Phys 4702 Intro QM II   Fall 2024   22 Oct 2024

* Homework #9 status.
* HW: Let's get back on track!
* Today: Easy, mainly review

Time-Dependent Hamiltonians

Review: Quantum Dynamics

$|\alpha\rangle = |\alpha; t=0\rangle$ "Initial state"

$|\alpha; t\rangle = U(t)|\alpha\rangle$ "Time evolution operator"

"Weyl's Trick": $U(dt) = 1 - \frac{i}{\hbar} H\, dt$

$H =$ "Hamiltonian" (a wisely chosen name!)

Finite times

$$U(t+dt) = U(dt)\,U(t)$$
$$= \left[1 - \frac{i}{\hbar} H dt\right] U(t)$$

$\times i\hbar$

$$U(t+dt) - U(t) = -\frac{i}{\hbar} \cancel{H dt}\, H U(t)\, dt$$

$$\Rightarrow i\hbar \frac{U(t+dt) - U(t)}{dt} = i\hbar \frac{dU}{dt} = H U(t)$$

$\times |\alpha\rangle$ i.e. $i\hbar \frac{d}{dt}|\alpha; t\rangle = H|\alpha; t\rangle$ "Schrödinger Equation"

Also $i\hbar \frac{d}{dt} \underline{U(t)|\alpha\rangle} = \underline{H U(t)|\alpha\rangle}$ $= |\alpha; t\rangle$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \underline{\langle \vec{r}\,'|\alpha; t\rangle} = \langle \vec{r}\,'|H|\alpha; t\rangle \quad = \psi(\vec{r}\,', t)$$

i.e. $i\hbar \frac{\partial}{\partial t} \psi(\vec{r}\,', t) = \left[-\frac{\hbar^2}{2m} \vec{\nabla}'^2 + V(\vec{r}\,')\right] \psi(\vec{r}\,', t)$

"Wave Equation"

<u>NOTES:</u> • Chose to project onto $|\vec{r}'\rangle$ because I assumed

$$H = \vec{p}^{\,2}/2m + V(\vec{r})$$

HW Prob #1

<u>But</u> other Hamiltonians are possible!

e.g. $H = -\vec{\mu}\cdot\vec{B} \Rightarrow$ Project onto appropriate spin basis

• we <u>assumed nothing about $H(t)$</u> until last step!!

Important consequence of <u>time-independence</u>:

$$i\hbar \frac{dU}{dt} = HU \Rightarrow U(t) = \exp\left[-\frac{i}{\hbar}Ht\right]$$

<u>If</u> $|a\rangle = |E\rangle$ "Energy Eigenstate"

then $|\alpha;t\rangle = U(t)|E\rangle = e^{-iEt/\hbar}|E\rangle$ "Stationary States"

The wave equation then becomes

$$i\hbar\left(-\frac{iE}{\hbar}\right)\psi(\vec{r}')\,e^{-iEt/\hbar} = \left[-\frac{\hbar^2}{2m}\vec{\nabla}'^2 + V(\vec{r}')\right]\psi(\vec{r}')\,e^{-iEt/\hbar}$$

$$\Rightarrow \underline{-\frac{\hbar^2}{2m}\vec{\nabla}'^2\psi(\vec{r}') + V(\vec{r}')\psi(\vec{r}') = E\psi(\vec{r}')}$$

This is what we've been doing so far!!

<u>Also recall</u> (HW Prob #2)

$$\frac{d}{dt}\langle A\rangle = \frac{d}{dt}\langle\alpha;t|A|\alpha;t\rangle$$ "State or A can change in time."

$$= \left[\frac{d}{dt}\langle\alpha;t|\right]A|\alpha;t\rangle + \langle\alpha;t|A\left[\frac{d}{dt}|\alpha;t\rangle\right] + \langle\alpha;t|\frac{dA}{dt}|\alpha;t\rangle$$

$$= \frac{i}{\hbar}\langle\alpha;t|[H,A]|\alpha;t\rangle$$

Time Dependent Hamiltonians

Back to $i\hbar \frac{d\bar{U}}{dt} = \underline{\underline{H(t)}}\, \bar{U}(t)$

Key Complication: Maybe $[H(t_1), H(t_2)] \neq 0$!!

$\Rightarrow$ $\bar{U}(t) = \lim_{N\to\infty} \left[1 - \frac{i}{\hbar} H\left(\frac{t}{N}\right)\right]^N$ has difficult cross terms!!

e.g. $H(t) = \cancel{B(t)}\; -\vec{\mu}\cdot[\,f(t)\, S_z \hat{z} + g(t)\, S_x \hat{x}\,]$

In principle $\bar{U}(t) = 1 + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots H(t_1) H(t_2) \cdots$

"Dyson Series"; Impractical!!

of course if $H(t)$ all commute, $\bar{U}(t) = \exp\left[-\frac{i}{\hbar}\int_0^t dt'\, H(t')\right]$

e.g. $H(t) = -\vec{\mu}\cdot B(t)\,\hat{z}$ [Would be HW but I couldn't think of a good problem!]

How to Solve? Two general approaches:

1) "Bull by the horns": Try to solve the specific problem
   eg. Magnetic Resonance (Thursday's class)

2) Approximation schemes
   a) Very fast time dependence (HW # Prob. 3)
   b) Very slow time dependence $\Rightarrow$ Berry's Phase
   c) Time-Dependent Perturbation theory

$$H = H_0 + V(t) \quad \text{w/ } V(t) \text{ "small"}$$

Detour: Pictures

We've only talked about state vectors that change with time. "Schrödinger Picture".

