Lecture 1

Wave Function, Schrodinger Equation

Wave Function $\psi(x, t)$

Probability interpretation

(Time dependent) Schrodinger Equation.

Solution of the Schrodinger Equation

$V(x)$ independent of t

$\downarrow$

Seperation of variable

$\downarrow$

time independent Schrodinger equation

Boundary condition

Initial condition

Expectation value

Momentum operator

Δx, Δp

uncertainty relation.

Oct 31

Lecture 1

An electron $\psi(x,t)$ $\downarrow$ wave function

Schrodinger equation

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

$$V(x,t) \longrightarrow V(x)$$

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

$\psi(x,0)$ + Schrodinger Equation

+ Boundary Condition

$\Longrightarrow$ $\psi(x,t)$

Physical interpretation of $\psi(x,t)$

$\underbrace{|\psi(x,t)|^2}_{\rho(x,t)} dx$ probability of finding the particle between x and $x+dx$ at time t.

$\rho(x,t)$ probability density

$S(x,t)$ probability current density

$$\frac{\partial}{\partial x}S(x,t) + \frac{\partial\rho}{\partial t} = 0 \quad \text{continuity equation.}$$

$\downarrow$

probability is conserved.

Normalization condition

$$\int_{-\infty}^{\infty}|\psi(x,t)|^2\,dx = 1$$

Boundary Condition

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$$

$\downarrow$

square integrable

Existence of $\rho(x,t)$, $S(x,t)$

$\Rightarrow$ $\psi(x,t)$ must be finite

$\psi(x,t)$ must be continuous

$\frac{\partial \psi(x,t)}{\partial x}$ must be finite

$\frac{\partial \psi}{\partial x}(x,t)$ must be continous

Specify the problem:

$V(x)$, $\psi(x,0)$

$\Rightarrow$ determine $\psi(x,t)$

$V(x,t) = V(x) \Rightarrow$ Seperation of variable. method

$$\psi_n(x,t) = e^{-iE_n t/\hbar} \psi_n(x)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} + V(x)\psi_n(x) = E_n \psi_n(x)$$

$\downarrow$

time-independent Schrodinger equation

$\psi_n(x)$ is the solution of time-independent Schrodinger equation.

Only certain E_n can we find acceptable solution i.e., satisfy the boundary condition and the time independent equation

$$\psi_n(x) \longleftrightarrow E_n$$

With these functions

$\Rightarrow \quad \Psi_n(x,t) = e^{-iE_n t/\hbar}\, \psi_n(x)$ is a solution of time-dependent Schrodinger equation.

Schrodinger equation is linear

$\sum_n c_n \Psi_n(x,t)$ is a general solution of the Schrodinger equation.

$$\psi(x,t) = \sum_n c_n \psi_n(x)\, e^{-iE_n t/\hbar}$$

$$\Rightarrow \quad \psi(x,0) = \sum_n c_n \psi_n(x)$$

$\downarrow$

initial condition.

$\Downarrow$

determine the c_n's $\Rightarrow$ wave function $\psi(x,t)$

Expectation value

$$\langle x \rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx$$

$$\langle f(x) \rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\, f(x)\, \psi(x,t)\, dx$$

$$\langle \hat{A} \rangle_t = \int \psi^*(x,t)\, \hat{A}\, \psi(x,t)\, dx$$

$$\hat{x} \leftarrow x$$
$$\widehat{f(x)} \leftarrow f(x)$$

Momentum operator $\hat{p} \rightarrow -i\hbar \frac{\partial}{\partial x}$

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) [-i\hbar \tfrac{\partial}{\partial x}] \psi(x,t)]\, dx$$

$$\langle \widehat{f(p)} \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) [f(-i\hbar \tfrac{\partial}{\partial x})] \psi(x,t)]\, dx$$

e.g., $\langle \hat{p}^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) [-\hbar^2 \frac{\partial^2}{\partial x^2}] \psi(x,t)\, dx$

$$\hat{E} \rightarrow i\hbar \frac{\partial}{\partial t}$$

Justification:

Ehrenfest's theorem

Schrodinger equation $\Rightarrow$ $\langle \frac{p^2}{2m} \rangle + \langle V \rangle = \langle E \rangle$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

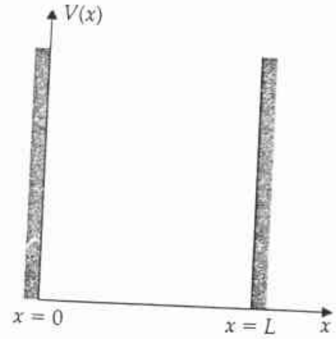
$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

Uncertainty Principle

$$\Delta x\, \Delta p \gtrsim \hbar/2$$

Example. The infinite well. (See the textbook)

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



The infinite-well potential has infinitely high potential-energy "walls" that confine a particle under its influence to the region $0 < x < L$. It is convenient to choose the bottom of the well to correspond to zero potential energy.

In the region $0 < x < L$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) = E\,u(x)$$

Boundary condition

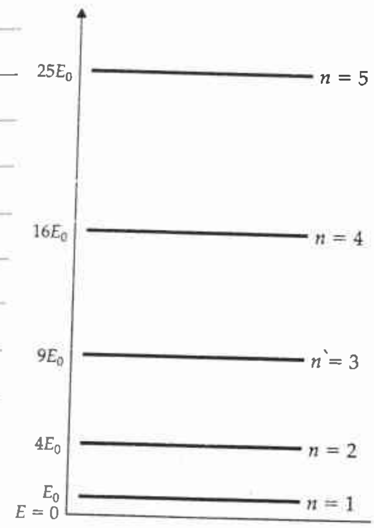
$$u(0) = u(L) = 0$$

$$u(x) = A \sin kx \qquad (u = 0 \text{ at } x = 0)$$

$$kL = n\pi \qquad n = 1, 2, \cdots$$

$$k = \frac{n\pi}{L}$$

$$\Rightarrow \quad E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2} \qquad n = 1, 2, \cdots$$



The energy spectrum (i.e., the allowed, or possible, energy values) for a particle of mass m in the infinite well of •Fig. 6–5. The ground-state energy is $E_0 = \frac{\hbar^2\pi^2}{2mL^2}$.

Normalization

$$|A|^2 \int_0^L \sin^2 kx \, dx = 1$$

$$\Rightarrow \quad A = \frac{\sqrt{2}}{L} e^{i\varphi}$$

$e^{i\varphi}$ does not appear in physical probabilities

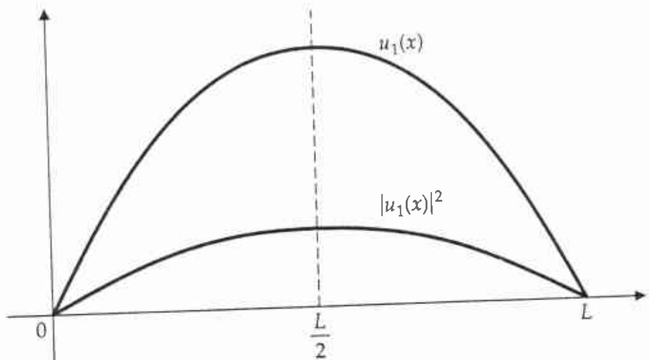
$$\int \psi^* \, L \, \psi \, dx$$

L: linear operator

the result is independent of φ

Ground state wave function

$$u_1(x) = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}$$



The ground-state wave function $u_1(x)$, as well as the associated probability distribution $|u_1(x)|^2$, for the infinite well is symmetric about the midpoint $x = L/2$.

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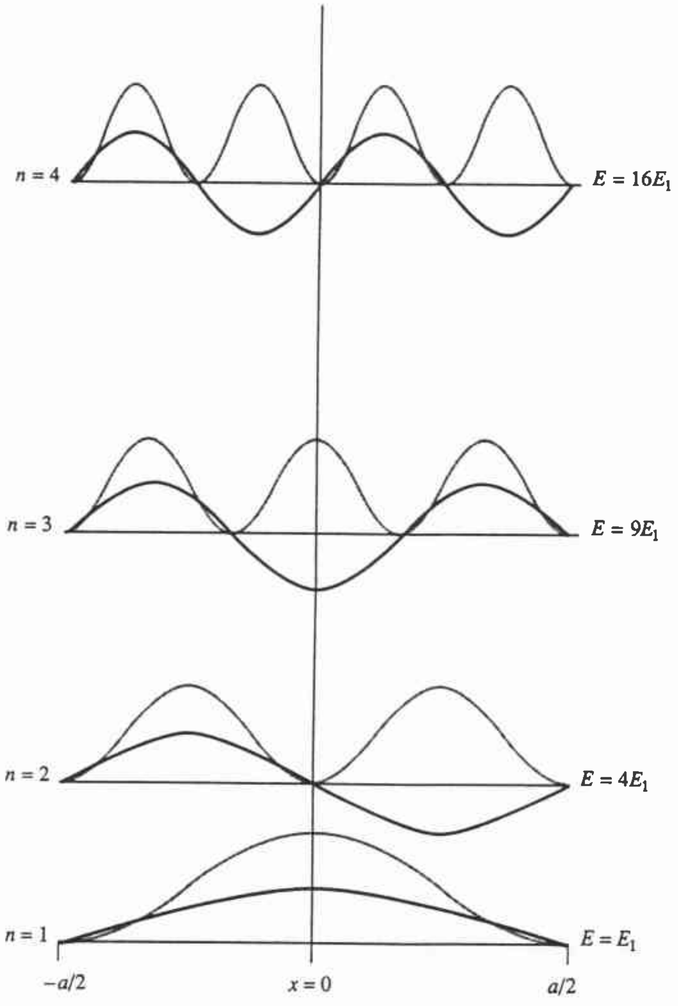

The wave functions (solid color) and probability densities (light color) for the ground state ($n = 1$) and first three excited states ($n = 2$, 3, and 4) of a particle confined to an infinite one-dimensional potential well of width a. Note that the wave functions are either odd or even functions of x.

