Lecture 3

23/2/11

Next we consider the harmonic oscillator, in ~~path~~ operator as well as path-integral formalism. This problem is ~~...~~ very basic and illustrates the physics of several more complicated problems.

Let us compute the propagator

$$\langle x'' | e^{-\frac{i}{\hbar} H (t''-t')} | x' \rangle$$

where $H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$

Thus we want to evaluate:

$$\langle x'' | e^{-\frac{i}{\hbar}\left(\frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2\right) T} | x' \rangle$$

where $T = t'' - t'$. This is more complicated than the free particle, because H has two terms that do not mutually commute.

Fortunately we can get around this using the creation & annihilation operator basis. In terms of $\hat{a}$, $\hat{a}^+$ the Hamiltonian is:

$$H = \hbar\omega\left(\hat{a}^+\hat{a} + \tfrac{1}{2}\right).$$

Now insert a complete set of energy eigenstates $|E_n\rangle$ satisfying

$$H|E_n\rangle = \hbar\omega\left(n + \tfrac{1}{2}\right)|E_n\rangle.$$

Then

$$\langle x''| e^{-\frac{i}{\hbar}HT} |x'\rangle =$$

$$\sum_{n=0}^{\infty} \langle x''| e^{-\frac{i}{\hbar}\cdot\hbar\omega(\hat{a}^{+}\hat{a}+\frac{1}{2})T} | E_n\rangle\langle E_n|x'\rangle$$

$$= \sum_{n=0}^{\infty} \langle x''| e^{-i\omega(n+\frac{1}{2})T} |E_n\rangle\langle E_n|x'\rangle$$

$$= \sum_{n=0}^{\infty} e^{-i\omega(n+\frac{1}{2})T} \langle x''|E_n\rangle\langle E_n|x'\rangle$$

Now $\langle x''|E_n\rangle$ is just the harmonic oscillator wave fn in the position basis (by definition!), namely:

$$\langle x''|E_n\rangle = \psi_n(x'')$$

$$= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} e^{-\beta^2 x^2/2} H_n(\beta x)$$

where $\beta = \sqrt{\frac{m\omega}{\hbar}}$ and H_n are the Hermite polynomials.

Hence $\langle x''| e^{-\frac{i}{\hbar}HT} |x'\rangle =$

$$\sqrt{\frac{\beta^2}{\pi}} \; e^{-\beta^2 x'^2/2 - \beta^2 x''^2/2} \times$$

$$\sum_{n=0}^{\infty} \frac{e^{-i\omega(n+\frac{1}{2})T}}{2^n n!} H_n(\beta x') H_n(\beta x'')$$

The sum can be evaluated by looking up Wikipedia, http://en.wikipedia.org/wiki/Hermite_polynomials.

There, we find the formula:

$$\sum_{n=0}^{\infty} \left(\frac{u}{2}\right)^n \frac{H_n(x) H_n(y)}{n!} = \frac{1}{\sqrt{1-u^2}} e^{\frac{2xyu - (x^2+y^2)u^2}{1-u^2}}$$

Thus, replacing $x \to \beta x'$, $y \to \beta x''$, $u = e^{-i\omega T}$, we have:

$$\Sigma = e^{-\frac{i\omega T}{2}} \times \frac{1}{\sqrt{1 - e^{-2i\omega T}}}$$

$$\times\ e^{\frac{m\omega}{\hbar}\left(\frac{2e^{-i\omega T} x'x'' - e^{-2i\omega T}(x'^2 + x''^2)}{1 - e^{-2i\omega T}}\right)}$$

$$= \frac{1}{\sqrt{e^{i\omega T} - e^{-i\omega T}}} \cdot e^{-\frac{m\omega}{\hbar}\left(\frac{e^{-i\omega T}(x'^2 + x''^2) - 2x'x''}{e^{i\omega T} - e^{-i\omega T}}\right)}$$

$$= \left(\frac{1}{2i \sin\omega T}\right)^{1/2} e^{\frac{im\omega}{2\hbar}\left(\frac{e^{-i\omega T}(x'^2 + x''^2) - 2x'x''}{\sin\omega T}\right)}$$

