Lecture 7

17/3/2011

Path integral formulation of variational principle.

In order to discuss this, we first add some observations to our previous discussion.

We had seen that

$$K(x'',t'';x',t') \equiv \langle x''| e^{-i\hat{H}(t''-t')} |x'\rangle$$

$$= \int [dx]\, e^{\frac{i}{\hbar}\int_{t'}^{t''} L\, dt}$$

where the integral is over paths $x(t)$ starting at x' at t' and ending at x'' at time t'':

$$x(t') = x', \quad x(t'') = x''.$$

We will find it useful henceforth to work with purely imaginary time. The reason is that the information contained in the path integral about energy eigenvalues becomes easier to extract.

Therefore, send $t \to -i\tau$ and let $(t''-t') = -i\beta\hbar$, β real and >0.

We also put $x'' = x'$

Thus we consider the object

$$K(x';\beta) \equiv \langle x' | e^{-\beta \hat{H}} | x' \rangle$$

Finally, integrate over all x'. The result depends only on β and is called the <u>partition</u> <u>function</u>:

$$Z(\beta) = \int dx' \; K(x';\beta)$$

$$= \int dx' \; \langle x' | e^{-\beta \hat{H}} | x' \rangle$$

The right hand side is analogous to the sum over all diagonal elements of a matrix, so we call it the <u>trace</u>:

$$Z(\beta) = \mathrm{tr}\; e^{-\beta H}$$

As with matrices, this trace is invariant under a change of basis. If $|\varphi\rangle$ forms some other basis satisfying completeness:

$$\int d\varphi \; |\varphi\rangle\langle\varphi| = \mathbb{1} \quad \text{(identity operator)}$$

(eg $|\varphi\rangle = |p\rangle$, the momentum basis) then

$$\int dx' \langle x' | e^{-\beta H} | x' \rangle =$$

$$\int dx' \langle x' | \int d\varphi \, |\varphi\rangle\langle\varphi| e^{-\beta \hat{H}} | x' \rangle$$

$$= \int d\varphi \, dx' \; \langle x' | \varphi \rangle \langle \varphi | e^{-\beta \hat{H}} | x' \rangle$$

$$= \int d\varphi \; \langle \varphi | e^{-\beta \hat{H}} \underbrace{\left(\int dx' \, |x'\rangle\langle x'| \right)}_{\text{identity op}} |\varphi\rangle = \int d\varphi \langle \varphi | e^{-\beta \hat{H}} | \varphi \rangle$$

Basis independence means we can insert a complete set of energy eigenstates instead, so:

$$Z(\beta) = \sum_n \langle \Psi_n | e^{-\beta H} | \Psi_n \rangle$$

$$= \sum_n e^{-\beta E_n}$$

Thus it counts the energy levels of the system (with degeneracies if any). Such a quantity in a statistical system is normally called the partition function, and here $\beta = \frac{1}{kT}$ where T is the temperature. Hence we borrow the same terminology for the present (quantum mechanics continued to imaginary time) problem.

In terms of path integrals we replace

$$S = \int_{t'}^{t''} L \, dt$$

by continuing $t \to -it$ in L and then integrating from 0 to $\beta\hbar$:

$$S = -i \underbrace{\int_0^{\beta\hbar} L(t \to -it) \, dt}_{S_E}$$

Let us refer to $L(t \to -it)$ as L_E (E for "Euclidean"). As an example, if

$$L(x, \dot{x}) = \frac{1}{2} m \dot{x}^2 - V(x)$$

then $$L_E(x, \dot{x}) = -\frac{1}{2} m \dot{x}^2 - V(x)$$

Thus $$S_E = -\int_0^{\beta\hbar} \left(\frac{1}{2} m \dot{x}^2 + V(x) \right) dt$$

So in the path integral,

$$e^{\frac{i}{\hbar} S} \longrightarrow e^{\frac{S_E}{\hbar}}$$

and also we note that S_E is typically negative definite.

(Note that S_E is not always real! The velocity-dependent magnetic field coupling $\dot{x}^i A_i$ becomes imaginary for $t \to -it$. We ignore such cases and assume real S_E.)