Since $V(x) = 0$ in the region where the particle can be found, the zero-point energy must be purely kinetic in this case. We could have estimated it using the Heisenberg uncertainty relation: Confining the particle to a region $\Delta x = a$ introduces a momentum uncertainty $\Delta p \sim \frac{\hbar}{\Delta x} = \frac{\hbar}{a}$, and a kinetic energy $\frac{(\Delta p)^2}{2m} \sim \frac{\hbar^2}{2ma^2}$. Since $V(x) = 0$ for $x \leq x \leq a$, and $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$ in this region, and $E = \frac{p^2}{2m}$ in **CM**, it appears that momentum is associated with the derivative $\frac{\partial}{\partial x}$ of the wavefunction, and kinetic energy with the curvature $\frac{\partial^2}{\partial x^2}$.

The eigenfunctions have the property that

$$\int_{-\infty}^{\infty} dx u_n^*(x) u_m(x) = \int_0^a dx \frac{2}{a} \sin\left(n\pi\frac{x}{a}\right) \sin\left(m\pi\frac{x}{a}\right) \tag{11-1}$$

$$= \frac{1}{a}\int_0^a dx \left\{\cos\left((n-m)\pi\frac{x}{a}\right) - \cos\left((n+m)\pi\frac{x}{a}\right)\right\} \tag{11-2}$$

$$= \frac{\sin((n-m)\pi)}{(n-m)\pi} - \frac{\sin((n+m)\pi)}{(n+m)\pi} \tag{11-3}$$

$$= \begin{cases} 0 & \text{for } n \neq m, \\ 1 & \text{for } n = m. \end{cases} \tag{11-4}$$

$$= \delta_{nm} \tag{11-5}$$

$$\boxed{\delta_{nm} = \begin{cases} 0 & \text{for } n \neq m, \\ 1 & \text{for } n = m. \end{cases}} \rightarrow \text{Kronecker delta} \tag{11-6}$$

This is a general property, not particular to this example: Eigenfunctions belonging to different eigenvalues are **orthogonal**, if the eigenfunctions are normalized we call them **orthonormal**.

$$\boxed{\int_{-\infty}^{\infty} dx u_n^*(x) u_m(x) = \delta_{mn}} \quad \text{orthonormality condition} \tag{11-7}$$

Complex conjugate not necessary for box potential, where eigenfunctions are real, but necessary in general.

$$\int u_n^* u_n dx = \int |u_n|^2 dx = 1 \quad \text{normalization} \tag{11-8}$$

Simple Harmonic Oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}\underset{\substack{\downarrow \\ m\omega^2}}{k}\, x^2$$

classical Hamiltonian for simple harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}$$

$\hat{p}$, $\hat{x}$ are operators

In x representation

$$\hat{p} \rightarrow -i\hbar \frac{\partial}{\partial x}$$

$$\hat{x} \rightarrow x$$

Time independent Schrodinger equation

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

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi$$

$$\psi_n(x) \longleftrightarrow E_n$$

$\Downarrow$

are acceptable solution

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Example: Simple harmonic oscillator

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

(See Griffiths' "Introduction to Quantum Mechanics" P. 37 to 43 ; and the textbook P. 143-144)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi$$

$$m\omega^2 = k$$

Let $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$ (changing variable to simplify the equation)

$$\Rightarrow \quad \frac{d^2\psi}{d^2\xi} = (\xi^2 - K)\psi \qquad K = \frac{2E}{\hbar\omega}$$

For large ξ

$$\Rightarrow \quad \frac{d^2\psi}{d\xi^2} \cong \xi^2\psi$$

$\Rightarrow$ approximate solution $\psi(\xi) \simeq A e^{-\xi^2/2} + B e^{+\xi^2/2}$

not normalizable

$$\psi(\xi) = h(\xi)\, e^{-\xi^2/2}$$

(hoping $h(\xi)$ has simpler functional form than $\psi(x)$)

$$\Rightarrow \quad \frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0$$

Solve the equation using the series expansion method

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j \xi^j$$

Task is to find $a_0, a_1, \cdots$

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots = \sum_{j=0}^{\infty} j a_j \xi^{j-1}$$

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2\cdot 3a_3\xi + 3\cdot 4a_4\xi^2 + \cdots = \sum_{j=0}^{\infty}(j+1)(j+2)a_{j+2}\xi^j$$

Put back into the differential equation

$$\sum_{j=0}^{\infty}\left[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j\right]\xi^j = 0$$

$$\Rightarrow \quad (j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j = 0$$

$$\Rightarrow \quad a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j$$

recursion relation

$a_0 \Rightarrow a_2, a_4, \cdots$ can be calculated
$a_1 \Rightarrow a_1, a_2, \cdots$ can be calculated

$$h(\xi) = h_{even}(\xi) + h_{odd}$$

$$h_{even}(\xi) = a_0 + a_2\xi^2 + a_4\xi^4 + \cdots \qquad \text{built on } a_0$$

$$h_{odd}(\xi) = a_1\xi + a_3\xi^3 + a_5\xi^5 + \cdots \qquad \text{built on } a_1$$

However, not all the solutions so obtained are normalizable

For large j, $a_{j+2} \simeq \frac{2}{j} a_j$

$$\downarrow$$

$$a_j \sim \frac{C}{(j/2)!}$$

$$h(\xi) \simeq C \sum \frac{1}{(j/2)!}\xi^j \simeq C \sum \frac{1}{k!}\xi^{2k} \simeq Ce^{\xi^2/2}$$

$$\downarrow$$

not acceptable

Therefore, the series must be terminate

$\downarrow$

There must occur some "highest" j (call it n)

$$K = 2n+1$$

$$\Downarrow$$

$$E_n = (n+\tfrac{1}{2})\hbar\omega \qquad n = 0, 1, 2, \cdots$$

$$\updownarrow$$

$$\psi_n(x) = \underbrace{\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}}_{\text{normalization constant}} \underbrace{H_n(\xi)}_{\text{Hermite polynomial.}} e^{-\xi^2/2}$$

Appendix A

Hermite Polynomials

From P. 6-10, we find

$$\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (K-1)H = 0$$

$(h \to H)$

Acceptable solutions can be found only if

$K = 2n+1 \qquad n = 0, 1, 2, \cdots$

$$\Rightarrow \quad \frac{d^2H_n}{d\xi^2} - 2\xi\frac{dH_n(\xi)}{d\xi} + 2n H_n(\xi) = 0$$

this is defining differential equation

Generating function and recursive relations

$$S(\xi, s) = e^{\xi^2-(s-\xi)^2} = e^{-s^2+2s\xi} = \sum_{n=0}^{\infty}\frac{H_n(\xi)}{n!}s^n$$

Expanding the exponential function in terms of powers of s and ξ, we see that the coefficients of the powers s^n are polynomials in terms of ξ – the Hermite polynomials. This can be shown as follows: we have

$$\frac{\partial S}{\partial \xi} = 2s\,e^{-s^2+2s\xi} = \sum_{n=0}^{\infty}\frac{2s^{n+1}}{n!}H_n(\xi)$$
$$= \sum_{n=0}^{\infty}\frac{s^n}{n!}\frac{\partial H_n(\xi)}{\partial \xi} \quad ,$$

$$\frac{\partial S}{\partial s} = (-2s+2\xi)\,e^{-s^2+2s\xi} = \sum_{n=0}^{\infty}\frac{(-2s+2\xi)s^n}{n!}H_n(\xi)$$
$$= \sum_{n=0}^{\infty}\frac{s^{n-1}}{(n-1)!}H_n(\xi) \quad . \tag{5}$$

Equating equal powers of s in the sums of these two equations, we obtain

$$\frac{\partial H_n(\xi)}{\partial \xi} = 2nH_{n-1}(\xi) \quad ,$$
$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi) \quad . \tag{6}$$

Therefore it follows that

$$\frac{\partial H_n(\xi)}{\partial \xi} = 2\xi H_n(\xi) - H_{n+1}(\xi) \quad , \tag{7}$$

and hence

$$\frac{\partial^2 H_n(\xi)}{\partial \xi^2} = 2H_n(\xi) + 2\xi\frac{\partial H_n(\xi)}{\partial \xi} - \frac{\partial H_{n+1}(\xi)}{\partial \xi}$$
$$= 2\xi\frac{\partial H_n(\xi)}{\partial \xi} + 2H_n(\xi) - (2n+2)H_n(\xi)$$

$$= 2\xi \frac{\partial H_n(\xi)}{\partial \xi} - 2nH_n(\xi) \quad . \tag{8}$$

This is exactly differential equation (3), proving that the $H_n(\xi)$ appearing in the generating function (4) are indeed Hermite polynomials.

