Lecture VIII: Quantum Dynamics

Up until this point our developement of the "structure" of quantum mechanics has had little connection with physics. The basic connection comes through the theory of symmetries, which we will study in more detail next semester, but begin here.

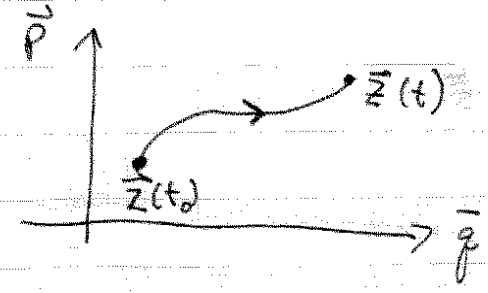
Symmetries and Conservation Laws

Noether's Theorem (1918): To every continuous symmetry (group) is associated a conserved quantity which "generates" that group

Symmetry	Conserved Quantity
• Time translation invariance	• Energy (Hamiltonian)
• Space translation invariance	• Momentum
• Rotational invariance	• Angular momentum

Classical Mechanics: flow on phase-space

$$\vec{Z}(t) = \begin{pmatrix} \vec{q}(t) \\ \vec{p}(t) \end{pmatrix} = \mathcal{J}(t,t_0) \begin{pmatrix} \vec{q}(t_0) \\ \vec{p}(t_0) \end{pmatrix}$$



Infinitesimal $\quad \frac{d}{dt}\vec{Z} = \{H, \vec{Z}\}$ ⇐ Poisson Bracket

<u>Wigner</u>: In quantum mechanics a continuous (Lie) group has a representation in terms of unitary operators (or possibly "anti-unitary" as we will see next semesters)

Consider the group of real numbers under addition

$$\mathbb{G} \equiv \{\lambda\}$$

- Group composition law $\lambda_1 \circledast \lambda_2 \equiv \lambda_1 + \lambda_2$
- Identity: I $\quad \lambda \circledast I = I \circledast \lambda = \lambda$

$$\Rightarrow \quad I = 0 \quad \text{(the number zero)}$$

- Inverse $\quad \lambda_{inv} \circledast \lambda = I \quad \Rightarrow \quad \lambda_{inv} = -\lambda$

Representation: To each element of $\mathbb{G}$, λ, we associate a unitary operator, $\hat{U}(\lambda)$

Define composition via operator multiplication

$$\hat{U}(\lambda_1) \circledast \hat{U}(\lambda_2) = \hat{U}(\lambda_1)\,\hat{U}(\lambda_2)$$

This is a <u>representation</u> of the group if

- Composition $\quad \hat{U}(\lambda_1)\,\hat{U}(\lambda_2) = \hat{U}(\lambda_1 + \lambda_2)$
- Inverse $\quad \hat{U}^{-1}(\lambda) = \hat{U}(\lambda_{inv}) = \hat{U}(-\lambda) = \underbrace{\left(\hat{U}^{\dagger}(\lambda)\right)}_{\text{unitary}}$
- Identity $\quad \hat{U}(\lambda = 0) = \hat{\mathbb{1}}$

"Near" unity group

Define $\hat{U}(\epsilon) = \hat{\mathbb{1}} + \epsilon \hat{A}$ where $\hat{A}^{\dagger} = -\hat{A}$ (anti-Hermitian)

and $\epsilon \equiv$ "infinitesemal" in the calculus sense

$$\Rightarrow \quad \epsilon^2 = 0$$

By convention let us write $\hat{A} = -i\hat{H}$ where

$\hat{H}^{\dagger} = \hat{H}$ is a Hermitian operator

This defines the "infinitesemal" group near $\hat{\mathbb{1}}$

First $\hat{U}(\epsilon)$ is unitary

$$\hat{U}^{\dagger}(\epsilon)\,\hat{U}(\epsilon) = (\hat{\mathbb{1}} + i\epsilon\hat{H})(\hat{\mathbb{1}} - i\epsilon\hat{H})$$

$$= \hat{\mathbb{1}} + \cancel{\epsilon^2 \hat{H}^2} \to 0 \quad = \hat{\mathbb{1}} \checkmark$$

Group properties:

