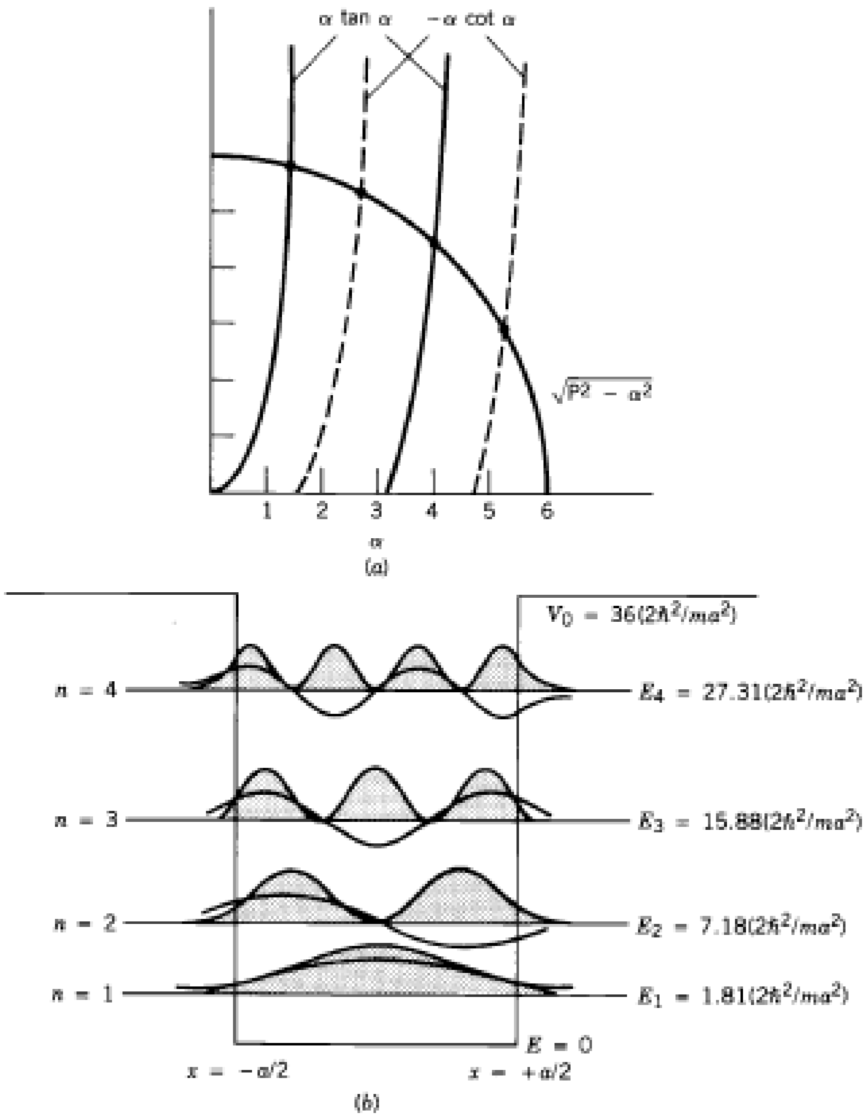
$$\alpha \tan \alpha = \left(P^2 - \alpha^2\right)^{1/2} \quad \Longleftrightarrow \quad -\alpha \cot \alpha = \left(P^2 - \alpha^2\right)^{1/2}$$

$$\alpha = \frac{k_2 a}{2} \qquad P = \left(\frac{m V_0 a^2}{2\hbar^2}\right)^{1/2}$$

1D problem: Finite well (3)

- Right side → circle of radius P ↔ left side → tangent function
- Solutions are given by the points where the circle intersects the tangent
- Therefore the number of solutions is determined by the radius P → by the depth V_0 of the well (for infinite well → infinite number of bound states)
- For $P < \pi/2$: only one bound state ↔ for $\pi/2 < P < \pi$: two bound states
- Technique that allows to estimate the depth of the nuclear potential → for deuteron: only one bound state

1D problem: Finite well (4)



Solutions for P = 6 (as an example) → 4 solutions at α = 1.345, 2.679, 3.985, 5.226

Images taken from: K.S. Krane, *Introductory Nuclear Physics*, Wiley, Oboken, 1988