The recurrence formulas (6) may be used to calculate the H_n and their derivatives. Another explicit expression directly obtainable from the generating function is quite useful; let us now establish this important relation. From (4) it follows instantly that

$$\left.\frac{\partial^n S(\xi, s)}{\partial s^n}\right|_{s=0} = H_n(\xi) \quad . \tag{9}$$

Now, for an arbitrary function $f(s-\xi)$, it also holds that

$$\frac{\partial f}{\partial s} = -\frac{\partial f}{\partial \xi} \quad . \tag{10}$$

Thus

$$\begin{aligned} \frac{\partial^n S}{\partial s^n} &= \mathrm{e}^{\xi^2} \frac{\partial^n \mathrm{e}^{-(s-\xi)^2}}{\partial s^n} \\ &= (-1)^n \mathrm{e}^{\xi^2} \frac{\partial^n}{\partial \xi^n} \mathrm{e}^{-(s-\xi)^2} \quad . \end{aligned} \tag{11}$$

Comparing (11) with (9) yields the very useful formula,

$$H_n(\xi) = (-1)^n = \mathrm{e}^{\xi^2} \frac{\partial^n}{\partial \xi^n} \mathrm{e}^{-\xi^2} \quad . \tag{12}$$

$$\lambda = \sqrt{\frac{m\omega}{\hbar}}$$

The $H_n(\xi)$ are polynomials of nth degree in ξ with the dominant term $2^n\xi^n$. The first five $H_n(\xi)$ calculated from (7.22) or (12) of the foregoing example are:

$$\begin{aligned} &H_0(\xi) = 1 \quad , \qquad H_1(\xi) = 2\xi \quad , \\ &H_2(\xi) = 4\xi^2 - 2 \quad , \quad H_3(\xi) = 8\xi^3 - 12\xi \quad , \quad H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \quad . \end{aligned} \tag{7.23}$$

The eigenfunctions (7.21) were combined by introducing the abbreviation $\xi = \sqrt{\lambda}x$ and using the Hermite polynomials in a way that holds for both even and odd n, i.e.

$$\psi_n(x) = N_n \mathrm{e}^{(-1/2)\xi^2} H_n(\xi) \quad , \quad \xi = \sqrt{\lambda}x \quad . \tag{7.24}$$

The constant N_n, which depends on the index n, is determined by the normalization condition

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, dx = 1 \quad , \tag{7.25}$$

since we require the position probability to be 1 for the particle in the entire configuration space. Thus

$$n=0:\psi_0(x)=\sqrt[4]{\frac{\lambda}{\pi}}\exp\left(-\frac{1}{2}\lambda x^2\right) \quad ,$$

$$n=1:\psi_1(x)=2\sqrt{\frac{1}{2}\sqrt{\frac{\lambda}{\pi}}}\exp\left(-\frac{1}{2}\lambda x^2\right)\sqrt{\lambda}x \quad ,$$

$$n=2:\psi_2(x)=\sqrt{\frac{1}{8}\sqrt{\frac{\lambda}{\pi}}}\exp\left(-\frac{1}{2}\lambda x^2\right)(4\lambda x^2-2) \quad . \tag{7.33}$$

From (7.24) and (7.30) it follows that, for space reflection, the eigenfunctions have the symmetry property

$$\psi_n(-x)=(-1)^n\psi_n(x) \quad . \tag{7.34}$$

This means

n even: $\psi(-x)=\psi(x)\rightarrow$ parity $+1$

n odd: $\psi(-x)=-\psi(x)\rightarrow$ parity -1 .

For the lowest H_n, it can easily be shown that they possess precisely n different real zeros and $n-1$ extremal values (see Fig. 7.1). With respect to (12) in Example 7.2, we have

$$H_{nk+1}=-e^{\xi^2}\frac{d}{d\xi}(e^{-\xi^2}H_n) \quad . \tag{7.35}$$

On the assumption that H_n possesses $n+1$ real extremal values, we can conclude the existence of $n+1$ extremal values for $e^{-\xi^2}H_n$ (since $e^{-\xi^2}\rightarrow 0$ for $\xi\rightarrow\infty$). The extremal values are identical with the zeros of the derivative $d/d\xi$; therefore H_{n+1} has precisely $n+1$ real zeros. This conclusion shows that the Hermite polynomials $H_n(\xi)$ – and, in consequence, the wave functions $\psi_n(\xi)$ – possess n different real zeros. This is a special case of a universally valid theorem which states that the principal quantum number of an eigenfunction is identical with the number of zeros.

In Fig. 7.1, some of the ψ_n are plotted together with an energy diagram. The energy eigenvalues are represented as horizontal lines with the quantum segments $E_n=\left(n+\frac{1}{2}\right)\hbar\omega$. For each of the lines there is a corresponding eigenfunction $\psi_n(x)$ drawn on an arbitrary scale.

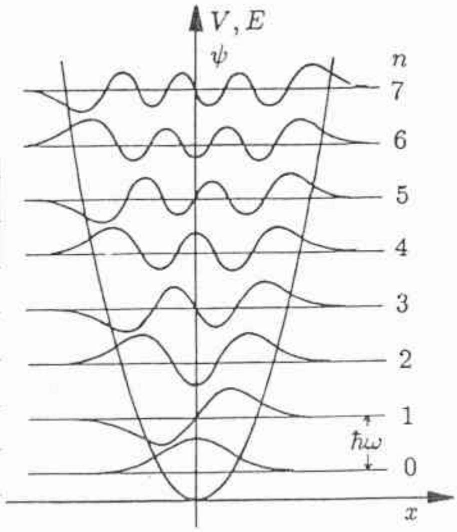

Fig. 7.1. Oscillator potential, energy levels and corresponding wavefunctions

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2\, dx = \frac{1}{\sqrt{\lambda}} N_n^2 \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2} H_n(\xi)^2\, d\xi = 1 \quad . \tag{7.26}$$

Using relation (12) of Example 7.2 to express one of the Hermite polynomials that appears in the integrand of the normalization integral, the evaluation of this integral becomes simply

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2\, dx = (-1)^n \frac{N_n^2}{\sqrt{\lambda}} \int_{-\infty}^{\infty} H_n(\xi) \frac{d^n}{d\xi^n} \mathrm{e}^{-\xi^2}\, d\xi \quad . \tag{7.27}$$

By partial integration we obtain

$$\begin{aligned} &\int_{-\infty}^{\infty} H_n(\xi) \frac{d^n}{d\xi^n} \mathrm{e}^{-\xi^2}\, d\xi \\ &\quad = \left[\left(\frac{d^{n-1}}{d\xi^{n-1}} \mathrm{e}^{-\xi^2} \right) H_n(\xi) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{dH_n}{d\xi} \frac{d^{n-1}}{d\xi^{n-1}} \mathrm{e}^{-\xi^2}\, d\xi \quad . \end{aligned} \tag{7.28}$$

The first term is, because of (12) in Example 7.2, equal to $(-1)^{n-1}\,\mathrm{e}^{-\xi^2} H_{n-1}(\xi) H_n(\xi)$. It vanishes at infinity, due to the exponential function.

Having carried out partial integration n times, we are left with

$$\int_{-\infty}^{\infty} H_n(\xi) \frac{d^n}{d\xi^n} \mathrm{e}^{-\xi^2}\, d\xi = (-1)^n \int_{-\infty}^{\infty} \frac{d^n H_n}{d\xi^n} \mathrm{e}^{-\xi^2}\, d\xi \quad . \tag{7.29}$$

Since $H_n(\xi)$ is a polynomial of nth order with the dominant term $2^n \xi^n$, for the nth derivative,

$$\frac{d^n}{d\xi^n} H_n(\xi) = 2^n n! \tag{7.30}$$

holds.

