Quantum states

$|\alpha\rangle$ - ket or $\langle\alpha|$ - bra

Normalization $\langle\alpha|\alpha\rangle = 1$

Orthogonality $\langle\alpha|\beta\rangle = 0$

Normally, we work with orthonormal basis $\{|n\rangle\}$ $\Rightarrow$ $\langle n|m\rangle = \delta_{nm}$

State decomposition $|\alpha\rangle = \sum_n C_n |n\rangle$

$C_n = \langle n|\alpha\rangle$ — probability amplitude

Probability to find a particle in a specific state $|n\rangle$

$P_n = |C_n|^2 = |\langle n|\alpha\rangle|^2 = |\langle\alpha|n\rangle|^2$ since $\langle n|\alpha\rangle = \langle\alpha|n\rangle^*$

Operators $\hat{A}$: $|\beta\rangle = \hat{A}|\alpha\rangle$

operators can modify states

Eigen values and eigenstates

$\hat{A}|n\rangle = A_n|n\rangle$ A_n – eigenvalue

$|n\rangle$ – eigenstate

Typically, we choose a basis to describe some quantum system to be eigenbasis for some operator (often Hamiltonian)

Expectation value / average value of $\hat{A}$ in $|\alpha\rangle$

$\langle\hat{A}\rangle = \langle\alpha|\hat{A}|\alpha\rangle$

Systems / operators . we considered
Angular momentum operators
Spin - 1/2 and Spin - 1 particles

Relevant operators $\hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{S}^2$

$\hat{S}_x, \hat{S}_y, \hat{S}_z$ do not commute

$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z \quad [\hat{S}_y, \hat{S}_z] = i\hbar \hat{S}_x \quad [\hat{S}_z, \hat{S}_x] = i\hbar \hat{S}_y$

$\hat{S}^2$ commute with everything, so normally we use a basis that is common eigenbasis for $\hat{S}^2$ and $\hat{S}_z$

$$\hat{S}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle$$
$$\hat{S}_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle$$

Same is ~~done~~ done for orbital ang. momentum $\hat{L}$ and total ang. momentum $\vec{J} = \vec{L} + \vec{S}$

$$\hat{L}^2 | l, m_l\rangle = \hbar^2 l(l+1) | l, m_l\rangle$$
$$\hat{L}_z | l, m_l\rangle = \hbar m_l | l, m_l\rangle$$

Hamiltonian $\hat{H}$ — energy operator

$$\hat{H} = \hat{K} + \hat{U} = \frac{\hat{p}^2}{2m} + \hat{U}$$

Eigen states — stationary states

$$\hat{H}|n\rangle = E_n|n\rangle$$

Hamiltonian determines <u>time-evolution</u> of any state

$$-i\hbar \frac{\partial|\alpha\rangle}{\partial t} = \hat{H}|\alpha\rangle$$

$$|\alpha(t)\rangle = e^{-i\hat{H}t/\hbar}|\alpha(t=0)\rangle$$

If we are in the eigenbasis of $\hat{H}$

$\hat{H}|n\rangle = E_n|n\rangle$, and $e^{-i\hat{H}t/\hbar}|n\rangle = e^{-iE_nt/\hbar}|n\rangle$

So if $|\alpha(t=0)\rangle = \sum_n c_n|n\rangle$ then

$$|\alpha(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}|n\rangle$$

Probability to find the particle in state n

$P_n(t) = |c_n e^{-iE_nt/\hbar}|^2 = |c_n|^2$ — doesn't depend on time

However

$\langle A\rangle(t) = \langle\alpha(t)|\hat{A}|\alpha(t)\rangle$ will depend on t unless $[\hat{A},\hat{H}]=0$

Particles with angular momentum in magnetic field

$$\hat{\vec{L}}, \hat{\vec{S}}, \hat{\vec{J}} \longrightarrow \hat{\vec{\mu}} \quad \text{magnetic moment}$$

$$\hat{\vec{\mu}} = \mu_B \cdot \hat{L} \quad \text{or} \quad \hat{\vec{\mu}} = g\mu_B \hat{S} \qquad g \approx 2 \text{ for } \bar{e}$$

$$\hat{H} = -\hat{\vec{\mu}}\vec{B} = -\hat{\mu}_z B_z = \omega_B \cdot L_z \ (\text{or } S_z \text{ or } J_z)$$

$$\hat{H}|s, m_s\rangle = \omega_B \hat{S}_z |s, m_s\rangle = \hbar\omega_B m_s |s, m_s\rangle$$

$$s = 1/2, \quad m_s = \pm 1/2 \qquad E_\pm = \pm \frac{\hbar\omega_B}{2}$$

$$s = 1, \quad m_s = 0, \pm 1 \qquad E = 0, \pm\hbar\omega_B$$

later

~~Orbital~~ Zeeman effect: electron energy level shift in magnetic field

$$\hat{H}|n l m_l\rangle = \omega_B \hat{L}_z |n l m_l\rangle = \underbrace{\hbar\omega_B m_l}_{\Delta E_{m_l}} |n l m_l\rangle$$