1D problem: Simple Harmonic Oscillator (1)

$$V(x) = \frac{1}{2}kx^2$$

- Any reasonably well-behaved potential can be expanded in a Taylor series about the point x_0 →

$$V(x) = V(x_0) + \left(\frac{dV}{dx}\right)_{x=x_0}(x - x_0) + \frac{1}{2}\left(\frac{d^2V}{dx^2}\right)_{x=x_0}(x - x_0)^2 + \ldots$$

- If x_0 is a potential minimum → the second term = 0 and since the first term is a constant → the interesting term is the third term
- Near its minimum the system behaves like a simple harmonic oscillator → The study of the simple harmonic oscillator is important for a large number of systems

1D problem: Simple Harmonic Oscillator (2)

- To solve the Schrödinger equation → change of ψ →

$$\psi(x) = h(x) \exp\left(-\alpha^2 x^2/2\right)$$

- $h(x)$ is a simple polynomial function in x and $\alpha^2 = (km)^{1/2}/\hbar$
- The degree of the polynomial → the highest power of x that appears is determined by the quantum number n that labels the energy states →

$$E_n = \hbar\omega_0 \left(n + \frac{1}{2}\right) \qquad \text{with } n = 0, 1, 2, \ldots$$

- where $\omega_0 = (k/m)^{1/2}$ is the classical angular frequency of the oscillator

1D problem: Simple Harmonic Oscillator (3)

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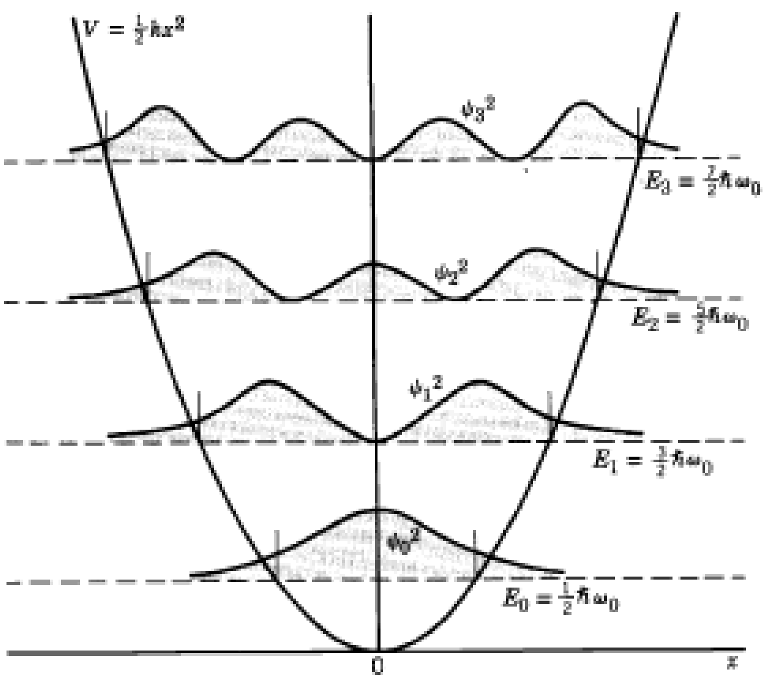
n	E_n	$\psi_n(x)$
0	$\frac{1}{2}\hbar\omega_0$	$\pi^{-1/4}\, e^{-\alpha^2 x^2/2}$
1	$\frac{3}{2}\hbar\omega_0$	$2^{-1/2}\pi^{-1/4}(2\alpha x)\, e^{-\alpha^2 x^2/2}$
2	$\frac{5}{2}\hbar\omega_0$	$2^{-3/2}\pi^{-1/4}(4\alpha^2 x^2 - 2)\, e^{-\alpha^2 x^2/2}$
3	$\frac{7}{2}\hbar\omega_0$	$(1/4\sqrt{3}\,\pi^{1/4})(8\alpha^3 x^3 - 12\alpha x)\, e^{-\alpha^2 x^2/2}$
4	$\frac{9}{2}\hbar\omega_0$	$(1/8\sqrt{6}\,\pi^{1/4})(16\alpha^4 x^4 - 48\alpha^2 x^2 + 12)\, e^{-\alpha^2 x^2/2}$

$$E_n = \hbar\omega_0(n + \tfrac{1}{2})$$

$$\psi_n(x) = (2^n n!\sqrt{\pi})^{-1/2} H_n(\alpha x)\, e^{-\alpha^2 x^2/2}$$

where $H_n(\alpha x)$ is a Hermite polynomial



- Results for the probabilities resemble those of finite well
- Energy levels are equally spaced
- Potential is infinitely deep → number of bound states is infinite