From this we find that

$$\int_{-\infty}^{\infty} H_n(\xi) \frac{d^n}{d\xi^n} \mathrm{e}^{-\xi^2}\, d\xi = (-1)^n (2^n) n! \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2}\, d\xi = (-1)^n (2^n) n! \sqrt{\pi} \quad , \tag{7.31}$$

and for the normalization constant,

$$N_n = \sqrt{\sqrt{\frac{\lambda}{\pi}} \frac{1}{2^n n!}} \quad .$$

The stationary states of the harmonic oscillator in quantum mechanics are therefore

$$\psi_n(x) = \sqrt{\frac{1}{2^n n!} \sqrt{\frac{\lambda}{\pi}}} \exp\left(-\frac{1}{2} \lambda x^2 \right) H_n(\sqrt{\lambda} x) \quad . \tag{7.32}$$

Here we have suppressed the phase factor $(-1)^n$, since it is not essential. To discuss the solution, we take a look at the first three eigenfunctions of the linear harmonic oscillator (see Fig. 7.1):

Now we shall solve the problem using the operator method

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2]\, u_n(x) = E_n\, u_n(x)$$

If this is multiplied by $2/\hbar\omega$ we get

$$\left[\frac{-\hbar}{m\omega}\frac{\partial^2}{\partial x^2}+\frac{m\omega}{\hbar}x^2\right]u_n(x) = \frac{2E_n}{\hbar\omega}u_n(x). \qquad (A)$$

Introducing the variables

$$y = \left(\frac{m\omega}{\hbar}\right)^{1/2} x,$$

$$\epsilon_n = E_n/\hbar\omega,$$

the equation becomes

$$\left(\frac{\partial^2}{\partial y^2}-y^2\right)u_n(y) = -2\epsilon_n u_n(y). \qquad (B)$$

So far, only change of variable is involved

Small exercise

$$\underline{\left(\frac{\partial}{\partial y}+y\right)\left(\frac{\partial}{\partial y}-y\right)} u_n(y)$$

$$= \left[\frac{\partial}{\partial y}\left(\frac{\partial}{\partial y}-y\right)+y\left(\frac{\partial}{\partial y}-y\right)\right]u_n(y) \qquad (\text{linear})$$

$$= \left[\frac{\partial^2}{\partial y^2}-\frac{\partial}{\partial y}y+y\frac{\partial}{\partial y}-y^2\right]u_n(y)$$

$$= \left[\frac{\partial^2}{\partial y^2}-y^2\right]u_n(y) - \underbrace{\frac{\partial}{\partial y}y\,u_n(y)}_{\parallel \; -y\frac{\partial}{\partial y}u_n(y)-u_n(y)} + y\frac{\partial}{\partial y}u_n(y)$$

$$-y\frac{\partial}{\partial y}u_n(y) - u_n(y) + y\frac{\partial}{\partial y}u(y)$$

$$= \underline{\left(\frac{\partial^2}{\partial y^2}-y^2-1\right)} u_n(y) \qquad (C1)$$

$$= \underline{[-2\epsilon_n - 1]}\, u_n(y)$$

Use the same method, we can show

$$\underline{\left(\frac{\partial}{\partial y}-y\right)\left(\frac{\partial}{\partial y}+y\right)u_n(y) = [-2\epsilon_n+1]\,u_n(y)} \qquad (C2)$$

Comment

(A) - (C) are the fundamental equations

$(\frac{\partial}{\partial y} - y)$ operates on (C1)

$$(\frac{\partial}{\partial y} - y)(\frac{\partial}{\partial y} + y)\underline{\underline{(\frac{\partial}{\partial y} - y)u_n(y)}}$$
$$= [-2\epsilon_n - 1]\underline{\underline{(\frac{\partial}{\partial y} - y)u_n(y)}} \qquad (D)$$

Let $(\frac{\partial}{\partial y} - y)u_n(y) = \tilde{u}_n(y)$

$$(\frac{\partial}{\partial y} - y)(\frac{\partial}{\partial y} + y)\tilde{u}_n(y) = [-2\epsilon_n - 1]\tilde{u}_n(y) \qquad (E)$$

There are two possiblities

(i) $\tilde{u}_n(y)$ does not exist, i.e.,

$\tilde{u}_n(y) = 0 \qquad (\frac{\partial}{\partial y} - y)u_n(y) = 0$

By inspection $e^{\frac{1}{2}y^2}$ is the solution

$\frac{\partial}{\partial y}e^{\frac{1}{2}y^2} = y e^{\frac{1}{2}y^2}$ ✓ not acceptible

(ii) $\tilde{u}_n(y)$ exists and equation (E) is satisfied

$$\Rightarrow (\frac{\partial^2}{\partial y^2} - y^2 - 1)\tilde{u}_n(y) = [-2(\epsilon_n + 1) - 1]\tilde{u}_n(y)$$

$$\Rightarrow (\frac{\partial^2}{\partial y^2} - y^2)\tilde{u}_n(y) = -2(\epsilon_n + 1)\tilde{u}_n(y)$$

$\tilde{u}_n(y) = (\frac{\partial}{\partial y} - y)u_n(y)$ is solution of (B)

with $\epsilon_n \to \epsilon_n + 1$

$\Rightarrow$ If we found a solution $u_n(y)$ with ϵ_n then by operating it with $\frac{\partial}{\partial y} - y$ we will get another solution $\tilde{u}_n(y)$ with $\tilde{\epsilon}_n = \epsilon_n + 1$

$$\tilde{u}_n(y) \longrightarrow \underset{\displaystyle \left(\frac{\partial}{\partial y} - y\right) u_n(y)}{\overset{}{u_{n+1}(y) \atop \|}} \quad \text{with} \quad \epsilon_{n+1} = \epsilon_n + 1$$

Comment

We can obtain other solutions with higher energy than $u_n(y) \leftrightarrow \epsilon_n$ by (repeatedly) operating $\left(\frac{\partial}{\partial y} - y\right)$ on $u_n(y)$

$\Rightarrow$ $\frac{\partial}{\partial y} - y$ is known as a raising operator.

Use the same method we can show that

$\frac{\partial}{\partial y} + y$ is a lowering operator, i.e.,

$\frac{\partial}{\partial y} + y$ operator on $u_n(y)$ with ϵ_n

with $u_{n-1}(y)$ with $\epsilon_{n-1} = \epsilon_n - 1$

This procedure can be repeated

until $\left(\frac{\partial}{\partial y} + y\right) u_0(y) = 0$

$$\Downarrow$$

$$u_0(y) = e^{-\frac{1}{2}y^2}$$

$\downarrow$ acceptable solution

Substitute back into (B) $\Rightarrow$ $\epsilon_0 = \frac{1}{2}$

$\downarrow$ ground state energy.

All $u_n(y)$ can be obtained

by repeadly applying the raising operators

on $u_0(y)$

After solving the time independent Schrodinger equation $\quad \psi_n(x) \longleftrightarrow \epsilon_n$

$\Rightarrow$ The most general form of the wave function

$$\psi(x,t) = \sum_n c_n \psi_n(x) e^{i \epsilon_n t/\hbar}$$

c_n is determined by the initial condition e.g. $\psi(x,0)$

The system is completely specified by $\psi(x,t)$

Stationary state

$\psi(x,0)$ is one of the ψ_n

$\downarrow$

$c_n = 1$, others $= 0$

$$\psi(x,t) = \psi_n e^{i \epsilon_n t/\hbar}$$

$$|\psi(x,t)|^2 = |\psi_n(x)|^2$$

$\downarrow$

independent of time.

Energy levels

Experimental "verification" : Frank - Hertz experiment.

Lecture 2

Operator

Physical Observer $\longleftrightarrow$ linear Hamitian operator

$$\hat{A} \longrightarrow \hat{A}^{+}$$

$\downarrow$ Hermitian adjoint

Hermitian operator $\hat{A} = \hat{A}^{+}$

$\langle A \rangle$ is real $\Rightarrow$ $\hat{A}$ is Hermilian

Eigenfunctions and Eigenvalues

Orthogonal. Theorem

Example

$$(\hat{A}\hat{B})^{+} = \hat{B}^{+}\hat{A}^{+}$$

Commutator $[\hat{A}, \hat{B}]$

Physical Meaning of Eigenfunctions and Eigenvalues

Simultaneous Eigenfunctions of $\hat{A}, \hat{B}$

$\updownarrow$

$$[\hat{A}, \hat{B}] = 0$$

Uncertainty Relation

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4} \langle i[\hat{A}, \hat{B}] \rangle$$

An operator $\hat{A}$ is a mapping

$$\hat{A}\,\psi(x) = \phi(x)$$

$\psi(x)$, $\phi(x)$ are square integral functions

Expectation Value of a Physical Observable

$$\langle A \rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\, A_{op}\, \psi(x,t)\, dx$$

We shall surpress the t - dependence.

$\langle A \rangle = \int \psi^*(x)\, A_{op}\, \psi(x)\, dx$ $\qquad$ ψ is square integrable

A_{op} is the operator which is somehow related to A

Example

$\langle x \rangle = \int \psi^*(x)\, x\, \psi(x)\, dx$ $\qquad$ $x_{op} \rightarrow x$

$\langle P_x \rangle = \int \psi^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right) \psi(x)\, dx$ $\qquad$ $P_{x,op} \rightarrow -i\hbar \frac{\partial}{\partial x}$

Physical observables $\longrightarrow$ linear Hermitian operators

An operator is linear

$\equiv$ $\qquad A\left[\alpha \psi_1(x) + \beta \psi_2(x)\right] = \alpha A \psi_1(x) + \beta A \psi_2(x)$

superposition principle.

It can be easily shown that x_{op}, $P_{x,op}$ are linear operators

Generalization.

$H = \frac{p^2}{2m} + V \longrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ $\quad$ one dimension

$-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$ $\quad$ three dimension.