With all this, we can write:

$$Z(\beta) = \int [dx]\, e^{\frac{S_E}{\hbar}}\, dx'$$

where the integral over $[dx]$ sums over all periodic paths in imaginary time from x' to x', and the integral over dx' sums over all the initial positions.

Sometimes one just writes $[dx]$ to represent the sum over all ~~paths~~ periodic paths with any starting point, in this latter definition the integral over dx' is subsumed.

It is sometimes convenient to work with the log of $Z(\beta)$: we define

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta)$$

and call it the "free energy". This is a stat-mech term which is relevant when we describe statistical systems via path integrals. Thus,

$$Z = e^{-\beta F}$$

Now let us see how the Rayleigh – Ritz variational principle discussed in the last two lectures can be incorporated in path integral language. Next we will ~~use~~ define that the path-integral version of the variational principle, which turns out to be more <u>general</u>.

Now put together two facts:

i) $E_0 \leq \langle H \rangle$ and is the absolute minimum of H,

ii) $Z(\beta \to \infty) \sim e^{-\beta E_0}$

The second follows from a result, derived in class, that

$$\cancel{K(t'', x'')} \; K(x'', t''; x', t') \xrightarrow{t''-t' = -i\tau,\ \tau \to \infty}$$

$$e^{-\frac{E_0 \tau}{\hbar}} \psi_0(x'') \psi_0^*(x') + \dots$$

Putting $x'' = x'$ and integrating over x' (also putting $\tau = \beta\hbar$) we have:

$$Z(\beta) \xrightarrow{\beta \to \infty} e^{-\beta E_0}$$

since $\int dx' \, \psi_0(x') \psi_0^*(x') = 1$ by normalisation.

<u>NB</u>: (Even if $x'' \neq x'$, the exponential dependence is still $\sim e^{-\beta E_0}$)

Now the idea is to vary, not the <u>wave function</u> (which does not appear directly in the path integral formalism) but the potential $V(x)$.

Thus consider a different action

$$\tilde{S}_E = -\int_0^{\beta\hbar} \left(\tfrac{1}{2} m \dot{x}^2 + \tilde{V}(x) \right) dt$$

Then
$$\int [dx]\, dx'\, e^{\frac{S_E}{\hbar}} = e^{-\beta F}$$
$$\int [dx]\, dx'\, e^{\tilde{S}_E/\hbar} = e^{-\beta \tilde{F}}$$

where $F, \tilde{F}$ are the free energies of two different systems (with potentials $V(x), \tilde{V}(x)$).

~~So~~ Taking the ratio,

$$\frac{\int [dx]\, dx'\, e^{\frac{S_E}{\hbar}}}{\int [dx]\, dx'\, e^{\tilde{S}_E/\hbar}} = e^{-\beta(F-\tilde{F})}$$

We write the numerator on the LHS as:

$$\int e^{S_E/\hbar} = \int e^{(S_E-\tilde{S}_E)/\hbar}\, e^{\tilde{S}_E/\hbar}$$

Then
$$\text{LHS} = \frac{\int [dx]dx'\, e^{(S_E-\tilde{S}_E)/\hbar}\, e^{\tilde{S}_E/\hbar}}{\int [dx]dx'\, e^{\tilde{S}_E/\hbar}}$$

$$= \left\langle e^{(S_E-\tilde{S}_E)/\hbar} \right\rangle_{\tilde{S}_E}$$: avg value of the exponential in the $\tilde{S}$ theory.