3D problem: Infinite Cartesian Well (1)

$$
\begin{aligned}
V(x) &= \infty \qquad x<0,\ x>a,\ \ y<0,\ y>a,\ \ z<0,\ z>a \\
&= 0 \qquad 0\le x\le a,\ \ 0\le y\le a,\ \ 0\le z\le a
\end{aligned}
$$

- The particle is confined to a cubic box of dimension *a*
- Inside the well → the Schrödinger equation is

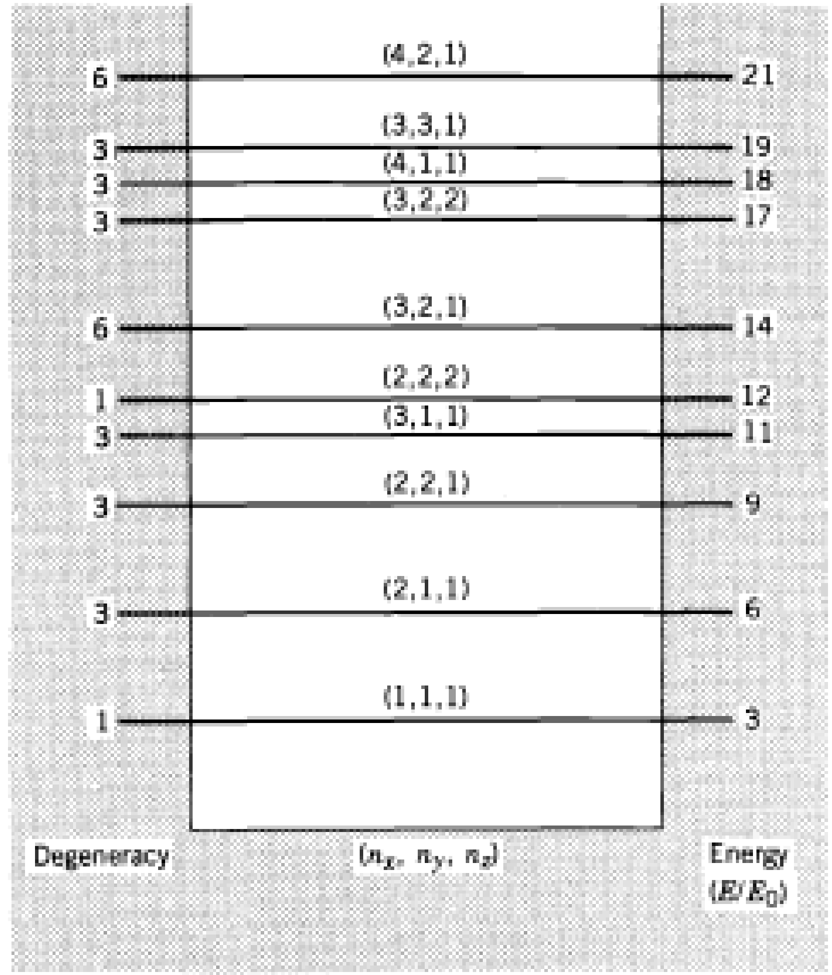
$$
-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)=E\psi(x,y,z)
$$

- With solutions →

$$
\begin{aligned}
\psi_{n_x,n_y,n_z}(x,y,z) &= \sqrt{\frac{8}{a^3}}\sin\frac{n_x\pi x}{a}\sin\frac{n_y\pi y}{a}\sin\frac{n_z\pi z}{a} \\
E_{n_x,n_y,n_z} &= \frac{\hbar^2\pi^2}{2ma^2}\left(n_x^2+n_y^2+n_z^2\right)
\end{aligned}
$$

3D problem: Infinite Cartesian Well (2)

- n_x, n_y, n_z are independent integers > 0
- The lowest state (ground state) has quantum numbers (n_x, n_y, n_z) = (1,1,1)
- The probability distribution has a maximum at the center of the box falling gradually to 0 at the walls like $\sin^2$



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3D problem: Infinite Cartesian Well (3)

- The first excited state has 3 possible sets of quantum numbers: (2,1,1), (1,2,1) and (1,1,2)
- Each of these distinct and independent states has a different wave function → a different probability density → different expectation values of the physical observables
- Attention → they have the same energy → situation called degeneracy
- Degeneracy is extremely important for atomic structure → how many electrons can be in each atomic subshell