Hamiltonian

Definition of Hermitian adjoint of the operator $A \rightarrow A^+$

$$\int dx\, (A\psi_2)^* \psi_1 = \int dx\, \psi_2^* A^+ \psi_1$$

A is Hermitian $\Leftrightarrow$ $A = A^+$

Example $\qquad A = x$

$$\int dx\, (x\psi_2)^* \psi_1 = \int dx\, x^* \psi_2^* \psi_1 = \int dx\, \psi_2^*\, x\, \psi_1$$

$\Rightarrow \quad A^{\dagger} = x = A$

thus x is a Hermitian operator

$A = p_{x,op} \Rightarrow -i\hbar \frac{\partial}{\partial x}$ (in one dimension $\frac{d}{dx}$)

$$\int_{-\infty}^{\infty} dx \, (-i\hbar \frac{\partial}{\partial x} \psi_2)^* \psi_1 = \int_{-\infty}^{\infty} dx \, (+i\hbar) \frac{\partial \psi_2^*}{\partial x} \psi_1$$

$$= i\hbar \, \psi_2^* \underset{\downarrow \, 0}{\psi} \Big|_{-\infty}^{\infty} - i\hbar \int dx \, \psi_2^* \frac{\partial}{\partial x} \psi_1$$

partial integration

$$= \int \psi_2^* \left(-i\hbar \frac{d}{dx}\right) \psi_1 \, dx$$

$$A^{\dagger} \longrightarrow -i\hbar \frac{d}{dx} \longrightarrow -i\hbar \frac{\partial}{\partial x} = A$$

p_x is also a Hermitian operator

$A = H_{op} = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$ in one dimension.

Exercise Show H is a Hermitian operator.

We want the operator to be Hermitian since we want $\langle A \rangle$ to be real

$$\langle A \rangle = \int \psi^* A \psi \, dx \underset{\downarrow}{=} \int (A\psi(x))^* \psi(x) \, dx$$

A is Hermitian

$\Rightarrow \langle A \rangle$ is real

$$\left[\int \psi^* A \psi \, dx \right]^* = \int \psi \, (A\psi)^* \, dx$$

Example : $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} k x^2$

Eigenfunctions and eigenvalue

$$\underset{\downarrow}{A\, u_n(x) = a_n u_n(x)}$$

eigenvalue equation

$$\int u_m^* A u_n \, dx = \int u_m^* a_n u_n \, dx$$

$\parallel$

$$\int (A u_m)^* u_n \, dx$$

$\parallel$

$$a_m^* \int u_m^* u_n \, dx$$

$$\Rightarrow \quad (a_n - a_m^*) \int u_m^* u_n \, dx = 0$$

$m = n \qquad (a_n - a_n^*) \int u_n^* u_n \, dx \quad \Rightarrow \quad a_n = a_n^*$

$m \neq n \qquad \int u_m^* u_n \, dx = 0$

$\downarrow$

u_m, u_n are orthogonal.

Example $\quad H\psi_n = E_n \psi_n \quad$ with $\quad H = -\frac{\hbar^2}{2m} + \frac{1}{2}kx^2$

$\downarrow$

simple harmonic oscillator.

we shall come to eigenfunctions and eigenvalues, after we have discussed the commutator

Theorem: $\quad (AB)^+ = B^+A^+$

Proof: $\quad \int \psi_2^* (AB)^+ \psi_1 = \int (AB\psi_2)^* \psi_1$

$$= \int (B\psi_2)^* (A^+ \psi_1)$$

$$= \int \psi_2^* B^+ A^+ \psi_1$$

$$\Rightarrow \quad (AB)^+ = B^+ A^+$$

A generalization of this is

$$(ABC \cdots Z)^+ = Z^+ \cdots C^+ B^+ A^+$$

Commutator $\quad [A, B] = AB - BA$

Example $\quad [x, p_x] = x(p_x) - p_x(x) = x(-i\hbar\frac{\partial}{\partial x}) + i\hbar\frac{\partial}{\partial x} x$

$$[x, p_x]\psi(x) = -x(i\hbar\frac{\partial}{\partial x}) + i\hbar\frac{\partial}{\partial x} x\psi(x) = i\hbar\,\psi(x)$$

$\downarrow$

any square integral function

$\Rightarrow \quad [x, p_x] = i\hbar \quad \rightarrow$ fundamental commutator relation

Note $[x, p_y] = 0$

$$[x, p_y] = x(-i\hbar\frac{\partial}{\partial y}) - (-i\hbar\frac{\partial}{\partial y})x$$

$$[x, P_y]\psi(x,y,z) = 0$$

for any $\psi(x,y,z)$ that is square integrable

$\Rightarrow [x, P_y] = 0$

these two operators are said to be commuting operator

The following properties of commutators can be easily shown.

(i) $[A, B] = -[B, A]$

(ii) $[A, B]^+ = (AB)^+ - (BA)^+ = B^+A^+ - A^+B^+$
$= [B^+, A^+]$

(iii) If A, B are Hermitian, so is $i[A, B]$
This follows directly from the proceding properties.

(iv) $[AB, C] = ABC - CAB = ABC - ACB + ACB - CAB$
$= A[B, C] + [A, C]B.$

Exercise: Establish that
$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$
this is known as Jocobi identity

Exercise: Show that for any operator A,
$A + A^+$, $i(A - A^+)$, AA^+
are Hermitian.

It can be shown that raising and lowering operator are not Hermitian. Still they are useful.

The Physical Meaning of Eigenfunctions and Eigenvalues

$$H_{op} u_E(x) = E\, u_E(x)$$

An operator operates on a function usually gives another function

Only when "proper" conditions are met, the new function is a constant multiply the original function

These original functions are said to be eigenfunctions of the operator, the multiplicative constants are known as the eigenvalues.

In the example of simple harmonic oscillator

$$\psi_n(x) = \left(\frac{m\omega}{n\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\xi^2/2}$$

$$\left[\ \omega = \sqrt{\frac{k}{\omega}}\ ,\quad \xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x\ \right]$$

are eigenfunctions of the operator $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$ with eigenvalues

$$E_n = (n + \tfrac{1}{2})\hbar\omega \quad \text{for } n = 0, 1, 2, \cdots$$

If we measure the expectation of H for a state at $\psi_n(x)$

$$\underset{\substack{\downarrow \\ \text{expectation value}}}{\langle H \rangle} = \int_{-\infty}^{\infty} \psi_n^* H \psi_n \, dx = E_n \int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx = E_n$$

$$\underset{\substack{\downarrow \\ \text{standard derivation}}}{\langle \sigma^2 \rangle} = \left(\langle (H - \langle H \rangle)^2 \rangle \right. = \langle H^2 \rangle - 2\langle H \rangle \langle H \rangle + \langle H \rangle^2$$

$$= \langle H^2 \rangle - \langle H \rangle^2$$

$\langle H^2 \rangle$ for a state in ψ_n is given by

$$\int_{-\infty}^{\infty} \psi_n^* H^2 \psi_n \, dx = E_n^2 \int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx = E_n^2$$

$\Rightarrow$ $\langle \sigma^2 \rangle = 0$

↓

no spread away from the average of energy

$\Rightarrow$ particle described by an eigenfunction $\psi_E(x, t)$ has a definite E

↳ real

$\psi_E^*(x,t)\,\psi(x,t)$ is independent of time.

Remarks.

· The argument applies to all observables.
$\updownarrow$
Hermitian, linear operator
$\downarrow$
they have real eigenvalues

$A\,u_\alpha = \alpha\,u_\alpha$

· u_α, α are the eigenfunctions and eigenvalues of A operator respectively

· A measurement $\longleftrightarrow$ operator A on a state u_α gives a definite value α.

$\Rightarrow$ energy could be discrete, $E_n = (n+\frac{1}{2})\hbar\omega$ for SHO
if the "particle" (electron) is in an eigenstate of energy with eigenvalue E_n, then it will have definite energy E_n
$\Rightarrow$ energy level.
furthermore, it will not decay
$\downarrow$
the probability of finding it in this state is independent of time

$\Rightarrow$ stationary state.

The Schrodinger equation in three dimension will be discussed in Chapter 9 (part I) next

The eigenfunction u_a corresponding to the eigenvalue a of the operator A

$$A u_a(x) = a u_a(x)$$

will be simultaneous eigenfunctions of another B when

$$B u_a(x) = b u_b(x)$$

$\Rightarrow$ $AB u_a(x) = A b u_a(x) = b A u_a(x) = ab u_a(x)$

$BA u_a(x) = B a u_a(x) = a B u_a(x) = ab u_a(x)$

$\Rightarrow$ $(AB - BA) u_a(x) = 0$

$\psi(x) = \sum_a C_a u_a(x)$

$(AB - BA)\psi(x) = (AB - BA)\sum_a C_a u_a(x)$

$= \sum_a C_a (AB - BA) u_a(x) = 0$

valid for any $\psi(x)$ $\Rightarrow$ $AB - BA = 0$

$\Rightarrow$ A, B commute

Conversely if A, B are two Hermitian operators

$$[A, B] = 0$$

$$A \underline{B u_a(x)} = B a u_a(x) = a \underline{B u_a(x)}$$

$B u_a(x)$ is also an eigenfunction of A corresponding to eigenfunction of A corresponding to the eigenvalue a.

