Physics 491
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Lecture #13 Dynamics

Recall Born collapse postulate.

Separation of variables solution to Schrodinger equation ()=Hamiltonian operator

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

$\Psi(x,t) = \phi_n e^{-iE_n t/\hbar}$ energy eigenstates, eigenvalues

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \right] \phi_n(x) = E_n \phi_n(x)$$

gives time evolution of any state in terms of expansion by energy eigenstates.

$$\Psi(x,t) = \sum_n C_n \phi_n(x) e^{-iE_n t/\hbar}$$

Formal approach - <u>unitary evolution</u> of state implies unitary time evolution operator

$$\hat{U}(t) \, |\psi(0)\rangle = |\psi(t)\rangle$$

$$\langle \psi(t)|\psi(t)\rangle = \langle \psi(0)|U^\dagger U|\psi(0)\rangle = \underset{=1}{\langle \psi(0)|\psi(0)\rangle}$$

Hermitian operator $\hat{H}$ is the generator

$$\lim_{\Delta t \to 0} \hat{U}(\Delta t) = 1 - \frac{i}{\hbar}\hat{H}\Delta t$$

$\hat{H}$ has dimensions of energy. Will turn out to be the Hamiltonian operator.

$\hat{U}$ evolution equation. We must be careful because we might have $\hat{H}(t)$ and possibly even
$$[\hat{H}(t_1), \hat{H}(t_2)] \neq 0.$$

$$\hat{U}(t+\Delta t) = \hat{U}(\Delta t)\,\hat{U}(t) =$$
$$\left(1 - \frac{i}{\hbar}\hat{H}\,\Delta t\right)\hat{U}(t)$$

so $$\frac{\hat{U}(t+\Delta t) - \hat{U}(t)}{\Delta t} = \frac{-i}{\hbar}\hat{H}\,\hat{U}(t)$$

taking the limit $\Delta t \to 0$

$$\boxed{\frac{d}{dt}\hat{U}(t) = \frac{-i}{\hbar}\hat{H}\,\hat{U}(t)}$$

This equation is true very generally. Therefore, the state evolves as

$$i\hbar\,\hat{U}(t)|\Psi(0)\rangle = i\hbar|\Psi(t)\rangle$$

differentiate to get $$\boxed{i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle}$$

General Schrödinger equation. Physics comes from $\hat{H}$.

Important simplifications. First, if $\hat{H}$ has no explicit time dependence,

$$\hat{U}(t) = \lim_{N\to\infty}\left[1 - \frac{i}{\hbar}\hat{H}\frac{t}{N}\right]^N = e^{-i\hat{H}t/\hbar}$$

Second, if $[\hat{H}(t_1), \hat{H}(t_2)] = 0$ then

$$\hat{U}(t) = \exp\left(\frac{-i}{\hbar}\int_0^t \hat{H}(t')\,dt'\right)$$

Otherwise, we must solve $\hat{U}$ evolution equation or Schrödinger equation explicitly.

<u>Energy Eigenstates</u> $|E_i\rangle$ form a complete set of states (basis)

$$\hat{H}|E_i\rangle = E_i|E_i\rangle$$

$$|\psi(0)\rangle = \sum_i |E_i\rangle \underbrace{\langle E_i|\psi(0)\rangle}_{\text{amplitudes } c_i}$$

then for $\hat{H}$ with no explicit time dependence,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = \sum_i c_i e^{-iE_it/\hbar}|E_i\rangle$$

This generalizes earlier wavefunction formula.

space>|spin>

Example 1 : charged particle $(q=-e)$ in magnetic field. From classical physics

$$E = -\vec{\mu}\cdot\vec{B}$$

Quantum mechanical operator is

$$\hat{H} = -\hat{\vec{\mu}}\cdot\vec{B} = -\left(\frac{-eg}{2mc}\hat{\vec{S}}\right)\cdot\vec{B}$$

$$= \left(\frac{eg}{2mc}\right)\hat{\vec{S}}\cdot\vec{B}$$ not it is rotational invariant