But a better connection to classical physics comes if we let observables change with time! "Heisenberg Picture"

i.e. $\langle A \rangle (t) = \langle \alpha; t | A | \alpha; t \rangle$
$$= \langle \alpha | U^+(t) A \, U(t) | \alpha \rangle$$

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i.e. $A \to A(t) = U^+(t) A(t=0) U(t)$ Time Independent

Sometimes we write $A^{(H)}(t) = U^+(t) A^{(S)} U(t)$

$$\Rightarrow \frac{dA^{(H)}}{dt} = \left[\frac{dU^+}{dt}\right] A^{(S)} U + U^+ A^{(S)} \left[\frac{dU}{dt}\right]$$

But $\frac{dU}{dt} = \frac{1}{i\hbar} HU \Rightarrow \frac{dU^+}{dt} = \left(\frac{1}{i\hbar}\right)^* U^+ H^+ = -\frac{1}{i\hbar} U^+ H$

$$\frac{dA^{(H)}}{dt} = -\frac{1}{i\hbar} U^+ H A^{(S)} U + U^+ A^{(S)} \frac{1}{i\hbar} H U$$

If the Hamiltonian is time-independent then

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar} \left\{ U^+ A^{(S)} U H - H U^+ A^{(S)} U \right\}$$

$$= \frac{1}{i\hbar} [A^{(H)}, H]$$ "Heisenberg Equation of Motion"

[... with a close connection to classical physics that you can look up, via "Poisson Brackets"

The Interaction Picture

$$* \quad H = H_0 + V(t) \qquad H_0 \text{ is time-independent}$$

Define $|\alpha;t\rangle_I \equiv e^{iH_0t/\hbar}\,|\alpha;t\rangle_S$

& Observables $A^{(I)}(t) \equiv e^{iH_0t/\hbar}\,A^{(S)}\,e^{-iH_0t}$

Now consider

$$i\hbar\frac{d}{dt}|\alpha;t\rangle_I = i\hbar\left(i\frac{H_0}{\hbar}\right)e^{iH_0t/\hbar}|\alpha;t\rangle_S + e^{iH_0t/\hbar}\,i\hbar\frac{d}{dt}|\alpha;t\rangle_S$$

$$= -H_0e^{iH_0t/\hbar}|\alpha;t\rangle_S + e^{iH_0t/\hbar}\,\underline{H}\,|\alpha;t\rangle_S \quad *$$

$$= e^{iH_0t/\hbar}\,V(t)\,|\alpha;t\rangle_S$$

$$i\hbar\frac{d}{dt}|\alpha;t\rangle_I = e^{iH_0t/\hbar}\,V(t)\,\underline{e^{-iH_0t}\,e^{iH_0t}}\,|\alpha;t\rangle_S$$

i.e. $$i\hbar\frac{d}{dt}|\alpha;t\rangle_I = V^{(I)}(t)\,|\alpha;t\rangle_I$$

• "Equation of Motion in Interaction Picture"

Time-Dependent Perturbation Theory

"Just a taste"

Work in the Interaction Picture:

$$|\alpha;t\rangle_I = \sum_m c_m(t)\,|m\rangle \qquad \text{w/ } H_0|n\rangle = E_n|n\rangle$$

$$\Leftrightarrow \quad c_n(t) = \langle n|\alpha;t\rangle_I$$

and $$i\hbar\frac{d}{dt}\langle n|\alpha;t\rangle_I = \langle n|V^{(I)}(t)|\alpha;t\rangle_I$$

Now use expansion for $|\alpha;t\rangle_I$ and insert $1 = \sum_m |m\rangle\langle m|$ after $V^{(I)}(t)$ to get

$$i\hbar \frac{d}{dt} \sum_m c_m(t) \underbrace{\langle n|m\rangle}_{\delta_{nm}} = \sum_m \langle n|V^{(I)}(t)|m\rangle \underbrace{\langle m|\alpha;t\rangle_I}_{c_m(t)}$$

Also $\langle n|V^{(I)}(t)|m\rangle = \langle n|e^{iH_0t/\hbar}\, V(t)\, e^{-iH_0t/\hbar}|m\rangle$

$$= \exp[i(E_n - E_m)t/\hbar]\, \langle n|V(t)|m\rangle$$

(Notation) $\equiv e^{i\omega_{nm}t}\, V_{nm}$

$$\Rightarrow i\hbar \dot{c}_n = \sum_m V_{nm}\, e^{i\omega_{nm}t}\, c_m(t)$$

No approximations so far! [Could approach any time-dependent Hamiltonian this way.] But...

Typical situation : $V_{nm} \ll |E_n - E_m|$ and ask for probability that you make a transition $|i\rangle \to |n\rangle$ $(i \neq n)$

Write $c_n(t) = c_n^{(0)} + c_n^{(1)} + c_n^{(2)} + \cdots$ "orders"

$$\Rightarrow \text{Prob} = |\langle n|U^{(I)}(t)|i\rangle|^2 = |c_n^{(1)}|^2 + \cdots$$

$$= -\frac{i}{\hbar}\int_0^t e^{i\omega_{ni}t'}\, V_{ni}(t')\, dt'$$

[Get a glimpse with HW Problem #5.]