If there is only eigenfunction of A corresponding to eigenvalue a, then $B u_n(x)$ must be proportional to $u_a(x)$

$\Rightarrow$ $B u_a(x) = b u_a(x)$

$\Rightarrow$ $u_a(x)$ is a simultaneous eigenfunction of A and B

If there is only eigenfunction of A, with eigenvalue a, then the eigenfunctions of A are not degenerate. (definition)

If there are two eigenfunctions of A corresponding to the eigenvalue a, i.e., we have two-fold degeneracy

$$A u_n^{(1)}(x) = a u_n^{(1)}(x)$$

$$A u_n^{(2)}(x) = a u_n^{(2)}(x)$$

$\Rightarrow$ $B\,u_a^{(1)}(x)$ and $B\,u_n^{(2)}(x)$ must be linear combination of $u_a^{(1)}(x)$ and $u_a^{(2)}(x)$

$$B\,u_a^{(1)}(x) = b_{11}\,u_a^{(1)}(x) + b_{12}\,u_a^{(2)}(x)$$

$$B\,u_a^{(2)}(x) = b_{21}\,u_a^{(1)}(x) + b_{22}\,u_a^{(2)}(x)$$

$$B(\underline{u_a^{(1)}(x) + \lambda u_a^{(2)}}) = (b_{11} + \lambda b_{21})\,u_a^{(1)} + (b_{12} + \lambda b_{22})\,u_a^{(2)}$$

Choose $\lambda = \dfrac{b_{12} + \lambda b_{22}}{b_{11} + \lambda b_{21}}$ (A)

$$= (b_{11} + \lambda b_{21})\underbrace{\left[u_a^{(1)} + \frac{b_{12} + \lambda b_{22}}{b_{11} + \lambda b_{12}}u_a^{(2)}\right]}_{\underline{u_a^{(1)} + \lambda u_a^{(2)}}}$$

Find λ by solving equation (A) $\Rightarrow$ two λ's

λ_1 $\quad u_a^{(1)} + \lambda_1 u_a^{(2)}$

$\downarrow$

eigenfunction of B
with eigenvalue $b_{11} + \lambda_1 b_{21}$
it is also an eigenfunction of
A with eigenvalue a

λ_2 $\quad u_a^{(1)} + \lambda_2 u_a^{(2)}$

eigenfunction of B
with eigenvalue $b_{11} + \lambda_2 b_{21}$
it is also eigenfunction of
A with eigenvalue a.

Thus we have found simultaneous eigenfunctions of A, B.

The procedure can be extended to higher degeneracy.

For a set of mutually commuting operators $A, B, C, \cdots M$ we can find a set of functions which are simultaneous eigenfunctions of $A, B, C, \cdots M$

These set of common eigenfunctions is called a complete set of commuting observable.

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Uncertainty relation

$$(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2 = \langle (A - \langle A\rangle)^2\rangle$$

$$(\Delta B)^2 = \langle B^2\rangle - \langle B\rangle^2 = \langle (B - \langle B\rangle)^2\rangle$$

Define $U = A - \langle A\rangle$
$V = B - \langle B\rangle$

Consider $\phi = U\psi + i\lambda V\psi$

$$I(\lambda) = \int dx\, \phi^*\phi \geq 0$$

$$= \int dx\, (U\psi + i\lambda V\psi)^* (U\psi + i\lambda V\psi)$$

$$= \int dx\, (U\psi)^*(U\psi) + \lambda^2 \int dx\, (V\psi)^*(V\psi)$$
$$+ i\lambda \int dx \{(U\psi^*)(V\psi) - (V\psi)^*(U\psi)\}$$

U, V are Hermitian

$$= \int dx\, \psi^* (U^2 + \lambda^2 V^2 + i\lambda \underbrace{[U, V]}_{\text{commutator}})\psi$$

$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \int dx\, \psi^* [U, V] \psi$$

$[U, V] = [A, B]$

$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \langle [A, B]\rangle \geq 0$$

Minimum occur at $\dfrac{dI(\lambda)}{d\lambda} = 0$

$$2\lambda (\Delta B)^2 + i\langle [A, B]\rangle = 0$$

$$\Rightarrow \quad \lambda = -i \frac{\langle [A, B]\rangle}{2(\Delta B)^2}$$

Substitute into $I(\lambda)$

$$\Rightarrow \quad (\Delta A)^2 - \frac{\langle [A,B]\rangle^2}{4(\Delta B)^2} + \frac{\langle [A,B]\rangle^2}{2(\Delta B)^2} \geq 0$$

$$\Rightarrow \quad (\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} \langle i[A, B]\rangle^2$$

this is the "uncertainty relation

$A \rightarrow x_{op}$, $B \rightarrow P_{op}$

$$[A, B] \rightarrow [x, p_x] = i\hbar$$

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$

this is the uncertainty relation
of Heisenberg.

Lecture 3

Uncertainty relation and wave-particle duality

Heisenberg's microscope

Momentum wave function

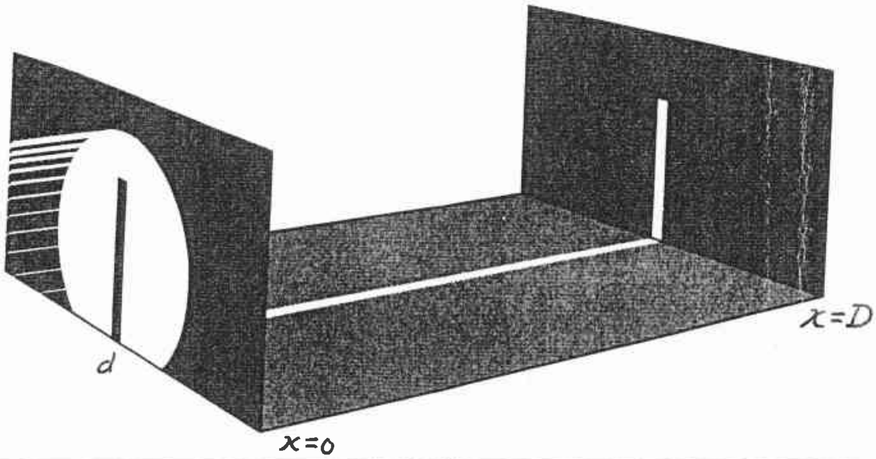
Application of uncertainty relation.

- No effect on macroscopic objects
- "Confinement" of electron
- "Zero point" energy
- Estimate of atomic size
- Unstable particle.
- Width of atomic spectral line.
- Range of strong force

Final questions

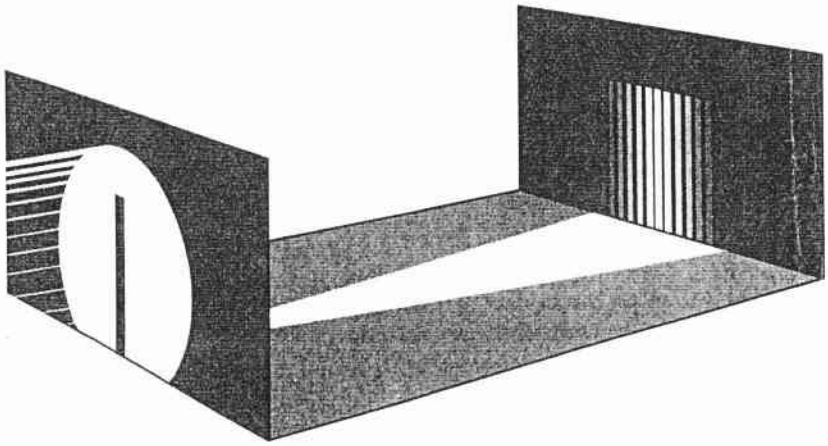
Uncertainty relation and wave-particle duality

Classical particle



A beam of particle of momentum P_x emerges from the slit $x=0$, $\Delta y = d$ they will strike the screen at $x=D$ within a marrow strip of width d.

According to classical mechanics, the image of a slit upon which a beam of particles is incident is the geometric projection of the slit.



If a slit is illuminated by waves (e.g., light), a diffraction pattern is seen on the screen.