3D problem: Infinite Spherical Well (1)

- In general → use of spherical coordinates with potential depending only on *r* (not θ or ϕ)
- Separable solutions of the form $\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$
- The central potential $V(r)$ appears only in the radial part of the equation $R(r)$ → the angular parts can be solved directly
- Differential equation for $\Phi(\phi)$ (with m_l^2 the separation constant) →

$$\frac{d^2\Phi}{d\phi^2} + m_l^2\Phi = 0$$

- The solution is

$$\Phi_{m_l}(\phi) = \frac{1}{\sqrt{2\pi}}\exp\left(im_l\phi\right)$$

- The $m_l = 0, \pm 1 \pm 2, \ldots$

3D problem: Infinite Spherical Well (2)

- The equation for $\Theta(\theta)$ →

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)-\frac{m_l^2}{\sin^2\theta}\right]\Theta=0$$

- Where l = 0,1,2,3… and m_l = 0, $\pm$ 1 $\pm$ 2,…
- The solutions $\Theta_{lm_l}(\theta)$ are expressed as a polynomial of degree l in sinθ or cosθ
- Together and normalized, $\Phi_{m_l}(\phi)$ and $\Theta_{lm_l}(\theta)$ give the spherical harmonics $Y_{lm_l}(\theta, \phi)$
- These functions give the angular part of the solution to the Schrödinger equation for any central potential $V(r)$
- For example → give the spatial properties of atomic orbitals responsible for molecular bonds

3D problem: Infinite Spherical Well (3)

ℓ	m_ℓ	$Y_{\ell m_\ell}(\theta,\phi) = \Theta_{\ell m_\ell}(\theta)\,\Phi_{m_\ell}(\phi)$
0	0	$(1/4\pi)^{1/2}$
1	0	$(3/4\pi)^{1/2}\cos\theta$
1	± 1	$\mp(3/8\pi)^{1/2}\sin\theta\, e^{\pm i\phi}$
2	0	$(5/16\pi)^{1/2}(3\cos^2\theta - 1)$
2	± 1	$\mp(15/8\pi)^{1/2}\sin\theta\cos\theta\, e^{\pm i\phi}$
2	± 2	$(15/32\pi)^{1/2}\sin^2\theta\, e^{\pm 2i\phi}$

$$\Phi_{m_\ell}(\phi) = \frac{1}{\sqrt{2\pi}}\, e^{i m_\ell \phi}$$

$$\Theta_{\ell m_\ell}(\theta) = \left[\frac{2\ell+1}{2}\,\frac{(\ell - m_\ell)!}{(\ell + m_\ell)!}\right]^{1/2} P_\ell^{m_\ell}(\theta)$$

where $P_\ell^{m_\ell}(\theta)$ is the associated Legendre polynomial

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3D problem: Infinite Spherical Well (4)

- For a given $V(r)$ → radial equation is

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

- The $l(l+1)$ term is an addition to the potential → « centrifugal potential » acts like a potential that keeps the particle away from the origin when $l > 0$
- Example of infinite spherical well →

$$\begin{aligned} V(x) &= \infty \qquad r > a \\ &= 0 \qquad r < a \end{aligned}$$

- Inside the well → solution are expressed in terms of the spherical Bessel functions $j_l(kr)$

3D problem: Infinite Spherical Well (5)

- Continuity condition at *r* = *a* to find the energy eigenvalues → $j_l(ka) = 0$
- Transcendental equation → numerical solutions → tables of the spherical Bessel functions to find the zeros for any given value of *l*
- For example → *l* = 0 → from the tables $j_0(x) = 0$ at *x* = 3.14, 6.28, 9.42, 12.57,…
- For *l* = 1 → first few zeros of $j_1(x)$ at x = 4.49, 7.73, 10.90, 14.07

$$j_0(kr) = \frac{\sin kr}{kr}$$

$$j_1(kr) = \frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr}$$

$$j_2(kr) = \frac{3\sin kr}{(kr)^3} - \frac{3\cos kr}{(kr)^2} - \frac{\sin kr}{kr}$$

$$j_\ell(kr) \cong \frac{(kr)^\ell}{1\cdot 3\cdot 5\cdots(2\ell+1)} \qquad kr \to 0$$

$$j_\ell(kr) \cong \frac{\sin(kr - \ell\pi/2)}{kr} \qquad kr \to \infty$$

$$j_\ell(kr) = \left(-\frac{r}{k}\right)^\ell \left(\frac{1}{r}\frac{d}{dr}\right)^\ell j_0(kr)$$