Similar for a quantum rotator

$$\hat{H}_0 = \frac{\hat{L}^2}{2I} \qquad \hat{H}_0 |l, m\rangle = \frac{\hbar^2 l(l+1)}{2I} |l, m\rangle$$

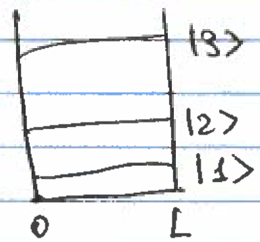
In the magnetic field

$$\hat{H} = \hat{H}_0 + \hat{H}_B = \frac{\hat{L}^2}{2I} + \omega_0 \hat{L}_z$$

$$\hat{H}|l, m\rangle = \left[\frac{\hbar^2 l(l+1)}{2I} + \hbar\omega_0 m_l\right] |l, m\rangle$$

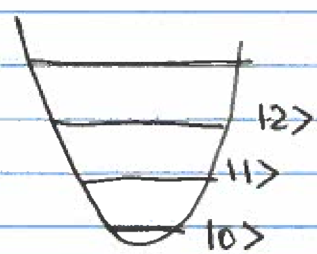
Spatially constrained quantum particles
descrete energy spectrum

1. Infinite well (1D)



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

2. ~~Coulumb~~ ~~potential~~ Harmonic oscillator



$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

Ladder operators

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

To calculate probability of particle distribution function in space, it is convenient to choose basis of eigenstate of position $\hat{x}$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \longrightarrow |\alpha\rangle \to \psi_\alpha(x) = \langle x|\alpha\rangle$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \qquad \underbrace{\hat{H}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi}_{\text{solutions } \psi_n(x),\ E_n}$$

Normalization/orthogonality $\displaystyle\int_{-\infty}^{+\infty} \psi_n^*(x)\psi_m(x)\,dx = \delta_{nm}$

$$\langle\hat{A}\rangle = \int_{-\infty}^{+\infty} \psi_n^*(x)\,\hat{A}\,\psi(x)\,dx$$

expectation value of $\hat{A}$ in the state $\psi(x)$

Probability to locate a particle $x \in [a, b]$

$$P_{a,b} = \int_a^b \psi^*(x)\,\psi(x)\,dx$$

Decomposition $\psi(x) = \sum_n c_n \psi_n(x)$

$$c_n = \int_{-\infty}^{+\infty} \psi_n^*(x)\,\psi(x)\,dx$$

Probability to find a particle in the state $|n\rangle\ [\psi_n(x)]$

$$P_n = \left| \int_{-\infty}^{+\infty} \psi_n^*(x)\,\psi(x)\,dx \right|^2 = |c_n|^2$$

3D potentials $\rightarrow$ need 3 quantum numbers to describe a quantum state

Cartesian coordinates $\rightarrow$ "square well"

$$\psi_{n_x, n_y, n_z}(\vec{r}) = \psi_{n_x}(x)\,\psi_{n_y}(y)\,\psi_{n_z}(z)$$

$$E_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2m} \left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right]$$

states can be degenerate, if the same value of energy correspons to different combination of indices.

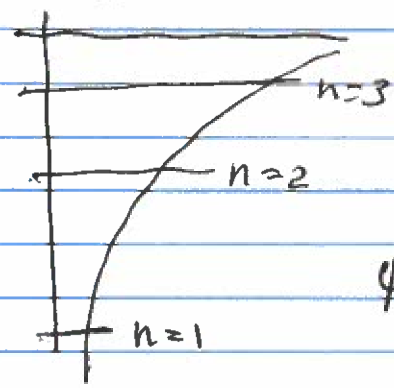
Spherically symmetric potential $U = U(r)$

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + U(r)\psi(\vec{r})$$

In this case $[\hat{H}, \hat{L}^2] = 0$ and $[\hat{H}, \hat{L}_z] = 0$

Convenient to work in the common basis of $\hat{H}, \hat{L}^2, \hat{L}_z$: $|n, \ell, m_\ell\rangle$