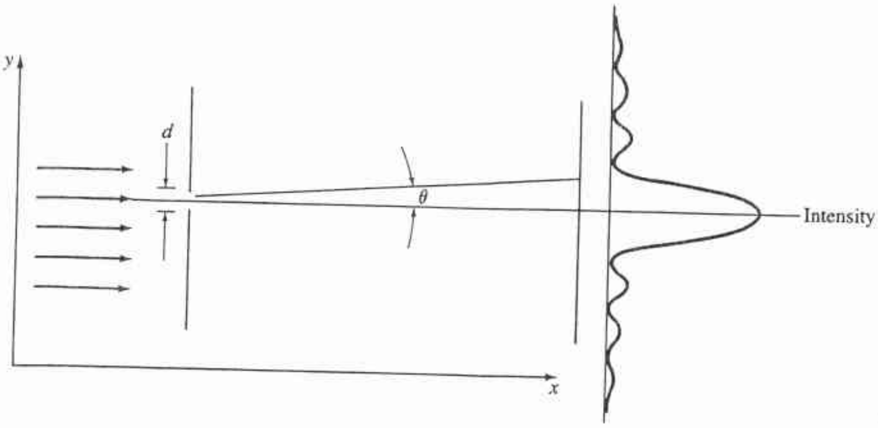
Wave $\Rightarrow$ the intensity of the wave will exhibit the typical diffraction pattern

The width of the pattern is defined by the angular seperation between the two minima bordering the central maximum. $= 2\theta$

$$\sin\theta \simeq \theta = \frac{\lambda}{d} = \frac{\lambda}{\Delta y} \qquad \text{for } \theta \ll 1 \qquad (\lambda \ll d)$$

See P. 701 of Alonso and Finn

$\Rightarrow$ the more we try to delimit the position of the wave at $x = 0$ by reducing the width of the slit the more we broaden the diffraction pattern



Particles exhibit wavelike behavior, we can use above equation and the de Broglie relation to determine ΔP_y (the spread in P_y)

$$\frac{\Delta P_y}{P_x} = \frac{\delta y}{D} = \tan\theta \sim \theta = \frac{\lambda}{\Delta y}$$

$$\frac{h}{P} \sim \frac{h}{P_x} = \lambda$$

$$\frac{\Delta P_y}{P_x} = \frac{h/P_x}{\Delta y}$$

$\Rightarrow \quad \Delta P_y \, \Delta y \simeq h \quad \rightarrow$ consistent with the uncertainty relation

Remark:

Uncertainty relation is a direct and necessary consequences of the wave nature of particles.

The uncertainty relation is independent of λ.

The beam of electrons is moving only in the x direction so before passing the slit it has no momentum component in the y direction ($P_y = 0$)

Since we know P_y exactly $(\Delta P_y = 0)$

$\Delta \quad = \infty$

we have no knowledge at all about
the particles along the y direction.

The diffraction (spreading) of a beam following passage through a slit is the effect of the uncertainty principle on our attempt to specify the location of the particle.

As we make the slit narrower P_y increases and the beam spread even more
The trade-off between observations of position and momentum is the core of the Heisenberg uncertainty principle.

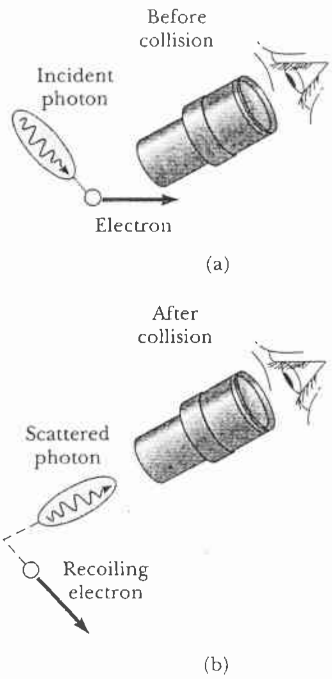
Heisenberg's microscope

This photograph of Werner Heisenberg was taken around 1924 (University of Hamburg). Heisenberg obtained his PhD in 1923 at the University of Munich where he studied under Arnold Sommerfeld and became an enthusiastic mountain climber and skier. Later, he worked as an assistant to Max Born at Göttingen and Niels Bohr in Copenhagen. While physicists such as de Broglie and Schrödinger tried to develop pictorialized models of the atom, Heisenberg, with the help of Born and Pascual Jordan, developed an abstract mathematical model called matrix mechanics to explain the wavelengths of spectral lines. The more successful wave mechanics by Schrödinger announced a few months later was shown to be equivalent to Heisenberg's approach. Heisenberg made many other significant contributions to physics, including his famous uncertainty principle, for which he received the Nobel prize in 1932, the prediction of two forms of molecular hydrogen, and theoretical models of the nucleus. During World War II he was director of the Max Planck Institute at Berlin where he was in charge of German research on atomic weapons. Following the war, he moved to West Germany and became director of the Max Planck Institute for Physics at Göttingen.

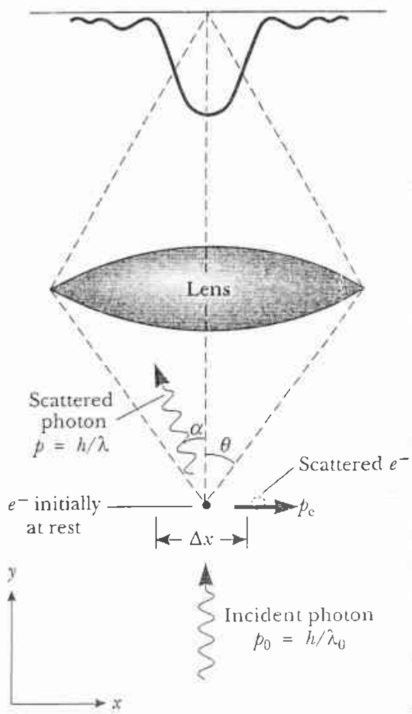
B I O G R A P H Y

WERNER HEISENBERG
(1901–1976)

(Photo courtesy of the University of Hamburg)



A thought experiment for viewing an electron with a powerful microscope. (a) The electron is shown before colliding with the photon. (b) The electron recoils (is disturbed) as a result of the collision with the photon.



The Heisenberg microscope. Conservation of momentum requires $p_{e^-} = (h \sin \alpha)/\lambda$. Because of diffraction by the lens opening, the electron may be anywhere in the region Δx.

Use the photon to measure the position of an electron.

Photon as wave

$\downarrow$

resolving the position to Δx
with wavelength λ, then

$$\Delta x = \frac{\lambda}{2\sin\theta}$$

where 2θ is the angle
subtended by the object lens

To be collected by the lens, the photon may be scattered through an angle from $-\theta$ to $+\theta$

$$\Delta p_x = 2p\sin\theta = 2\frac{h}{\lambda}\sin\theta$$

$\updownarrow$

the uncertainty of p_x
imparts to the electron
(momentum conservation)

$$\Rightarrow \quad \Delta p_x \, \Delta x = \frac{2h}{\lambda}\sin\theta \cdot \frac{\lambda}{2\sin\theta}$$

$$= h.$$

· Again, we see that it is a consequence of particle-wave duality

· The result is independent of λ.

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Take the case of $H = \frac{p^2}{2m}$ in one dimension

It can be readily show that $[H, P] = 0$

$\Rightarrow$ one can find simultaneous eigenfunctions of H, P

Eigenvalue problem for momentum operator

$$-i\hbar \frac{d}{dx} \; u_p(x) = p\, u_p(x)$$

$$\Rightarrow \quad \underbrace{u_p(x)}_{\text{eigenfunction}} = A e^{ipx/\hbar}$$

It is a plane wave solution

$$\underbrace{\int_{-\infty}^{\infty} u_p^*(x)\, u_p(x)\, dx}_{\text{it cannot be normalized.}} = |A|^2 \int_{-\infty}^{\infty} dx$$

Solution exists for $\underbrace{\text{all}}_{\text{continuous spectrum}}$ real p

Localized particle $\rightarrow$ wave packet.

$$\psi_n(x,t) = u_n(x)\, e^{-iE_n t}$$

$$\psi(x,t) = \sum_n c_n u_n(x)\, e^{-iE_n t}$$

$$\rightarrow \int \underbrace{A(p)}_{\text{this is equation (7.12) of the textbook}} e^{i(px - Et)/\hbar} dp$$

Look at the situation at $t=0$

$$\psi(x) = \int A(p)\, e^{ipx/\hbar} dp$$

Next we want to find the meaning of $A(p)$

$$\int e^{-ip'x/\hbar}\, \psi(x)\, dx = \iint A(p)\, e^{ipx/\hbar}\, e^{-ip'x/\hbar}\, dx\, dp$$

$$\int e^{ipx/\hbar} e^{-ip'x/\hbar} dx = 2\pi\hbar\delta(p-p')$$

See notes on Dirac δ-function

$$\int_{-\infty}^{\infty} e^{i(p-p')y} dy = \delta(p-p')$$

$$\int e^{-ip'x/\hbar} \psi(x) dx = \int A(p) \, 2\pi\hbar\delta(p-p') dp = 2\pi\hbar A(p')$$

$$\langle p \rangle = \int dx \, \psi^*(x) \frac{\hbar}{i} \frac{\partial \psi(x)}{\partial x}$$

$$= \int dx \, \psi^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \int A(p) e^{ipx/\hbar} dp$$

$$= \int dp \, A(p) p \int dx \, \psi^*(x) e^{ipx/\hbar}$$

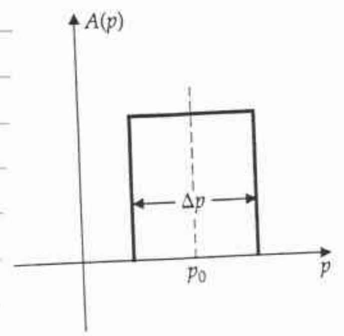
$$= 2\pi\hbar \int dp \, A(p) p \, A^*(p)$$

$\Rightarrow$ $2\pi\hbar \, |A(p)|^2 dp =$ probability that the momentum will be found between p and $p+dp$

(7-15) of the textbook.