Let $\vec{B} = B\hat{z}$, $\omega_0 \equiv \frac{egB}{2mc}$ angular frequency

$$\hat{H} = \omega_0 \hat{S}_z \xrightarrow[z\ \text{basis}]{} \omega_0 \frac{\hbar}{2}\hat{\sigma}_z = \frac{\omega_0\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

Suppose $|\psi(0)\rangle = |+x\rangle = \frac{1}{\sqrt{2}}\left(|+z\rangle + |-z\rangle\right)$

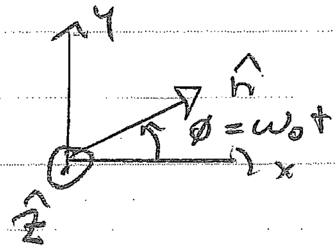
$\hat{H}$ has no explicit time dependence for constant B

$$\hat{U}(t)|\pm z\rangle = e^{-i\hat{H}t/\hbar}|\pm z\rangle = e^{\mp\frac{\omega_0 t}{2}}|\pm z\rangle$$

factor out $e^{-i\frac{\omega_0 t}{2}}$ to pick out phase difference

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}e^{-i\omega_0 t/2}\left(|+z\rangle + e^{+i\omega_0 t}|-z\rangle\right)$$

State precesses about magnetic field direction $\hat{z}$ with frequency $f = \omega_0/2\pi$.



$$P(\pm z) = \left| \langle \pm z | \psi(t) \rangle \right|^2 = \frac{1}{2}$$

$$P(+x) = \left| \langle +x | \psi(t) \rangle \right|^2$$

$$\langle +x | \psi(t) \rangle = e^{-i\omega_0 t/2} \frac{1}{2} \left(\langle +z| + \langle -z| \right) \left(|+z\rangle + e^{i\omega_0 t} |-z\rangle \right)$$

$$= e^{-i\omega_0 t/2} \frac{1}{2} (1, 1) \begin{pmatrix} 1 \\ e^{i\omega_0 t} \end{pmatrix}$$

$$= \frac{1}{2} \left(e^{-i\omega_0 t/2} + e^{+i\omega_0 t/2} \right) = \cos\left(\frac{\omega_0 t}{2}\right)$$

$$P(+x) = \cos^2\left(\frac{\omega_0 t}{2}\right)$$

Similarly $P(-x) = \sin^2(\omega_0 t/2)$
from which you can calculate $\langle S_x \rangle$

$$\langle S_x \rangle = \frac{\hbar}{2}\left[\cos^2\left(\frac{\omega_0 t}{2}\right) - \sin^2\left(\frac{\omega_0 t}{2}\right)\right]$$

$$= \frac{\hbar}{2} \cos(\omega_0 t)$$

Expectation Values

$$\frac{d}{dt}\langle \hat{A} \rangle = \frac{d}{dt}\langle \psi(t) | \hat{A} | \psi(t) \rangle$$

$$= \left(\frac{d}{dt}\langle \psi(t)|\right) \hat{A} \, |\psi(t)\rangle$$

$$+ \quad \langle \psi(t) | \frac{\partial \hat{A}}{\partial t} | \psi(t) \rangle$$

$$+ \quad \langle \psi(t) | \hat{A} \frac{d}{dt} | \psi(t) \rangle$$

$$= \langle \psi(t) | \left[\frac{+i\hat{H}t}{\hbar} \hat{A} - \hat{A}\left(\frac{i\hat{H}t}{\hbar}\right)\right] | \psi(t) \rangle$$

$$+ \quad \frac{\partial}{\partial t}\langle \hat{A} \rangle$$

We can write this as an operator equation

$$\boxed{\frac{d}{dt}\hat{A} = \frac{i}{\hbar}\left[\hat{H}, \hat{A}\right] + \frac{\partial \hat{A}}{\partial t}}$$

We see that if $\hat{A}$ commutes with $\hat{H}$ and has no explicit time dependence,

$\langle \hat{A} \rangle$ is conserved.