- Composition $\quad \hat{U}(\epsilon_1)\,\hat{U}(\epsilon_2) = \hat{\mathbb{1}} - i(\epsilon_1 + \epsilon_2)\hat{H}$

$$= \hat{U}(\epsilon_1 + \epsilon_2) \checkmark$$

- Inverse $\quad \hat{U}^{-1}(\epsilon) \overset{?}{=} \hat{U}(-\epsilon) = \hat{U}^{\dagger}(\epsilon)$

$$\hat{U}^{\dagger}(\epsilon) = \hat{\mathbb{1}} - i\epsilon\hat{H} = \hat{U}(-\epsilon) \checkmark$$

- Identity $\quad \hat{U}(0) = \hat{\mathbb{1}} \checkmark$

Time Translation Operator $\hat{U}(t, t_0)$

$$|\psi(t)\rangle = \hat{U}(t, t_0)\, |\psi(t_0)\rangle$$

continuous parameter fix

Infinitesimal version:

$$\hat{U}(t_0 + dt,\ t_0) = \hat{\mathbb{1}} - i\,\hat{\Omega}\, dt$$

$\hat{\Omega}$ is Hermitian, units $(\text{time})^{-1}$ = frequency

Noether: Time Translation invariance $\Rightarrow$ Energy conservation

$\Rightarrow$ Energy is the "generator" of time translation

$$\Rightarrow \hat{\Omega} = \alpha \hat{H} \qquad \hat{H} = \text{Hamiltonian (energy)}$$

α: constant of nature

Units $[\alpha] = (\text{energy} \cdot \text{time})^{-1} = (\text{"action"})^{-1}$

Fundamental unit of action:

$$\hbar = \frac{h}{2\pi} = 1.05 \times 10^{-27}\ \text{erg} \cdot \text{s}$$

$$\Rightarrow \boxed{\hat{U}(t_0 + dt,\ t_0) = \hat{\mathbb{1}} - \frac{i}{\hbar}\hat{H}\, dt}$$

Differential equation: (Next page)

$$\cancel{\frac{d}{dt}\hat{U}(t) = \lim_{\Delta t \to 0} \frac{\hat{U}(t+\Delta t, t_0) - \hat{U}(t, t_0)}{\Delta t} = -\frac{i}{\hbar}\hat{H}}$$

Differential equation for $\hat{U}(t,t_0)$

Aside: $\hat{U}(t+dt, t_0) = \hat{U}(t+dt, t)\ \hat{U}(t, t_0)$

$$\Rightarrow \frac{d}{dt}\hat{U}(t,t_0) = \lim_{\Delta t \to 0} \frac{\hat{U}(t+\Delta t, t_0) - \hat{U}(t,t_0)}{\Delta t}$$

$$= \lim_{\Delta t \to 0} \left(\frac{\hat{U}(t+\Delta t) - \hat{1}}{\Delta t} \right) \hat{U}(t,t_0)$$

$$\Rightarrow \boxed{\frac{d}{dt}\hat{U}(t,t_0) = -\frac{i}{\hbar}\hat{H}\ \hat{U}(t,t_0)}$$ "Schrodinger equation"

Solution: $\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$

if $\hat{H}$ is not explicitly fnct of time

"propagator"

Differential equation for state vector:

$$|\psi(t)\rangle = \hat{U}(t,t_0)\ |\psi(t_0)\rangle$$

$$\Rightarrow \frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}\hat{H}\ \hat{U}(t,t_0)\ |\psi(t_0)\rangle$$

$$\Rightarrow \boxed{\frac{\hbar}{-i}\frac{d}{dt}|\psi(t)\rangle = \hat{H}\ |\psi(t)\rangle}$$

Time dependent Schrödinger equation

Solving for the time evolution of states

Stationary states $\equiv$ Eigenstates of $\hat{H}$

$$\boxed{\hat{H}|u_\lambda\rangle = E_\lambda |u_\lambda\rangle}$$ Time Independent Schrödinger Equation (TISE)