Example

$$A(p) = \begin{cases} 0 & \text{for } p < p_0 - \Delta p/2 \\ C & \text{for } p_0 - \frac{\Delta p}{2} < p < p_0 + \frac{\Delta p}{2} \\ 0 & \text{for } p > p_0 + \Delta p/2 \end{cases}$$



The weight function $A(p)$ for Eq. (7–16).

$$\psi(x) = \int_{-\infty}^{\infty} A(p) e^{ipx/\hbar} dp = C \int_{p_0 - \Delta p/2}^{p_0 + \Delta p/2} e^{ipx} dx$$

$$q = p - p_0$$

$$= C e^{ip_0/\hbar} \int_{-\Delta p/2}^{\Delta p/2} e^{iqx/\hbar}$$

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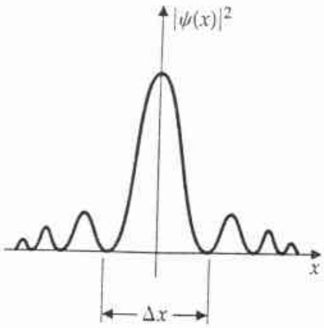
$$= c\, e^{ip_0 x/\hbar} \frac{\hbar}{ix} \left[e^{x\Delta p/2\hbar} - e^{-ix\Delta p/2\hbar} \right]$$

$$= 2c\, e^{ip_0 x} \frac{\hbar}{x} \sin \frac{x\Delta p}{2\hbar}$$

$$|\psi(x)|^2 = \frac{4c^2\hbar^2}{x^2} \sin^2 \frac{x\Delta p}{2\hbar}$$



The probability density $|\psi(x)|^2$ obtained in Eq. (7–18) that results from the superposition of plane waves with the weight function $A(p)$ of Eq. (7–16). Our choice of "width"—the distance between the first two minima of the distribution—is shown in the figure.

The first minimum occur at $x = \pm x_0$

$$\frac{x_0 \Delta p}{2\hbar} = \pi$$

$$x_0 = \frac{2\pi\hbar}{\Delta p}$$

$$\Rightarrow \quad \Delta x = 2x_0 = \frac{4\pi\hbar}{\Delta p} \quad \Rightarrow \quad \Delta p \Delta x = 2h$$

From the correspondence

$$p \leftrightarrow E$$
$$x \leftrightarrow t$$

$$\Rightarrow \quad \Delta E \Delta t \geq \frac{\hbar}{2}$$

time - energy uncertainty relation

It asserts that a state of finite duration Δt cannot have a precisely defined energy in E specified by
$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$

Applying the uncertainty principle

· It is a useful tool, not a just a negative statement

· It is a great help in understanding many phenomena in quantum level.

· It gives a qualitative estimates

· The lower limit of $\frac{\hbar}{2}$ for $\Delta x \Delta p_x$ is rarely attained.

· The uncertainty principle changing nothing for macroscopic objects
racquetball 100 g confined to a room of 15 m on a side. the ball is moving at 2 m/sec along x axis

$$\Delta p_x \geq \frac{\hbar}{2\Delta x} = \frac{1.05 \cdot 10^{-34} \, J \cdot sec}{2 \cdot 10 m}$$

$$= 3.5 \cdot 10^{-36} \, kg \, m/sec$$

$$\Delta v_x = \frac{\Delta p_x}{m} \sim 3.5 \cdot 10^{-35} \, m/sec$$

$$\frac{\Delta v_x}{v_x} = 1.8 \cdot 10^{-35}$$
↳ certainly unmeasurable

· Estimate the minimum kinetic energy of an electron confined by the electromagnetic force to be inside an atom
$\Delta x \simeq 0.1 \, nm$ → atomic radius
$m = 0.5 \, MeV/c^2$
$$\langle E_k \rangle_{min} = \frac{\hbar^2}{8m(\Delta x)^2} \sim 1 eV$$

Estimate the minimum kinetic energy of the proton to be inside the nucleus
$\Delta x \simeq 2 fm$ → nuclear radius
$\Rightarrow \langle E_k \rangle_{min} \sim 1 MeV.$

· Do electron exist within the nucleus

Nuclear size is take to be $1 \cdot 10^{-14}$ m

$$\Rightarrow \quad \Delta p = \underset{\substack{\downarrow \\ 20\ \mathrm{MeV}/c}}{2 \cdot 10^{7}} \frac{eV}{c} \sim p \quad \sim 20\ \mathrm{MeV}/c$$

Need relativity

$$\cancel{E^2 = p^2c^2 + (m_e e)^2}$$

$$E \geq 20\ \mathrm{MeV} \qquad K = E - m_e c^2 \geq 19.2\ \mathrm{MeV}$$

Since electron emitted in radioactive decay of the nucleus (β decay) have energies much less than 19.2 MeV (about 1 MeV or less) and is known no other mechanism could carry off an internuclear electron's energy during the decay process

$\Rightarrow$ electrons observed in β-decay do not come from within the nucleus but are actually created at the instant of decay.

· "Zero-point" energy of a harmonic oscillator

$$\cancel{(\Delta p)^2 = \langle (p - \langle p \rangle)^2 \rangle = \langle (p^2 - 2p\underset{0}{\langle p \rangle} + \underset{0}{\langle p \rangle^2}) \rangle = \langle p \rangle^2}$$

$$\langle K.E. \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{(\Delta p)^2}{2m}$$

Same argument $\quad \langle P.E. \rangle = \frac{1}{2} m\omega^2 (\Delta x)^2$

$$\Rightarrow \quad E = \frac{1}{2} m\omega^2 (\Delta x)^2 + \frac{(\Delta p)^2}{2m}$$

$$\Delta p\, \Delta x \geq \frac{\hbar}{2}$$

$$\Rightarrow \quad E \geq \frac{1}{2} m\omega^2 (\Delta x)^2 + \frac{\hbar^2/8m}{(\Delta x)^2}$$

$$\frac{\partial E}{\partial (\Delta x)} = 0 \quad \Rightarrow \quad (\Delta x)_{min} = \sqrt{\frac{\hbar}{2m\omega}}$$

$$\Rightarrow E_{min} = \frac{1}{2} \hbar \omega$$

Exercise Estimate the size of hydrogen atom

$$E = \frac{p^2}{2m} - \frac{ke^2}{r} \qquad k = \frac{1}{4\pi\epsilon_0}$$

$\Delta x = r$

$(\Delta p)^2 = \langle p^2 \rangle \geq \frac{\hbar^2}{r^2}$

$E = \frac{\hbar^2}{2mr^2} - \frac{ke^2}{r}$

$\frac{dE}{dr} = 0 \Rightarrow r_{min} = \frac{\hbar^2}{ke^2 m} = a_0$
↳ Bohr radius

$\Rightarrow E_{min} = -\frac{k^2e^4m}{2\hbar^2} = -13.6\,eV$

· Unstable particle

Many elementary particles are unstable
For example, the Δ has an average lifetime of only $3\cdot 10^{-24}$ sec.
The average mass of the Δ is $1232\ MeV/c^2$
What is the uncertainty in the measurement of the mass of the Δ?

$\Delta E \geq \frac{\hbar}{2\Delta t} \simeq 110\ MeV$
↓
the uncertainty in its rest energy

$\Rightarrow m_\Delta = 1232 \pm 110\ MeV/c^2$

· Width of atomic spectral lines.

When an atom is raised to an excited state, it usually decays to the ground state in about $\Delta t \sim 10^{-8}$ sec.
Consequently, there is an uncertainty in the short-lived excited state and a corresponding uncertainty in the wavelength of the radiation emitted as the atom returns to the ground state

$$\lambda = \frac{hc}{E_i - E_f}$$

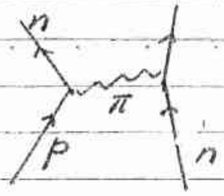
$E_i \rightarrow$ initial, excited state
$E_f \rightarrow$ final, ground state

$$\frac{d\lambda}{dE_i} = -\frac{hc}{(E_i - E_f)^2} = -\frac{\lambda}{E_i - E_f}$$

$$\Rightarrow \frac{\Delta\lambda}{\lambda} = -\frac{\Delta E}{E_i - E_f}$$

$$\Delta E \geq \frac{\hbar}{2\Delta t}$$

Range of the Forces



In order to produce π meson

$$\Delta E \gtrsim 140\ \text{MeV} = m_\pi c^2$$

It can "live"

$$\Delta t = \frac{h}{2\Delta E} = \frac{h}{2 m_\pi c^2}$$

It at most travel a distance

$$R = c\Delta t = \frac{hc}{2\Delta E} = \frac{\hbar}{2 m_\pi c^2}$$

↓

mass - range relation

Nuclear force has a range ~ 1-2 fm $\Rightarrow$ m_π can be estimated

↓

Yukawa.

Eigenstate of position operator

$$x\, u_{x_0}(x) = x_0\, u_{x_0}(x)$$

$$\Rightarrow \quad u_{x_0}(x) = \delta(x - x_0)$$

$$[L_x, L_y] = i\hbar L_z$$

$$\Downarrow$$

$$\Delta L_x \, \Delta L_y \gtrsim \langle \hbar L_z \rangle$$

If a state is in the eigenstate of $L_x \Rightarrow \Delta L_x = 0$

But for this state, we can prove $\langle L_z \rangle = 0$

The uncertainty relation is still valid.