FYS245

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Chapter 1: Light

Chapter 2: Wave mechanics

Chapter 3: The time-independent Schrödinger equation

Separation of variables

When V(x) is independent of t, we can solve Schrödinger's equation by separation of variables.

$$\Psi(x,t) = \psi(x)f(t) \quad \Rightarrow \quad \frac{\delta^2\Psi(x,t)}{\delta x^2} = f(t)\frac{d^2\psi(x)}{dx^2} \quad \text{and} \quad \frac{\delta\Psi(x,t)}{\delta t} = \psi(x)\frac{df(t)}{dt} \tag{1}$$

This leads to the time-independent Schrödinger's equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{2}$$

And a solution to the time-dependent Schrödinger's equation:

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \tag{3}$$

Where $\psi(x)$ is the solution to the time-independent equation. This is a stationary state, because the probability density

$$|\Psi(x,t)|^2 = \psi^*(x)e^{iEt/\hbar}\psi(x)e^{-iEt/\hbar} = |\psi(x)|^2 \tag{4}$$

is independent of time.

Particle in a box

The potential inside the box $(0 < x < L)$ is 0. This leads to the general solution:

$$\psi(x) = Asin(kx) + Bcos(kx) \tag{5}$$

for $0 < x < L$. And the boundary conditions $\psi(0) = \psi(L) = 0$ are used to find A and B. Which lead to the solution for the allowed energies and corresponding wave functions:

$$E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}, \quad \psi_n(x) = A_n sin(\frac{n\pi x}{L}) \quad \text{for } n = 1,2,3,\dots \tag{6}$$

where A_n is found by normalizing the equation. $A_n = \sqrt{2/L}$:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}sin(\frac{n\pi x}{L}) & 0 < x < L \\ 0 & elsewhere \end{cases} \quad n = 1,2,3,\dots \tag{7}$$

Statistical interpretation

The wave function can be expressed as a superposition:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x) \quad c_n = A\phi(t) \quad \phi(t) = e^{-iE_nt/\hbar} \tag{8}$$

Where A is the normalization coefficient, and $|c_n|^2 = |A|^2$ is the probability P_n of obtaining E_n if a measurement is made.

$$\langle E\rangle = \sum_{n=1}^{\infty}|c_n|^2E_n \tag{9}$$

Orthonormality

If

$$\int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x)dx = \delta_{mn} \tag{10}$$

where

$$\delta_{mn} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases} \tag{11}$$

is the "Kronecker delta", then the wave functions ψ_n form an orthonormal set.

Eigenvalues and Eigenfunctions

$$A_{op}\psi_a = a\psi_a \tag{12}$$

where a is the eigenvalue and ψ_a is the eigenfunction of the operator A_{op}.a

	Position:	x_{op}	x
Common operators:	Momentum:	$p_{x_{op}}$	$\frac{\hbar}{i}\frac{\delta}{\delta x}$
	Energy:	$H \equiv E_{op}$	$\frac{(p_{x_{op}})^2}{2m} + V(x_{op}) \equiv -\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + V(x)$

This yields:

$$\langle E \rangle = \int_{-\infty}^{\infty} \Psi^* H \Psi dx \tag{13}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi|^2 dx = \int_{-\infty}^{\infty} \Psi^* x \Psi dx \tag{14}$$

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \Psi^* p_{x_{op}} \Psi dx \tag{15}$$

Chapter 4: One-dimensional potentials (confined particles)

Finite square well

$$V(x) = \begin{cases} 0 & |x| < a/2 \\ V_0 & |x| > a/2 \end{cases} \tag{16}$$

Inside well ($V_0 = 0$)

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{17}$$

$$k = \frac{\sqrt{2mE}}{\hbar} \tag{18}$$

Outside well ($0 < E < V_0$)

$$\psi(x) = \begin{cases} Ce^{\kappa x} & x < -a/2 \\ De^{-\kappa x} & x > a/2 \end{cases} \tag{19}$$

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \tag{20}$$

Dirac delta function

$$\delta(x) = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases} \tag{21}$$

$$\int_{-\infty}^{\infty} f(x)\delta(x)dx = f(0)\int_{-\infty}^{\infty} \delta(x)dx = f(0) \tag{22}$$