Hydrogen atom $U(r) = -\frac{ke^2}{r}$



$$E_n = -\frac{E_R}{n^2}$$

Eigenstates $|n, \ell, m_\ell\rangle$

$$\psi_{n\ell m_\ell} = \frac{U_{n\ell}(r)}{r} \underbrace{Y_{\ell m}(\theta, \varphi)}_{\text{spherical functions}}$$

eigenfunctions of $\hat{L}^2, \hat{L}_z$

Zeeman effect : energy level splitting in magnetic field

$$\hat{H}_0 |n, \ell, m\rangle = E_n |n, \ell, m\rangle$$

$$\hat{H} = \hat{H}_0 + \hat{H}_B = \hat{H}_0 + \omega_B \hat{L}_z$$

$$\hat{H} |n, \ell, m\rangle = (E_n + \hbar\omega_B m_\ell) |n, \ell, m\rangle = E_{n, m_\ell} |n, \ell, m\rangle$$

for $m_\ell = -\ell, .. 0, .. \ell$, in magnetic field single energy level splits into $(2\ell+1)$ sublevels

Free-moving particles (1D)

Eigenstate of $\hat{p}_x \to \frac{1}{\sqrt{2\pi\hbar}} e^{-ip_x \cdot x/\hbar} = \psi_{p_x}(x)$

$\hat{H} = \frac{\hat{p}^2}{2m}$ $\qquad \hat{p}_x \psi_{p_x}(x) = p_x \psi_{p_x}(x)$

$\hat{H}\psi_{p_x}(x) = \frac{\hat{p}^2}{2m}\psi_{p_x}(x) = \frac{p_x^2}{2m}\psi_{p_x}(x)$

Wave-vector $p_x = \hbar k$.

$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{\pm ikx}$ $\qquad \hat{H}\psi_k(x) = \frac{\hbar^2 k^2}{2m}\psi_k(x) =$
$= E\psi_k(x)$

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

Constant potential $E > U_0$

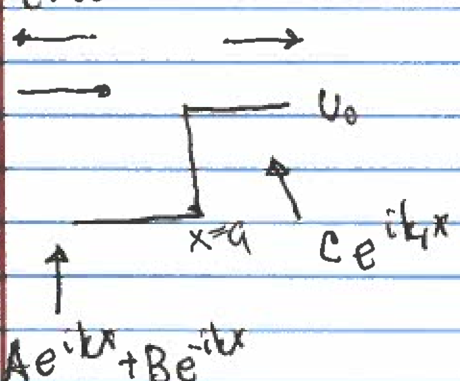
$k_1 = \sqrt{\frac{2m(E-U_0)}{\hbar^2}}$ real wave

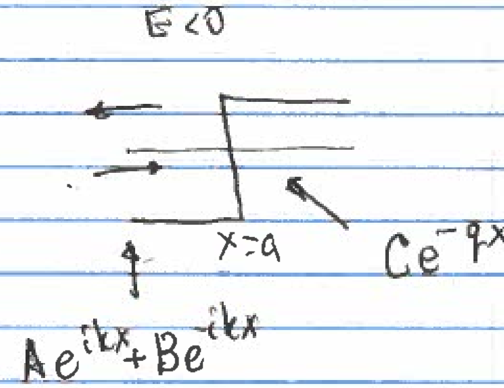
$E < U_0$ — evanescent (non-propagating wave)

$q = \sqrt{\frac{2m(U_0-E)}{\hbar^2}}$

$\psi_q(x) \propto e^{\pm qx}$

$E > U_0$ $\qquad\qquad$ $E < U_0$





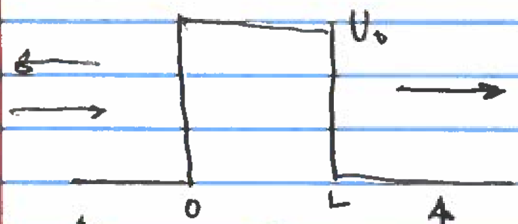
Boundary conditions (for non-infinite potential)

$\psi(x=a-0) = \psi(x=a+0)$ continuous

$\psi'(a-0) = \psi'(a+0)$ smooth

Barriers & wells

$E<U_0$



Reflection

$$R = \left|\frac{B}{A}\right|^2$$

$Ae^{ikx}+Be^{-ikx}$ $\quad$ $Fe^{ik(x-L)}$

Transmission

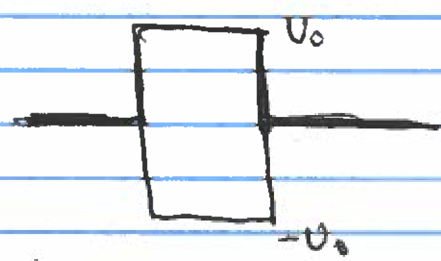
$$T = \left|\frac{F}{A}\right|^2$$

$Ce^{qx}+De^{-qx}$

$E>U_0$

Two boundaries $(x=0, L)$

Four boundary conditions



$Ae^{ikx}+Be^{-ikx}$ $\quad$ $Fe^{ik(x-L)}$

$Ce^{ik_1x}+De^{-ik_1x}$