Suppose at $t=0$ $|\psi(0)\rangle = |u_\lambda\rangle$

$$\Rightarrow |\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|u_\lambda\rangle$$

$$= e^{-\frac{i}{\hbar}E_\lambda t}|u_\lambda\rangle = e^{-i\omega_\lambda t}|u_\lambda\rangle$$

where $\hbar\omega_\lambda = E_\lambda$

$$\Rightarrow |\psi(t)\rangle = e^{-i\phi_\lambda(t)}|\psi(0)\rangle$$

Irrevalent overall phase: does not effect predictions of any measurement

However: Suppose $|\psi(0)\rangle = c_1|u_1\rangle + c_2|u_2\rangle$

Not a stationary state

$$\Rightarrow |\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = c_1\hat{U}(t)|u_1\rangle + c_2\hat{U}(t)|u_2\rangle$$

$$= c_1 e^{-\frac{i}{\hbar}E_1 t}|u_1\rangle + c_2 e^{-\frac{i}{\hbar}E_2 t}|u_2\rangle$$

$$= e^{-iE_1/\hbar\, t}\left(c_1|u_1\rangle + c_2 \underbrace{e^{-i\frac{(E_2-E_1)t}{\hbar}}}_{\text{relevant phase}}|u_2\rangle\right)$$

Note: Dynamics depend only on energy differences

Solving for the time-evolution operator

We have implicitly assumed that the Hamiltonian operator was independent of time. Then the solution to $\frac{\partial}{\partial t}\hat{U}(t;t_0) = -\frac{i}{\hbar}\hat{H}\hat{U}(t;t_0)$ is $\hat{U}(t;t_0) = \exp\{-\frac{i}{\hbar}\hat{H}(t-t_0)\}$.

Check $\hat{U}(t_0;t_0) = \hat{\mathbb{1}}$, $\hat{U}(t;t_0) = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{(t-t_0)^n}{n!}\hat{H}^n \Rightarrow \frac{\partial}{\partial t}\hat{U}(t-t_0) = \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{n}{n!}(t-t_0)^{n-1}\hat{H}^n$

$$= \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^{n+1}\frac{n+1}{(n+1)!}(t-t_0)^n\hat{H}^{n+1} = \frac{-i}{\hbar}\hat{H}\sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n\frac{1}{n!}(t-t_0)^n\hat{H}^n = -\frac{i}{\hbar}\hat{H}\hat{U}(t;t_0)$$

<u>Aside</u>: Note every unitary operator is of the form $\hat{U} = e^{\hat{A}}$ ($\hat{A}$ anti Hermitian) $= e^{-i\hat{H}}$ ($\hat{H}$, Hermitian)

$$\hat{U}^\dagger = (e^{\hat{A}})^\dagger = e^{\hat{A}^\dagger} = e^{-\hat{A}} = \hat{U}^{-1} \quad \checkmark$$

What if $\hat{H}$ is a function of time, e.g. $\hat{H}(t) = \hat{H}[\vec{B}(t)]$ time-dependent magnetic field

(Note, here we are treat $\vec{B}(t)$ as a classical field. This is a very subtle point because all fields themselves are quantum in nature. But in some cases it is an excellent approximation to treat this field as a classical object ("c-number"). To fully understand this requires quantum field theory beyond the scope of the course, so for now, take my word on it. Nonetheless, this is strange. It is an example of a open quantum system whose evolution is still unitary and deterministic when $\vec{B}(t)$ is deterministic. The classical fields are the handles through we we can attempt to "control" quantum systems).

Now $\frac{\partial}{\partial t}\hat{U}(t;t_0) = -\frac{i}{\hbar}\hat{H}(t)\hat{U}(t;t_0)$. What is the solution to this differential equation?