Step potential

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases} \tag{23}$$

$$k = \frac{\sqrt{2mE}}{\hbar} \tag{24}$$

$$k_0 = \frac{\sqrt{2m(E - V_0)}}{\hbar} \tag{25}$$

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ik_0x} + De^{-ik_0x} \equiv Ce^{ik_0x} & x > 0 \end{cases} \tag{26}$$

Continous requirements lead to

$$A + B = C + D \equiv A + B = C \quad \text{and} \quad ik(A - B) = ik_0(C - D) \equiv ik(A - B) = ik_0C \tag{27}$$

Because we are not interested in D, we set this to 0.
This yields the probability currents

$$j_x = \begin{cases} \frac{\hbar k}{m}(|A|^2 - |B|^2) & x < 0 \\ \frac{\hbar k_0}{m}|C|^2 & x > 0 \end{cases} \tag{28}$$

And the reflection and transmission coefficients:

$$R = \frac{(k - k_0)^2}{(k + k_0)^2} \quad \text{and} \quad T = \frac{4kk_0}{(k + k_0)^2} \tag{29}$$

Where R + T = 1.

Tunneling

E < V_0.

$$T \cong \left(\frac{4\kappa k}{k^2 + \kappa^2}\right)^2 e^{2\kappa a} \tag{30}$$

Chapter 5: Principles of quantum mechanics

Parity operator Π

$$\Pi\psi(x) = \psi(-x) \tag{31}$$

This means that the parity operator is an eigenequation, with eigenvalues ± 1.

$$\Pi\psi_{\lambda=1}(x) = \psi_{\lambda=1}(x) \quad \Rightarrow \quad \psi_{\lambda=1}(-x) = \psi_{\lambda=1}(x) \tag{32}$$

and

$$\Pi\psi_{\lambda=-1}(x) = -\psi_{\lambda=-1}(x) \quad \Rightarrow \quad \psi_{\lambda=-1}(-x) = -\psi_{\lambda=1}(-x) \tag{33}$$

Where the eigenfunction with $\lambda = -1$ is an odd function and $\lambda = 1$ is an even function.

Hermitian operators

All operators that lead to an observable (measurable value & real eigenvalues) are Hermitian operators.

$$\langle A\rangle = \int_{-\infty}^{\infty} \Psi^* A_{op} \Psi dx \qquad \text{and} \qquad \langle A^2\rangle = \int_{-\infty}^{\infty} \Psi^* A_{op}^2 \Psi dx \tag{34}$$

$$(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2 = \int_{-\infty}^{\infty} \Psi^* A_{op}^2 \Psi dx - \left(\int_{-\infty}^{\infty} \Psi^* A_{op} \Psi dx\right)^2 \tag{35}$$

Commutation

$$[A_{op}, B_{op}] \equiv A_{op}B_{op} - B_{op}A_{op} \tag{36}$$

Commuting operators

When two Hermitian operators commute, they have a complete set of eigenfunctions in common. We can then know both of these dynamical variables simultaneously, without uncertainty.

Noncommuting operators

$$[A_{op}, B_{op}] = iC_{op} \tag{37}$$

$$\Delta A \Delta B \geq \frac{|\langle C\rangle|}{2} \tag{38}$$

Time development

$$\frac{d\langle A\rangle}{dt} = \frac{i}{\hbar} \int_{-\infty}^{\infty} \Psi^* \left[H, A_{op}\right] \Psi dx + \int_{-\infty}^{\infty} \Psi^* \frac{\delta A_{op}}{\delta t} \Psi dx \tag{39}$$

Where A is the observable assosiated with a linear Hermitian operator A_{op}.