Now put in the pre-factors:

$$\sqrt{\frac{\beta^2}{\pi}}\, e^{-\frac{\beta^2}{2}x'^2 - \frac{\beta^2}{2}x'^2}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{m\omega}{2\hbar}(x'^2 + x''^2)}$$, to get:

$$\left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{\frac{1}{2}} e^{\frac{im\omega}{2\hbar \sin\omega T}\left((i\sin\omega T + e^{-i\omega T})(x'^2 + x''^2) - 2x'x''\right)}$$

Using $i \sin\omega T + e^{-i\omega T}$

$= i\sin\omega T + (\cos\omega T - i\sin\omega T)$

$= \cos\omega T$, we finally have:

$$\langle x''| e^{-\frac{i}{\hbar}HT} |x'\rangle =$$

$$\left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{\frac{1}{2}} e^{\frac{im\omega}{2\hbar\sin\omega T}\left((x'^2+x''^2)\cos\omega T - 2x'x''\right)}$$

A very nice check of this result is to take the limit $\omega \to 0$. Then we have:

$$\lim_{x\to 0} \frac{\sin x}{x} = 1 = \lim_{\omega\to 0} \frac{\sin\omega T}{\omega T} = 1, \text{ so}$$

$$\lim_{\omega\to 0} \frac{\omega}{\sin\omega T} = \frac{1}{T}, \text{ and } \lim_{\omega\to 0} \cos\omega T = 1, \text{ so.}$$

$$\langle x''| e^{-\frac{i}{\hbar}HT} |x'\rangle \xrightarrow{\omega\to 0}$$

$$\left(\frac{m}{2\pi i\hbar T}\right)^{\frac{1}{2}} e^{\frac{im}{2\hbar T}(x'-x'')^2}$$

which is precisely the free particle result!

Now consider the path integral.

$$\int [dx]\, e^{\frac{i}{\hbar} S[x]}$$

The integral is over all paths $x(t)$ which start at $x(t') = x'$ and end at $x(t'') = x''$.

To evaluate it, we shift variables.

$$x(t) = x_{cl}(t) + \eta(t)$$

where $x_{cl}(t)$ is a solution of the classical equations of motion, with the above boundary conditions, and η satisfies $\eta(t') = \eta(t'') = 0$.

Since $x_{cl}(t)$ is a fixed path, we have $[dx] = [d\eta]$ and:

$$\int [dx]\, e^{\frac{i}{\hbar} S[x]} = \int [d\eta]\, e^{\frac{i}{\hbar}\left(S[x_{cl}] + \int \frac{\delta S}{\delta x}\Big|_{x_{cl}} \eta + \int \frac{\delta^2 S}{\delta x^2} \eta^2\right)}$$

Now $\frac{\delta S}{\delta x}\Big|_{x=x_{cl}} = 0$ due to the eqn of motion. Also the last term is $\int_{t'}^{t''} dt \left(\frac{1}{2} m \dot{\eta}^2 - \frac{1}{2} m\omega^2 \eta^2\right) = S[\eta]$. Thus

$$\int_{t'}^{t''} [dx]\, e^{\frac{i}{\hbar} S[x]} = e^{\frac{i}{\hbar} S_{cl}} \int [d\eta]\, e^{\frac{i}{\hbar} S[\eta]}$$

~~Now consider the path integral~~ Let us now evaluate the first factor, S_{cl}. The action:

$$S = \int_{t'}^{t''} \left(\tfrac{1}{2} m \dot{x}^2 - \tfrac{1}{2} m\omega^2 x^2\right) dt$$

has the familiar equation of motion:

$$\ddot{x} = -\omega x$$

whose general solution is:

$$x = a \cos\omega t + b \sin\omega t$$

Here a and b are constants determined by: $x(t') = x'$, $x(t'') = x''$.

Since there is no preferred origin of time, we will take $t' = 0$, $t'' = T$.