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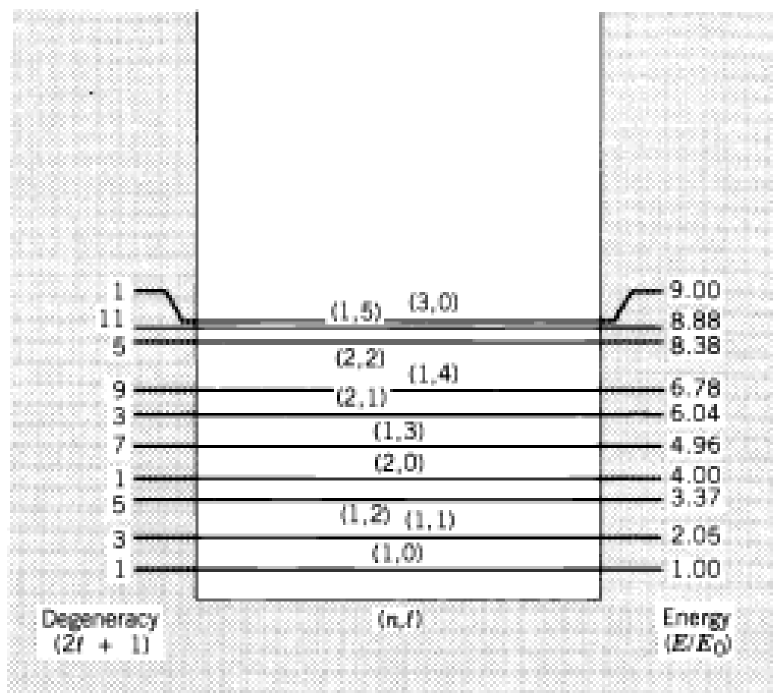
3D problem: Infinite Spherical Well (6)

- Since $E = \hbar^2 k^2/2m \rightarrow$ solutions for the allowed values of E energies
- Repeating process for $l = 2$, $l = 3$,… → construction of the spectrum of the energy states



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3D problem: Infinite Spherical Well (7)

- The levels are also degenerate → since E depends only on l → the wave functions with different m_l values all have the same energy

- Since m_l is restricted to the values 0, $\pm$ 1, $\pm$ 2, …, $\pm l$ → there are exactly $2l + 1$ possible Y_{lm_l} for a given l → each level has a degeneracy of $2l + 1$

3D problem: Simple Harmonic Oscillator (1)

- Central oscillator potential → $V(r)=1/2kr^2$
- For all central potentials → the angular part of the solution to the Schrodinger equation is $Y_{lm_l}(\theta, \phi)$ → we have only to find the solution to the radial equation
- As in 1D → the solution is the product of an exponential and a finite polynomial
- The energy levels are given by

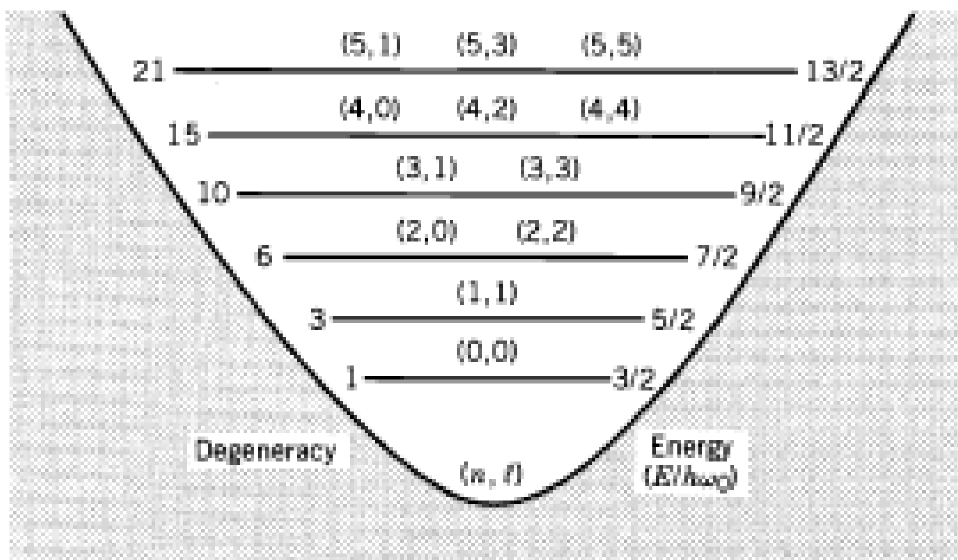
$$E_n = \hbar\omega_0 \left(n + \frac{3}{2}\right) \quad \text{with } n = 0, 1, 2, ...$$

