Physics 506 Lecture 21

Time-dependent problems

Schroedinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

suppose we are in the state $|\psi(t_0)\rangle$ at time t_0.
What state are we in at time t?

1.) Suppose $\hat{H}$ is independent of time.

Introduce eigenfunctions $|n\rangle$ such that $\hat{H}|n\rangle = E_n|n\rangle$.
and $\langle n|m\rangle = \delta_{nm}$.

Then expand

$$|\psi(t_0)\rangle = \sum_n c_n(t_0)\, |n\rangle$$

The TDSE becomes

$$\sum_n i\hbar \frac{\partial}{\partial t} c_n(t)\, |n\rangle = \sum_n E_n\, c_n(t)\, |n\rangle$$

multiply by $\langle m|$ to get

$$i\hbar \frac{\partial}{\partial t} c_m(t) = E_m\, c_m(t)$$

or

$$c_m(t) = c_m(t_0)\, e^{-i E_m (t-t_0)/\hbar}$$

Hence

$$\boxed{|\psi(t)\rangle = \sum_m c_n(t_0)\, e^{-i E_m (t-t_0)/\hbar}\, |n\rangle}$$

An alternate way to view this is as follows

$$|\psi(t)\rangle = e^{-i\hat{H}(t-t_0)/\hbar}\,|\psi(t_0)\rangle$$

$$e^{-i\hat{H}(t-t_0)/\hbar}\,|n\rangle = e^{-iE_n(t-t_0)/\hbar}\,|n\rangle$$

so $$|\psi(t)\rangle = \sum_n C_n(t_0)\, e^{-iE_n(t-t_0)/\hbar}\,|n\rangle$$

as before.

2.) $\hat{H}(t)$ is time dependent $\left[\frac{\partial \hat{H}}{\partial t} \neq 0\right]$

method a introduce a complete set of states $|n\rangle$ (time independent)

$$|\psi(t)\rangle = \sum_n C_n(t)\,|n\rangle$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \sum_n i\hbar\frac{\partial}{\partial t}C_n(t)\,|n\rangle = \hat{H}(t)|\psi(t)\rangle = \sum_n C_n(t)\,\hat{H}(t)\,|n\rangle$$

multiply by $\langle m|$ to get

$$i\hbar\frac{\partial}{\partial t}C_m(t) = \sum_n C_n(t)\,\underbrace{\langle m|\hat{H}(t)|n\rangle}_{=H_{mn}(t)}$$

$$i\hbar\frac{\partial}{\partial t}C_m(t) = \sum_n H_{mn}(t)\,C_n(t)$$

This is a matrix differential equation. Need matrix elements $H_{mn}(t)$ to solve it — this is often complicated except for small finite sized problems.

method b introduce instantaneous eigenstates

$$\hat{H}(t)\,|n(t)\rangle = E_n(t)\,|n(t)\rangle$$

state and energy can both vary with time, but

$\langle m(t)|n(t)\rangle = \delta_{mn}$ and $\sum_m |m(t)\rangle\langle m(t)| = \mathbb{1}$ still.

let $|\psi(t)\rangle = \sum_n c_n(t)\,|n(t)\rangle$

$$\sum_n i\hbar \frac{\partial}{\partial t} c_n(t)\,|n(t)\rangle + \sum_n i\hbar\, c_n(t) \frac{\partial}{\partial t}|n(t)\rangle = \sum_n c_n(t)\,E_n(t)\,|n(t)\rangle$$

multiply by $\langle m(t)|$ to get

$$i\hbar \frac{\partial c_m(t)}{\partial t} + i\hbar \sum_n c_n(t)\,\langle m(t)|\frac{\partial}{\partial t}|n(t)\rangle = c_m(t)\,E_m(t)$$

In general it is hard to calculate the middle term. But note

$\langle m(t)|n(t)\rangle = \delta_{mn}$

$\partial_t\langle m(t)|\,n(t)\rangle + \langle m(t)|\partial_t|n(t)\rangle = 0$

$\hat{H}(t)|n(t)\rangle = E_n(t)\,|n(t)\rangle$

$$\partial_t \hat{H}(t)\,|n(t)\rangle + \hat{H}(t)\,\partial_t|n(t)\rangle = \partial_t E_n(t)\,|n(t)\rangle + E_n(t)\,\partial_t|n(t)\rangle$$

multiply by $\langle m(t)|$ to get

$$\langle m(t)|\partial_t \hat{H}(t)|n(t)\rangle + E_m(t)\,\langle m(t)|\partial_t|n(t)\rangle = \partial_t E_n(t)\,\delta_{mn} + E_n(t)\,\langle m(t)|\partial_t|n(t)\rangle$$

If $m=n$, we find $\langle n(t)|\partial_t\hat{H}(t)|n(t)\rangle = \partial_t E_n(t)$

If $m\neq n$ we find $\dfrac{\langle m(t)|\partial_t\hat{H}(t)|n(t)\rangle}{E_n(t)-E_m(t)} = \langle m(t)|\partial_t n(t)\rangle$

So
$$i\hbar\frac{\partial c_m(t)}{\partial t} + i\hbar\, c_m(t)\,\langle m(t)|\partial_t|m(t)\rangle + i\hbar\sum_{n\neq m} c_n(t)\,\frac{\langle m(t)|\partial_t\hat{H}(t)|n(t)\rangle}{E_n(t)-E_m(t)} = c_m(t)\,E_m(t)$$

derivative still hard to deal with.