Then

$$x' = a$$

$$x'' = a\cos\omega T + b \sin\omega T$$

$$\Rightarrow \quad a = x', \quad b = \frac{x'' - x'\cos\omega T}{\sin\omega T}$$

Now let us compute the classical action for this particle:

$$S_{cl} = \int_0^T dt \left(\tfrac{1}{2} m\dot{x}^2 - \tfrac{1}{2} m\omega^2 x^2\right)$$

$$= \tfrac{1}{2} m \int_0^T dt \Big[(-\omega a \sin\omega t + \omega b \cos\omega t)^2 - \omega^2 (a\cos\omega t + b \sin\omega t)^2 \Big]$$

$$= \frac{1}{2} m\omega^2 \int_0^T dt \left[(b^2-a^2)\cos 2\omega t - 2ab \sin 2\omega t \right]$$

$$= \frac{m\omega}{4} \left[(b^2-a^2) \sin 2\omega t \Big|_0^T + 2ab \cos 2\omega t \Big|_0^T \right]$$

Now
$$b^2 - a^2 = \frac{x'^2 \cos 2\omega T + x''^2 - 2x'x'' \cos\omega T}{\sin^2\omega T}$$

$$2ab = \frac{2(x'x'' - x'^2 \cos \omega T)}{\sin \omega T}$$

So above $= \dfrac{m\omega}{4} \Big\{$

$$\frac{x'^2}{\sin^2\omega T}\left[\cos 2\omega T \sin 2\omega T + \ldots - 2 \cos\omega T \sin\omega T (\cos 2\omega T - 1) \right]$$

$$+ \frac{x''^2}{\sin^2\omega T}\left[\sin 2\omega T \right]$$

$$+ \frac{2x'x''}{\sin^2\omega T}\left[-\cos\omega T \sin 2\omega T + \sin\omega T (\cos 2\omega T - 1) \right] \Big\}$$

$$= \frac{m\omega}{4\sin^2\omega T}\left\{ (x'^2 + x''^2)\sin 2\omega T - 4x'x''\sin\omega T \right\}$$

$$= \frac{m\omega}{2\sin\omega T}\left[(x'^2 + x''^2)\cos\omega T - 2x'x'' \right]$$

Hence
$$e^{iS_{cl}/\hbar} = e^{\frac{im\omega}{2\hbar \sin\omega T}\left[(x'^2+x''^2)\cos\omega T - 2x'x'' \right]}$$

which is precisely the phase part of the propagator!

We can try to fix the prefactor as before, but with less success. If we take

$$\lim_{T\to 0} e^{\frac{im\omega}{2\hbar \sin\omega T}\left[(x'^2 + x''^2)\cos\omega T - 2x'x''\right]}$$

we find this is equal to

$$\lim_{T\to 0} e^{\frac{im\omega}{2\hbar \sin\omega T}(x''-x')^2} + \ldots$$

which suggests that the prefactor is

$$\left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{1/2}$$ — which is the correct answer.

However we could have instead concluded that the prefactor was

$$\left(\frac{m}{2\pi i\hbar T}\right)^{1/2},$$ which is <u>not</u> the right answer (as we see from the operator calculation) but has the same limit as $T \to 0$.

So, except for the free particle case, requiring $\langle x'', t'' | x', t' \rangle \xrightarrow{t''\to t'} \delta(x''-x')$ does <u>not</u> determine the prefactor.

To find the prefactor let us re-consider the path integral, for which we showed that:

$$\langle x'', t'' | x', t' \rangle = e^{\frac{i}{\hbar} S_{cl}} \int [d\eta]\, e^{\frac{i}{\hbar}\int_{t'}^{t''} \left(\frac{m}{2}\dot{\eta}^2 - \frac{m\omega^2}{2}\eta^2\right) dt}$$

and let us try to evaluate the second integral.

Here we ~~...~~ encounter a key point. The integral is over functions $\eta(t)$ with $\eta(t') = \eta(t'') = 0$. It is quite easy to find a normalised basis for such functions:

$$y_n(t) = \sqrt{\frac{2}{t''-t'}}\, \sin\frac{n\pi t}{t''-t'}$$

therefore we can write $\eta(t) = \sqrt{\frac{2}{t''-t'}} \sum_{n=1}^{\infty} a_n \sin\frac{n\pi t}{t''-t'}$

where a_n are the Fourier coefficients. It follows that, upto an over normalisation (which we anyway do not know),

$$[d\eta] = \prod_{n=1}^{\infty} da_n$$

and

$$\int_{t'}^{t''} dt \left(\frac{m}{2}\dot{\eta}^2 - \frac{m\omega}{2}\eta^2\right)$$

$$= \frac{m}{2}\sum_n \left(\frac{n^2\pi^2}{T^2} - \omega^2\right) a_n^2$$

Thus we want to evaluate:

$$\int \prod_{n=1}^{\infty} da_n \; e^{\frac{im}{2\hbar}\sum_{n=1}^{\infty}\left(\frac{n^2\pi^2}{T^2}-\omega^2\right)a_n^2}$$

$$= \prod_{n=1}^{\infty}\left[\int_{-\infty}^{+\infty} da_n \; e^{\frac{im}{2\hbar}\left(\frac{n^2\pi^2}{T^2}-\omega^2\right)a_n^2}\right]$$

$$= \prod_{n=1}^{\infty} \frac{\sqrt{\pi}}{\sqrt{\frac{im}{2\hbar}\left(\frac{n^2\pi^2}{T^2}-\omega^2\right)}}$$

Let's write this as:

$$\prod_{n=1}^{\infty} \sqrt{\frac{2\pi\hbar}{im}} \; \prod_{n=1}^{\infty}\left(\frac{T}{n\pi}\right) \prod_{n=1}^{\infty} \frac{1}{\sqrt{1-\frac{(\omega T)^2}{n^2\pi^2}}}$$

Now the first two factors are divergent, but independent of ω. The last factor is finite, as we see by using

$$\prod_{n=1}^{\infty}\left(1-\frac{x^2}{n^2\pi^2}\right) = \frac{\sin x}{x}.$$

Hence we find that

$$\int [d\eta]\, e^{\frac{i}{\hbar}\int_{t'}^{t''}\left(\frac{m}{2}\dot{\eta}^2-\frac{m\omega}{2}\eta^2\right)dt}$$

$$= (\text{infinite constant}) \times \sqrt{\frac{\omega T}{\sin \omega T}}$$

Now we take the point of view that the "infinite constant", combined with the other normalisation factors in the definition of $[dx]$, gives an unknown but ω-independent constant.

This constant can be fixed by comparing with the free particle as $\omega \to 0$, hence finally we get

$$\sqrt{\frac{m}{2\pi i \hbar T}} \sqrt{\frac{\omega T}{\sin \omega T}} = \sqrt{\frac{m\omega}{2\pi i \hbar \sin \omega T}}$$

which is the correct answer.

Physical properties of the propagator

$\langle x'', t'' | x', t' \rangle$.

i) Convolution property:

$$\int d\bar{x} \quad \langle x'', t'' | \bar{x}, \bar{t} \rangle \langle \bar{x}, \bar{t} | x', t' \rangle$$
$$= \langle x'', t'' | x', t' \rangle$$

The proof trivially follows from completeness.

$$\int d\bar{x} \; | \bar{x}, \bar{t} \rangle \langle \bar{x}, \bar{t} | = \mathbb{1}$$

ii) Viewed as a function x'' and t'' at fixed x', t', the propagator satisfies the Schrödinger eqn:

$$H\left(-i\hbar \frac{\partial}{\partial x''}, x''\right) \langle x'', t'' | x', t' \rangle = i\hbar \frac{\partial}{\partial t''} \langle x'', t'' | x', t' \rangle$$

<u>Proof</u>: We have $\hat{H}(\hat{p}, \hat{x}) | x, t \rangle = H\left(-i\hbar \frac{\partial}{\partial x}, x\right) | x, t \rangle$

Since H is hermitian, we also have

$$\langle x, t | \hat{H}(\hat{p}, \hat{x}) = H\left(-i\hbar \frac{\partial}{\partial x}, x\right) \langle x, t |$$

Now $\quad i\hbar \frac{\partial}{\partial t''} \langle x'', t'' | x', t' \rangle = i\hbar \frac{\partial}{\partial t''} \langle x'' | e^{-\frac{i}{\hbar} \hat{H}(t''-t')} | x' \rangle$

$$= \langle x'' | \hat{H} e^{-\frac{i}{\hbar} \hat{H}(t''-t')} | x' \rangle$$

$$= H\left(-i\hbar \frac{\partial}{\partial x''}, x''\right) \langle x'', t'' | x', t' \rangle$$

which proves the result.

iii) The propagator provides the time evolution of any wave-function $\psi(x)$ prepared at an initial instant.