Recall for "classical functions" $\frac{d}{dt}f(t) = g(t)f(t) \Rightarrow \int_{t_0}^{t}\frac{df(t')}{f(t')} = \int_{t_0}^{t}dt'g(t') \Rightarrow \ln\left(\frac{f(t)}{f(t_0)}\right) = \int_{t_0}^{t}g(t')dt'$

$$\Rightarrow f(t) = f(t_0)\,e^{\int_{t_0}^{t}dt'\,g(t')}$$

So a good guess is $\hat{U}(t;t_0) = \exp\{-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t')\}$ (since $\hat{U}(t_0;t_0) = \hat{\mathbb{1}}$)

However $\exp\{-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t')\} = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t') - \frac{1}{2\hbar^2}\left[\int_{t_0}^{t}dt'\,\hat{H}(t')\right]\left[\int_{t_0}^{t}dt'\,\hat{H}(t')\right] + \cdots$

$$\Rightarrow \frac{\partial}{\partial t}\exp\{-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t')\} = -\frac{i}{\hbar}\hat{H}(t') - \frac{1}{\hbar^2}\int_{t_0}^{t}\left(\frac{\hat{H}(t')\hat{H}(t) + \hat{H}(t)\hat{H}(t')}{2}\right) + \cdots$$

$$\boxed{\hat{U}(t;t_0) = \exp\{-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t')\} \text{ iff } [\hat{H}(t), \hat{H}(t')] = 0 \ \forall t,t'}$$

General approach to solving Time Dependent S.E.

Given $|\psi(0)\rangle$, expand in energy eigenstates

$$|\psi(0)\rangle = \sum_\lambda |u_\lambda\rangle\langle u_\lambda|\psi(0)\rangle = \sum_\lambda c_\lambda |u_\lambda\rangle$$

$$\Rightarrow \boxed{|\psi(t)\rangle = \sum_\lambda c_\lambda e^{-\frac{i}{\hbar}E_\lambda t} |u_\lambda\rangle}$$

This is the "normal mode" expansion for <u>linear</u> waves: Note $P_\lambda(t) = |c_\lambda|^2$ all <u>times</u>

Formal solution of the propagator:

$$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} = \sum_{\lambda,\lambda'} |u_\lambda\rangle \underbrace{\langle u_\lambda| e^{-\frac{i\hat{H}(t-t_0)}{\hbar}} |u_{\lambda'}\rangle}_{e^{-\frac{iE_\lambda(t-t_0)}{\hbar}}\delta_{\lambda\lambda'}} \langle u_{\lambda'}|$$

$$\boxed{\hat{U}(t,t_0) = \sum_\lambda e^{-\frac{iE_\lambda(t-t_0)}{\hbar}} |u_\lambda\rangle\langle u_\lambda|}$$

Stationary states diagonalize $\hat{U}(t,t_0)$

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle = \sum_\lambda e^{-\frac{iE_\lambda(t-t_0)}{\hbar}} |u_\lambda\rangle \underbrace{\langle u_\lambda|\psi(t_0)\rangle}_{c_\lambda(t_0)}$$

$$\Rightarrow \boxed{|\psi(t)\rangle = \sum_\lambda c_\lambda(t_0) e^{-\frac{iE_\lambda(t-t_0)}{\hbar}} |u_\lambda\rangle}$$

<u>Example:</u> Larmor precession of a spin in a magnetic field.

Interaction of magnetic moment $\hat{\vec{\mu}}$ with "Classical" $\vec{B}$ field

$$\hat{H} = -\hat{\vec{\mu}} \cdot \vec{B}$$

$\uparrow \vec{B} \uparrow \vec{\mu}$ min energy

$\uparrow \vec{B}$, $\downarrow \vec{\mu}$ max energy

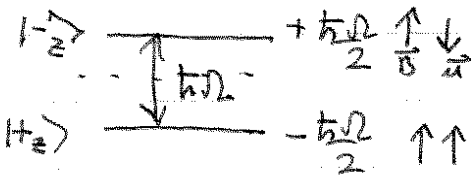
<u>Intrinsic</u> $\hat{\vec{\mu}} : \gamma \hat{\vec{S}}$

γ ← gyromagnetic ratio

$\hat{\vec{S}} = \frac{\hbar}{2} \hat{\vec{\sigma}}$ spin, eigenvalues $\pm \frac{\hbar}{2}$

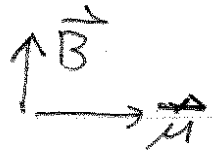
Take $\vec{B} = B_z \vec{e}_z$ $\Rightarrow$ $\boxed{\begin{array}{l} \hat{H} = -\frac{\hbar\Omega}{2} \hat{\sigma}_z \\ \Omega = \gamma B_z \end{array}}$