3D problem: Simple Harmonic Oscillator (2)

- No dependence on l for the energy but not all l values are permitted
- From the mathematical solution of the radial equation → l can be at most equal to n and takes only even or only odd values as n is even or odd
- Example → For $n = 5$, the permitted values of l are 1, 3, and 5
- Since E do not depend on m_l → additional degeneracy of $2l + 1$ for each l
- For $n = 5$ level has a degeneracy of [(2 * 1 + 1) + (2 * 3 + 1) +
- (2 * *5* + 1)] = 21
- Degeneracy equals to 1/2(n+1)(n+2)

3D problem: Simple Harmonic Oscillator (3)

n	ℓ	E_n	$R(r)$
0	0	$\frac{3}{2}\hbar\omega_0$	$(2\alpha^{3/2}/\pi^{1/4})\, e^{-\alpha^2 r^2/2}$
1	1	$\frac{5}{2}\hbar\omega_0$	$(2\alpha^{3/2}\sqrt{2}/\sqrt{3}\,\pi^{1/4})(\alpha r)\, e^{-\alpha^2 r^2/2}$
2	0	$\frac{7}{2}\hbar\omega_0$	$(2\alpha^{3/2}\sqrt{2}/\sqrt{3}\,\pi^{1/4})(\frac{3}{2} - \alpha^2 r^2)\, e^{-\alpha^2 r^2/2}$
2	2	$\frac{7}{2}\hbar\omega_0$	$(4\alpha^{3/2}/\sqrt{15}\,\pi^{1/4})(\alpha^2 r^2)\, e^{-\alpha^2 r^2/2}$
3	1	$\frac{9}{2}\hbar\omega_0$	$(4\alpha^{3/2}/\sqrt{15}\,\pi^{1/4})(\frac{5}{2}\alpha r - \alpha^3 r^3)\, e^{-\alpha^2 r^2/2}$
3	3	$\frac{9}{2}\hbar\omega_0$	$(4\alpha^{3/2}\sqrt{2}/\sqrt{105}\,\pi^{1/4})(\alpha^3 r^3)\, e^{-\alpha^2 r^2/2}$
4	0	$\frac{11}{2}\hbar\omega_0$	$(4\alpha^{3/2}\sqrt{2}/\sqrt{15}\,\pi^{1/4})(\frac{15}{8} - \frac{5}{2}\alpha^2 r^2 + \frac{1}{2}\alpha^4 r^4)\, e^{-\alpha^2 r^2/2}$
4	2	$\frac{11}{2}\hbar\omega_0$	$(4\alpha^{3/2}\sqrt{2}/\sqrt{105}\,\pi^{1/4})(\frac{7}{2}\alpha^2 r^2 - \alpha^4 r^4)\, e^{-\alpha^2 r^2/2}$
4	4	$\frac{11}{2}\hbar\omega_0$	$(8\alpha^{3/2}/3\sqrt{105}\,\pi^{1/4})\, \alpha^4 r^4\, e^{-\alpha^2 r^2/2}$



Images taken from: K.S. Krane, *Introductory Nuclear Physics*, Wiley, Oboken, 1988

Commutator

- Mathematical definition of Commutator →

$$[A, B] = AB - BA$$

- This is equal to 0 if they commute and something else if they do not commute
- It is known that you cannot know the value of two physical values at the same time if they do not commute (Heisenberg's principle)
- If we can find a set of operators commuting with *H* → this set is complete in the sense that all energy eigenstates are uniquely labelled by the eigenvalues of the above operators
- A key property of central potential problems is that the angular momentum operators commute with the Hamiltonian

(Orbital) Angular momentum (1)

- In solutions of the 3D Schrödinger equation → prominent role of the quantum number *l*
- In atomic physics → label the different electron wave functions and give information about their spatial behaviour
- This angular momentum quantum number has the same function in all 3D problems involving central potentials *V*(*r*)
- In classical physics → $\boldsymbol{l} = \boldsymbol{r} \times \boldsymbol{p}$
- In quantum mechanics → components of ***p*** have to be replaced by their equivalent operators:

$$p_i = -i\hbar \frac{\partial}{\partial x}$$

(Orbital) Angular momentum (2)