Suppose we are given an abstract state vector $|\psi\rangle$ at the initial instant $t=0$. After a time T, this evolves to:

$$e^{-\frac{i}{\hbar}HT}|\psi\rangle$$

Now in position space, the initial wave function is $\langle x'|\psi\rangle = \psi(x')$. The final wave fn is $\langle x''|e^{-\frac{i}{\hbar}HT}|\psi\rangle$

$$= \int dx' \, \langle x''|e^{-\frac{i}{\hbar}HT}|x'\rangle\langle x'|\psi\rangle$$

$$= \int dx' \, \langle x''|e^{-\frac{i}{\hbar}HT}|x'\rangle\,\psi(x')$$

iv) The propagator can be used to "extract" the energy eigenfunctions and eigenvalues, as follows. It can be written:

$$\langle x''|e^{-\frac{i}{\hbar}HT}|x'\rangle = \sum_n e^{-\frac{i}{\hbar}E_nT}\langle x''|E_n\rangle\langle E_n|x'\rangle$$

$$= \sum_n e^{-\frac{i}{\hbar}E_nT}\,\psi_n(x'')\,\psi_n^*(x')$$

~~Suppose further~~ Let $T = -i\tau$ and take $\tau \to \infty$. Then:

$\langle x'', t'' | x', t' \rangle \longrightarrow$

$$\sum_n e^{-\frac{1}{\hbar} E_n T} \psi_n(x'') \psi_n^*(x')$$

$$\xrightarrow{T\to\infty} e^{-\frac{E_0}{\hbar} T} \psi_0(x'') \psi_0^*(x') + \text{exponentially suppressed terms}$$

Thus from the leading exponential, we can read off the ground-state energy E_0. Similarly the corrections give us the other energies E_n.

For each definite power $e^{-\frac{E_n}{\hbar} T}$, the coefficient has to be of the product form $\psi_n(x'') \psi_n^*(x')$. This allows us to read off the eigenfunctions $\psi_n(x)$.

Example: For the SHO we have:

$$\langle x'', T | x', 0 \rangle = \left(\frac{m\omega}{2\pi i \hbar \sin\omega T} \right)^{1/2} \times$$

$$e^{\frac{i m \omega}{2\hbar \sin\omega T} \left[(x'^2 + x''^2) \cos\omega T - 2 x' x'' \right]}$$

$$= \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} \frac{1}{\left(e^{i\omega T} - e^{-i\omega T} \right)^{1/2}} e^{-\frac{m\omega}{\hbar} \frac{1}{e^{i\omega T} - e^{-i\omega T}} \left[(x'^2 + x''^2) \frac{\left(e^{i\omega T} + e^{-i\omega T}\right)}{2} - 2x'x'' \right]}$$

$$= \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\frac{i\omega T}{2}} \left(1 - e^{-2i\omega T} \right)^{-1/2} \times$$

$$e^{-\frac{m\omega}{2\hbar} \left[(x'^2 + x''^2)(1 + e^{-2i\omega T})(1 - e^{-2i\omega T})^{-1} - 4x'x'' e^{-i\omega T} (1 - e^{-2i\omega T})^{-1} \right]}$$

Now this is set up as a power series in $e^{-in\omega T}$ with an overall coefficient $e^{-i\omega T/2}$. Hence $E_0 = \frac{1}{2}\hbar\omega$, $E_n = (n+\frac{1}{2})\hbar\omega$

The leading term is (as $T \to -i\infty$):

$$\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-i\omega T/2} \, e^{-\frac{m\omega}{2\hbar}(x'^2 + x''^2)}$$

$$= e^{-i\omega T/2} \left[\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x'^2}\right]\left[\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x''^2}\right]$$

which gives $\psi_0(x') = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x'^2}$

It is instructive to go to the next order:

$$\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-i\omega T/2} \, e^{-i\omega T} \left\{ e^{-\frac{m\omega}{2\hbar}(x'^2 + x''^2)} \cdot \frac{2m\omega}{\hbar} x' x'' \right.$$

$$= e^{-3i\omega T/2}\left[\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \sqrt{\frac{2m\omega}{\hbar}} \, x' \, e^{-\frac{m\omega}{2\hbar}x'^2}\right]\left[x' \to x'' \right]$$

So $E_1 = \frac{3}{2}\hbar\omega$ and

$$\psi_1(x) = \sqrt{\frac{2m\omega}{\hbar}} \, x \, \psi_0(x)$$

Thus, all Hermite polynomials are reproduced!