Stationary states: $|\pm_z\rangle$, $E_\pm = \mp \frac{\hbar\Omega}{2}$



Suppose $|\psi(0)\rangle = |+_x\rangle$

find $|\psi(t)\rangle$



Expand $|\psi(0)\rangle = \frac{1}{\sqrt{2}}|+_z\rangle + \frac{1}{\sqrt{2}}|-_z\rangle$

$$\Rightarrow \boxed{|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-iE_+ t/\hbar} |+_z\rangle + \frac{1}{\sqrt{2}} e^{-iE_- t/\hbar} |-_z\rangle}$$

(Next Page)

$$\Rightarrow \boxed{|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{+i\frac{\Omega t}{2}} |+_z\rangle + \frac{1}{\sqrt{2}} e^{-i\frac{\Omega t}{2}} |-_z\rangle}$$

For "fun", reëxpress in $|\pm_x\rangle$ basis

$$|\psi(t)\rangle = |+_x\rangle\langle +_x|\psi(t)\rangle + |-_x\rangle\langle -_x|\psi(t)\rangle$$

$$= \frac{1}{2}\left(e^{i\frac{\Omega t}{2}} + e^{-i\frac{\Omega t}{2}}\right)|+\rangle + \frac{1}{2}\left(e^{i\Omega t} - e^{-i\Omega t}\right)|-\rangle$$

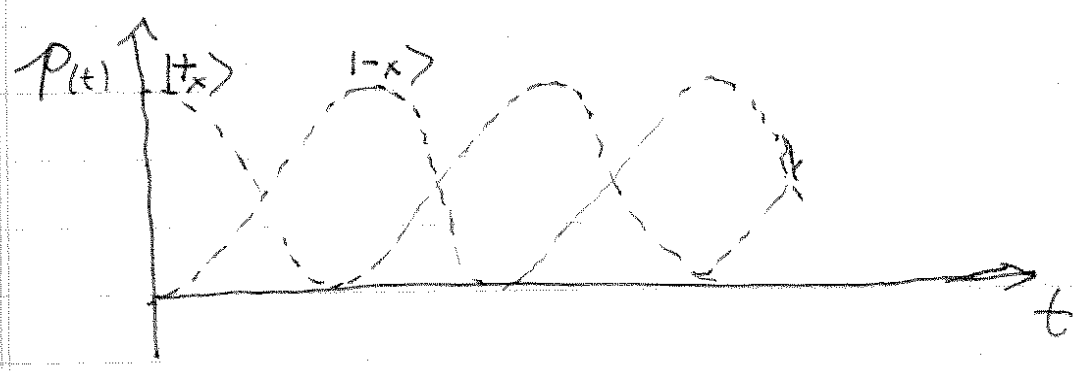
$$\boxed{|\psi(t)\rangle = \cos\left(\frac{\Omega}{2}t\right)|+_x\rangle + i\sin\left(\frac{\Omega t}{2}\right)|-_x\rangle}$$

Evolution of probabilities as a fnct of time:

$$P_{\pm_z}(t) = |\langle \pm_z|\psi(t)\rangle|^2 = \frac{1}{2} \quad \text{indep of time}$$

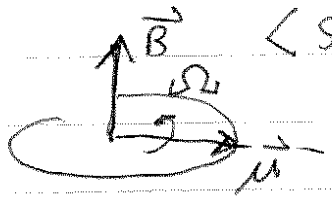
$$P_{+_x}(t) = |\langle +_x|\psi(t)\rangle|^2 = \cos^2\left(\frac{\Omega t}{2}\right) = \frac{1+\cos(\Omega t)}{2}$$

$$P_{-_x}(t) = |\langle -_x|\psi(t)\rangle|^2 = \sin^2\left(\frac{\Omega t}{2}\right) = \frac{1-\cos(\Omega t)}{2}$$



$$\langle S_z(t)\rangle = 0 \qquad \langle S_x(t)\rangle = \sum_{m_x} P_{m_x}\, m_x = \cos(\Omega t)$$

$$\langle S_y(t)\rangle = \sin(\Omega t)$$



Larmor precession at $\Omega = \gamma B$