Chapter 6: In three dimensions

With three dimensions we separate the variables

$$\psi(x,y,z) = X(x)Y(y)Z(z) \qquad \text{where} \qquad E = E_x + E_y + E_z \tag{40}$$

Where the eigenvalues and eigenfunctions are:

$$E_{n_x,n_y,n_z} = \frac{(n_x^2 + n_y^2 + n_z^2)\hbar^2\pi^2}{2mL^2} \qquad \text{and} \qquad \psi_{n_x,n_y,n_z} = \left(\frac{2}{L}\right)^{3/2} sin\frac{n_x \pi x}{L} sin\frac{n_y \pi y}{L} sin\frac{n_z \pi z}{L} \tag{41}$$

Orbital angular momentum

$$\mathbf{p}_{op} = \frac{\hbar}{i}\nabla \qquad \text{where} \qquad \nabla = \frac{\delta}{\delta x} + \frac{\delta}{\delta y} + \frac{\delta}{\delta z} \tag{42}$$

Spherical coordinates

$$\begin{gathered} x = r sin\theta cos\phi \\ y = r sin\theta sin\phi \\ z = r cos\theta \\ \textstyle\int dxdydz = \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} r^2 sin\theta dr d\theta d\phi \end{gathered} \tag{43}$$

Spherical harmonics

Eigenfunctions: $Y_{l,m_l}(\theta,\phi)$ satisfy

$$\begin{aligned} L_{zop}Y_{l,m_l}(\theta,\phi) &= m_l\hbar Y_{l,m_l}(\theta,\phi) \qquad && \mathrm{m}_l = -l,-l+1,\ldots,l-1,l \\ \mathbf{L}_{op}^2 Y_{l,m_l}(\theta,\phi) &= l(l+1)\hbar^2 Y_{l,m_l}(\theta,\phi) && l=0,1,2,\ldots \end{aligned} \tag{44}$$

The uncertainty relation inangular momentum is

$$\Delta L_x \Delta L_y \geq \frac{\hbar}{2}|\langle L_z\rangle| \tag{45}$$

Quantum numbers

Number	Symbol	Possible values
Principal Quantum Number	n	1, 2, 3, ...
Angular Momentum Quantum Number	l	0, 1, 2, ..., $(n-1)$
Magnetic Quantum Numer	m_l	$-l,\ldots,-1,0,1,\ldots,l$
Spin Quantum Number	m_S	$+1/2$, $-1/2$

The shell depends on the value of l. s, p, d and f corresponds to ($l=$) 0, 1, 2 and 3.
Allowed Quantum Numbers:

n	**l**	**m$_l$**	**# orbitals**	**Orb. name**	**# electrons**
1	0	0	1	1s	2
2	0	0	1	2s	2
	1	$-1,0,+1$	3	2p	6
3	0	0	1	3s	2
	1	$-1,0,+1$	3	3p	6
	2	$-2,-1,0,+1,+2$	5	3d	10
$\vdots$					

Hydrogen atom

$$\Psi(r,\theta,\phi) = R(r)Y_{l,m_l}(\theta,\phi) \tag{46}$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\right] + \frac{l(l+1)\hbar^2}{2mr^2}R - \frac{Ze^2}{4\pi\epsilon_0 r}R = ER \tag{47}$$

Where $Z=1$ for hydrogen, and e is the charge.

$$E_n = -\frac{mZ^2e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2} = -\frac{(13.6eV)Z^2}{n^2} \tag{48}$$

Emission

$$h\nu = E_{n_{initial}} - E_{n_{final}} \tag{49}$$

Chapter 7: Identical particles

Exchange operator

$$P_{1,2}\Psi(1,2) = \Psi(2,1) \qquad P_{1,2}\psi_{n_1}(x_1)\psi_{n_2}(x_2) = \psi_{n_1}(x_2)\psi_{n_2}(x_1) \tag{50}$$

For identical particles this leads to

$$P_{1,2}\Psi(1,2) = \lambda\Psi(1,2) \tag{51}$$

with the allowed eigenvalues $\lambda = \pm 1$. It is $=1$ for symmetric states (bosons), and $=-1$ for antisymmetric states (fermions).

Pauli principle

No two electrons can have the exact same quantum numbers, n, l, m_l, m_S.

Fermi energy

The highest energy state (level) occupied.

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3} \tag{52}$$

Where

$$N = \frac{V(2mE_F)^{3/2}}{3\hbar^3\pi^2} \tag{53}$$

$$E_{total} = \frac{3}{5}NE_F \tag{54}$$

Chapter 8: Solid-state physics