Follows that if $\hat{H}$ has no explicit time dependence, $E = \langle \hat{H} \rangle$ is conserved.

Example 2 $\hat{H} = \omega_0 \hat{S}_z$

We immediatly see that $\langle \hat{S}_z \rangle$ is conserved but not $\langle \hat{S}_x \rangle$ or $\langle \hat{S}_y \rangle$.

$$\frac{d}{dt}\hat{S}_x = \frac{i}{\hbar}\left[\hat{H}, \hat{S}_x\right] = \frac{i\omega_0}{\hbar}\underbrace{\left[\hat{S}_z, \hat{S}_x\right]}_{i\hbar \hat{S}_y} = -\omega_0 \hat{S}_y$$

so $\frac{d}{dt}\langle \hat{S}_x \rangle = -\omega_0 \langle \hat{S}_y \rangle$ for any state.

Take $|\psi(0)\rangle = |+x\rangle \xrightarrow[z]{} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$|\psi(t)\rangle \xrightarrow[z]{} \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\omega_0 t/2} \\ e^{+i\omega_0 t/2} \end{pmatrix}$$

$$\langle \hat{S}_x \rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \left(e^{+i\omega_0 t/2}, e^{-i\omega_0 t/2}\right) \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} e^{-i\omega_0 t/2} \\ e^{i\omega_0 t/2} \end{pmatrix}$$

$$= \frac{1}{2}\left(\frac{\hbar}{2}\right)\left(e^{i\omega_0 t} + e^{-i\omega_0 t}\right) = \frac{\hbar}{2}\cos(\omega_0 t)$$

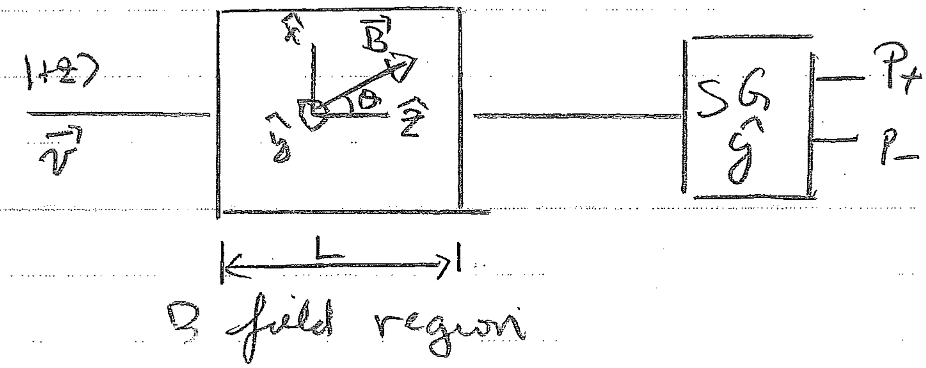
$$\langle \hat{S}_y \rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \left(e^{i\omega_0 t/2}, e^{-i\omega_0 t/2}\right) \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} e^{-i\omega_0 t/2} \\ e^{+i\omega_0 t/2} \end{pmatrix}$$

$$= \frac{1}{2}\left(\frac{\hbar}{2}\right)\frac{1}{i}\left(e^{i\omega_0 t} - e^{-i\omega_0 t}\right) = \frac{\hbar}{2}\sin(\omega_0 t)$$

so $\frac{d}{dt}\langle \hat{S}_x \rangle = -\omega_0 \frac{\hbar}{2}\sin\omega_0 t = -\omega_0 \langle \hat{S}_y \rangle$

as it should.