- Result for which a central potential is considered → having a wave function $R(r)Y_{lm_l}(\theta, \phi)$ → independent of the form of $R(r)$
- It is simple to calculate $\boldsymbol{l}^2$ →

$$\langle \boldsymbol{l}^2 \rangle = \hbar l(l+1)$$

- As in classical physics for central potentials → the angular momentum is a constant of the motion
- The atomic substates with a given l value are labeled using spectroscopic notation → same spectroscopic notation in nuclear physics: s for $l = 0$, p for $l = 1$, …

ℓ value	0	1	2	3	4	5	6
Symbol	s	p	d	f	g	h	i

Image taken from: K.S. Krane, *Introductory Nuclear Physics*, Wiley, Oboken, 1988

(Orbital) Angular momentum (3)

- Direction of *l* → barrier imposed by the uncertainty principle in quantum mechanics → it is permitted to know exactly only one component of *l* at a time → when one component is known the other two components are completely indeterminate

- By convention → *z* component is chosen →

$$\langle l_z \rangle = \hbar m_l$$

with m_l = 0, $\pm$ 1 $\pm$ 2,…

Spin angular momentum

- Spin angular momentum = Intrinsic angular momentum = Spin
- Nucleons (like electrons) have spin quantum number *s* = ½
- Usual calculations for angular momenta →

$$\langle \boldsymbol{s}^2 \rangle = \hbar s(s+1)$$

$$\langle s_z \rangle = \hbar m_s \qquad (m_s = \pm \tfrac{1}{2})$$

- Useful to imagine the spin as a vector **s** with possible *z* components = $\pm$ ½$\hbar$

Total angular momentum (1)

- The total angular momentum ***j*** combines both the spin and orbital angular momentum of a particle or system →

$$\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$$

- Behaviour of total angular momentum →

$$\langle \boldsymbol{j}^2 \rangle = \hbar j(j+1)$$

$$\langle j_z \rangle = \langle j l_z + s_z \rangle = \hbar m_j$$

- We have $m_j = -j, -j + 1, . . . , j - 1, j$ (j is the total angular momentum quantum number)

Total angular momentum (2)

- As $m_s = \pm½ \rightarrow m_j = m_l + m_s = m_l \pm ½$
- m_l is always an integer $\rightarrow$ m_j is half-integral $\rightarrow$ j is half-integral $\rightarrow$

$$j = l + \frac{1}{2} \quad \text{or} \quad j = l - \frac{1}{2}$$

- The j value is noted as a subscript in spectroscopic notation
- For $l = 1$ (p states) $\rightarrow$ two possible j values: $l + 1/2 = 3/2$ and $l - 1/2 = 1/2$
- These states are written as $p_{3/2}$ and $p_{1/2}$

General addition of angular momenta

- General rules for the addition of two angular momenta $\boldsymbol{J_1}$ and $\boldsymbol{J_2}$ → $\boldsymbol{J} = \boldsymbol{J_1} + \boldsymbol{J_2}$
- When j_1 and j_2 (corresponding quantum numbers) are “added” the maximal and minimal values of j are $j_{max} = j_1 + j_2$ and $j_{min} = |j_1 - j_2|$
- The allowed j-values in this interval are j = $|j_1 - j_2|$, $|j_1 - j_2| + 1, \dots, j_1 + j_2$
- If both j_1 and j_2 are half-integral or if both are integers → the possible quantum numbers j are integers ↔ in the opposite case the resulting j-values become half-integral
- Properties known as triangular inequality and noted →