Time evolution operator

Define $U(t, t_0)$ from

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

U evolves from time t_0 to time t.

If $\hat{H}(t)$ is independent of time $\left(\frac{\partial \hat{H}}{\partial t} = 0\right)$ then

$$U(t, t_0) = \exp\left[-\frac{i}{\hbar}\hat{H}\,(t - t_0)\right]$$

as we derived earlier.

$U(t, t_0)$ satisfies a set of general properties even if $\hat{H}$ depends on time.

1.) $U(t_0, t_0) = \mathbb{1}$ obvious from definition

2.) $U(t, t')\, U(t', t_0) = U(t, t_0)$

3.) Hermiticity of $\hat{H} \Rightarrow \hat{H}^\dagger = \hat{H}$

$$i\hbar\, \partial_t |\psi(t)\rangle = \hat{H}(t)\, |\psi(t)\rangle$$

$$\langle\psi(t)|\, -i\hbar \overleftarrow{\partial_t} = \langle\psi(t)|\, \hat{H}(t)$$

$$\Rightarrow \frac{\partial}{\partial t} \langle\psi(t)|\psi(t)\rangle = \langle\psi(t)|\, \frac{\overleftarrow{\partial}}{\partial t}\, |\psi(t)\rangle + \langle\psi(t)|\, \frac{\partial}{\partial t}\, |\psi(t)\rangle$$

$$= \frac{i}{\hbar} \langle\psi(t)|\hat{H}(t)|\psi(t)\rangle - \frac{i}{\hbar} \langle\psi(t)|\hat{H}(t)|\psi(t)\rangle$$

$$= 0$$

$\Rightarrow$ normalized states stay normalized.

but $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$

$\langle\psi(t)| = \langle\psi(t_0)|U^\dagger(t,t_0)$

so $\langle\psi(t_0)|U^\dagger(t,t_0)\,U(t,t_0)|\psi(t_0)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle$

$\Rightarrow \quad U^\dagger(t,t_0)\,U(t,t_0) = \mathbb{1}$ unitary operator.

4.) $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$

$i\hbar\frac{\partial}{\partial t}U(t,t_0)|\psi(t_0)\rangle = \hat{H}(t)\,U(t,t_0)|\psi(t_0)\rangle$

true for all $|\psi(t_0)\rangle \Rightarrow$

$$\boxed{i\hbar\frac{\partial}{\partial t}U(t,t_0) = \hat{H}(t)\,U(t,t_0)}$$

called the equation of motion.

5.) Integrate

$i\hbar\left[U(t,t_0) - U(t_0,t_0)\right] = \int_{t_0}^{t}\hat{H}(t')\,U(t',t_0)\,dt'$ $\qquad U(t_0,t_0)=\mathbb{1}$

$U(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,U(t',t_0)\,dt'$

Iterate equation

$U(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,dt' + \left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\,\hat{H}(t_1)\hat{H}(t_2)$

$+ \ldots$

$= \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t}dt_1\,T\left(\hat{H}(t_1)\right) + \left(\frac{-i}{\hbar}\right)\frac{1}{2!}\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\,T\left[\hat{H}(t_1)\hat{H}(t_2)\right]$

$+ \ldots$

The time-ordered product T is defined by

$$T(\hat{A}(t_1)) = \hat{A}_1(t_1)$$
$$T(\hat{A}_1(t_1)\,\hat{A}_2(t_2)) = \Theta(t_1-t_2)\,\hat{A}_1(t_1)\,\hat{A}_2(t_2) + \Theta(t_2-t_1)\,\hat{A}_2(t_2)\,\hat{A}_1(t_1)$$

etc.

The rule is to put <u>later</u> times to the <u>left</u>

proof of this formula is simple.

each time ordered piece gives the same result as the original series. There are $n!$ different time orderings of n operators so this cancels the $\frac{1}{n!}$

We write $U(t,t_0) = T\, e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')}$

$$= \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n\, T\left(\hat{H}(t_1)\,\hat{H}(t_2)\cdots\hat{H}(t_n)\right)$$

This is a power series in $\hat{H}$ not in some time dependent perturbation $V(t)$, hence it often is not useful for applications.

Note that property 4 says

$$i\hbar \frac{\partial}{\partial t} T\, e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')} = \hat{H}(t)\, T\, e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')}$$

so time ordered products generalize to operators the fundamental property of an exponential function – namely that the derivative of an exponential is the derivative of the argument times the exponential. This is non trivial because the operators may not commute at different times.