Example 3 Beam of spin-$\frac{1}{2}$, $q=-e$ particles



$$\vec{B} = B\left(\sin\theta\,\hat{x} + \cos\theta\,\hat{z}\right)$$

$$\hat{H} = \omega_0 \vec{S}\cdot\left(\sin\theta\,\hat{x} + \cos\theta\,\hat{z}\right) = \omega_0 \sin\theta\,\hat{S}_x + \omega_0\cos\theta\,\hat{S}_z$$

$$\xrightarrow[z]{} \frac{\omega_0\hbar}{2}\left(\sin\theta\,\vec{\sigma}_x + \cos\theta\,\vec{\sigma}_z\right)$$

$$= \frac{\omega_0\hbar}{2}\begin{pmatrix}\cos\theta & +\sin\theta\\ \sin\theta & -\cos\theta\end{pmatrix}$$

Rather than solving this eigenvalue problem, rotate to basis ($\vec{B}$) where $\hat{H}$ is diagonal. $\hat{R}^S(+\theta\hat{y})$ rotates basis, $\hat{R}^S(-\theta\hat{y})$ rotates components.

$$\hat{R}^S(+\theta\hat{y}) \Rightarrow \cos\tfrac{\theta}{2}\,\hat{I} - i\,\hat{\sigma}_y \sin\tfrac{\theta}{2} = \begin{pmatrix}\cos\theta/2, & -\sin\theta/2\\ \sin\theta/2, & \cos\theta/2\end{pmatrix}$$

so the operator transforms as

$$\left[\hat{H}\right]_B = \hat{R}^S(-\theta\hat{y})\left[\hat{H}\right]_z R^S(+\theta\hat{y}) = \frac{\omega_0\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

which we already knew.

Components of $|+z\rangle$ in B-basis

$$|\psi(0)\rangle = |+z\rangle \xrightarrow[z]{} \begin{pmatrix}1\\0\end{pmatrix}_z$$

applying $\hat{R}^s(-\theta \hat{y})$

$$\begin{pmatrix}a(0)\\b(0)\end{pmatrix}_B = \begin{pmatrix}c & s\\-s & c\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}_z = \begin{pmatrix}\cos\theta/2\\-\sin\theta/2\end{pmatrix}_B$$

Then $|\psi(t)\rangle \xrightarrow[B]{} \begin{pmatrix}\cos\frac{\theta}{2}\, e^{-i\omega_0 t/2}\\-\sin\frac{\theta}{2}\, e^{+i\omega_0 t/2}\end{pmatrix}_B$

at $t = L/v$

State $|+y\rangle$ in B-basis just acquires overall phase which can be ignored.

$$|+y\rangle \xrightarrow[B]{} \hat{R}(-\theta\hat{y})\,\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}_z = \frac{1}{\sqrt{2}}\begin{pmatrix}c+is\\-s+ic\end{pmatrix}$$

$$= e^{\frac{i\theta}{2}}\,\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}_B$$

Now we have everything in the B-basis.

$$\langle +y|\psi(t)\rangle = \frac{1}{\sqrt{2}}(1, -i)\begin{pmatrix}\cos\theta/2\, e^{-i\omega_0 t/2}\\-\sin\theta/2\, e^{+i\omega_0 t/2}\end{pmatrix}$$

$$= \frac{1}{\sqrt{2}}\left(\cos\frac{\theta}{2}e^{-i\omega_0 t/2} + i\sin\frac{\theta}{2}e^{i\omega_0 t/2}\right)$$

$$P_{+y}(t) = \left| \langle +y | \psi(t) \rangle \right|^2$$

$$= \frac{1}{2}\left[1 + i \cos\theta/_2 \sin\theta/_2 \left(e^{i\omega_0 t} - e^{-i\omega_0 t} \right) \right]$$

$$= \frac{1}{2}\left[1 - \sin\theta \sin\omega_0 t \right]$$

<u>Analogous to classical precession</u>:

$$\frac{d\vec{S}}{dt} = \vec{\tau} = \vec{\mu} \times \vec{B} = \left(\frac{-eg\vec{S}}{2mc} \right) \times \vec{B} = \omega_0 \hat{B} \times \vec{S}$$

precesses about $\hat{B}$ with frequency ω_0