$$|j_1 - j_2| \leq j \leq j_1 + j_2$$

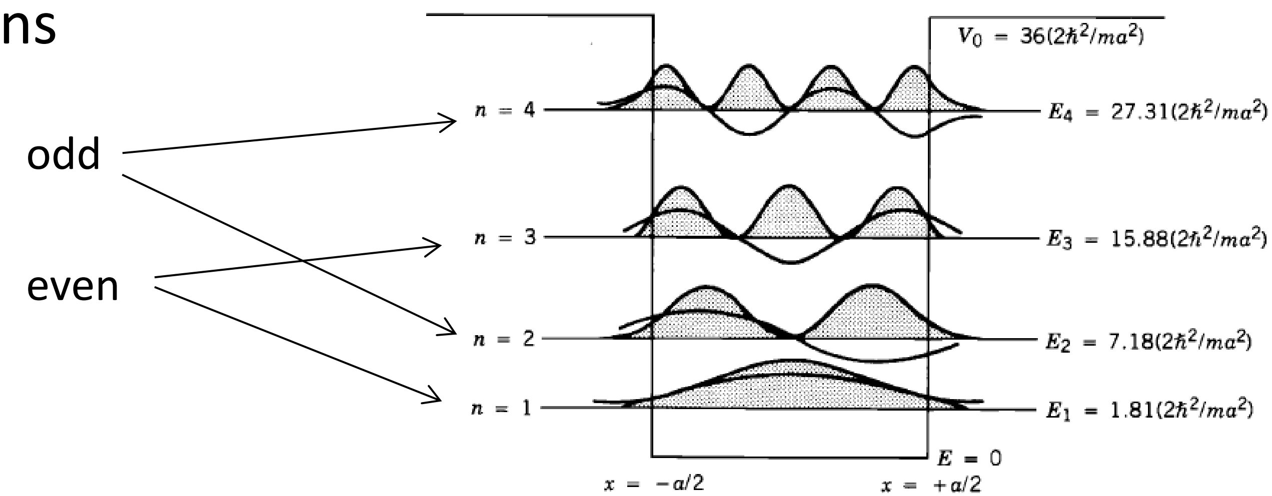
Parity (1)

- The parity operation causes a reflection of all of the coordinates through the origin: $\boldsymbol{r} \rightarrow -\boldsymbol{r}$
- In Cartesian coordinates → $x \rightarrow -x$ / $y \rightarrow -y$ / $z \rightarrow -z$
- In spherical coordinates → $r \rightarrow r$ / $\theta \rightarrow \pi - \theta$ / $\phi \rightarrow \phi + \pi$
- If a system is left unchanged by the parity operation → none of the properties should change as a result of the reflection
- The values of the observable quantities depend on $|\psi|^2$ →

$$\text{If} \quad V(\boldsymbol{r}) = V(-\boldsymbol{r}) \rightarrow |\psi(\boldsymbol{r})|^2 = |\psi(-\boldsymbol{r})|^2$$

Parity (2)

- Consequence → $\psi(-\boldsymbol{r}) = \pm\psi(\boldsymbol{r})$
- In case $\psi(-\boldsymbol{r}) = +\psi(\boldsymbol{r})$ → positive or even parity
- In case $\psi(-\boldsymbol{r}) = -\psi(\boldsymbol{r})$ → negative or odd parity
- If the potential V(***r***) is unchanged by the parity operation → the resulting wave functions must have either even or odd parity (mixed-parity wave functions are not permitted)
- For finite well → potential symmetric with respect to the parity operation: V(*x*) = V(-*x*) → even or odd parity for the solutions



Parity (3)

- In 3D the parity operation applied to $Y_{lm_l}(\theta, \phi)$ gives →

$$Y_{lm_l}(\pi - \theta, \phi + \pi) = (-1)^l Y_{lm_l}(\theta, \phi)$$

- Central potentials depend only on the magnitude of ***r*** are thus invariant with respect to parity → their wave functions have odd arity if *l* is odd and even parity if *l* is even

Parity (4)

- The wave function for a system of many particles = the product of the wave functions for the individual particles → the parity of the combined wave function is even if the combined wave function represents any number of even-parity particles or an even number of odd-parity particles ↔ it is odd if there is an odd number of odd-parity particles
- Thus nuclear states can be assigned a definite parity (odd or even) → indicated along with the total angular momentum for that state → example:

$$\frac{3}{2}^{+} \text{ or } \frac{5}{2}^{-}$$

Fermi’s golden rule

- Fermi's golden rule is a formula that describes the transition rate (probability of transition per unit time) from one energy eigenstate of a quantum system into other energy eigenstates effected by a weak perturbation
- We consider the system to begin in an eigenstate $|i>$ of a given Hamiltonian H_0
- We consider the effect of a (possibly time-dependent) perturbing Hamiltonian H' .
- The transition probability per unit of time λ from the state $|i>$ to a set of final states $|f>$ is given to first order in the perturbation by

$$\lambda = \frac{2\pi}{\hbar} | \langle f | \, H' \, | i \rangle \, |^2 \rho$$

- ρ is the density of final states (number of continuum states per unit of energy)