Hence

$$e^{-\beta(F-\tilde{F})} = \langle e^{(S_E-\tilde{S}_E)/\hbar} \rangle_{\tilde{S}_E}$$

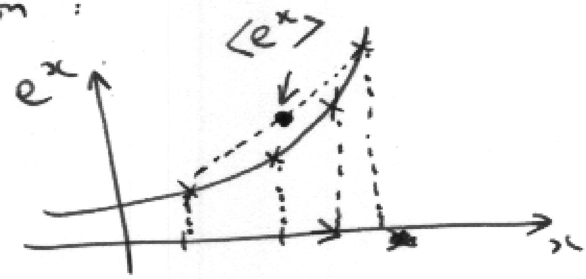
and moreover,

$$S_E - \tilde{S}_E = -\int_0^{\beta\hbar} (V-\tilde{V})\, dt$$

Next, use a powerful result in probability theory: for any random variable x,

$$\langle e^x \rangle \geqslant e^{\langle x \rangle}$$

This follows from concavity of the exponential function:



For this distribution of (say) four equal point masses, the value of $e^{\langle x \rangle}$ lies on the curve, while $\langle e^x \rangle$ is above the curve, as shown, located at the "centre of gravity" of the four points on the curve.

Thus we have

$$\langle e^{(S_E-\tilde{S}_E)/\hbar} \rangle_{\tilde{S}_E} \geqslant e^{\frac{1}{\hbar}\langle S_E-\tilde{S}_E \rangle_{\tilde{S}_E}} \quad \text{where:}$$

$$\langle S_E - \tilde{S}_E \rangle_{\tilde{S}_E} = \frac{\int [dx]\, dx' \, (S_E - \tilde{S}_E)\, e^{\tilde{S}_E/\hbar}}{\int [dx]\, dx' \, e^{\tilde{S}_E/\hbar}}$$

Therefore

$$e^{\frac{1}{\hbar}\langle S_E - \tilde{S}_E \rangle_{\tilde{S}}} \leq e^{-\beta(F - F')}$$

From monotonic nature of the exponential, we get:

$$F \leq \tilde{F} - \underbrace{\frac{1}{\beta\hbar} \langle S_E - \tilde{S}_E \rangle_{\tilde{S}}}_{= \delta}$$

Thus if we consider a family of potentials $\tilde{V}$ (which are easier to solve than the true potential V) then we can compute

$$\tilde{F} - \frac{1}{\beta\hbar} \langle S_E - \tilde{S}_E \rangle_{\tilde{S}_E}$$

over this family and try to minimize it — this takes us closer and closer to the ~~true~~ F.

Now we use the fact that as $\beta \to \infty$, $F \to E_0$. Thus at very large β,

$$E_0 \leq E_0' - \delta .$$

Now the quantity δ can be written in a simpler way by using that S_E, $\tilde{S}_E$ differ only in their potential terms:

$$S_E - \tilde{S}_E = -\int_0^{\beta\hbar} \left[V(x(t)) - \tilde{V}(x(t)) \right] dt$$

So

$$\delta = -\frac{1}{\beta\hbar} \frac{\int [dx]\, dx'\, e^{\tilde{S}/\hbar} \int_0^{\beta\hbar} dt \left[V(x(t)) - \tilde{V}(x(t)) \right]}{\int [dx]\, dx'\, e^{\tilde{S}/\hbar}}$$

Next we assume that the quantity $V(x(t)) - \tilde{V}(x(t))$ has a ~~[illegible]~~ ~~[illegible]~~ ~~depen~~ very gradual dependence on t, so that we can approximate

$$-\frac{1}{\beta\hbar} \int_0^{\beta\hbar} dt \left[V(x(t)) - \tilde{V}(x(t)) \right] \simeq -\left(V(x(\bar{t})) - \tilde{V}(x(\bar{t})) \right)$$

where $\bar{t}$ is some time intermediate between 0 and $\beta\hbar$, say $\frac{\beta\hbar}{2}$.

~~Hence we~~ As $\beta \to \infty$, the denominator of δ is $\sim e^{-\beta E_0}$. For the numerator we use that

$$\int [dx]\, dx'\, e^{\tilde{S}/\hbar} f(x(\bar{t}))$$

~~a~~ Applying a formula derived earlier:

above $= \int dx' \int dx \, \langle x', \beta\hbar \,|\, x, \bar{t} \rangle f(x(\bar{t})) \langle x, \bar{t} \,|\, x', 0 \rangle$

This is equal to

$$\int dx'\,dx \sum_n e^{-\frac{\bar{t}}{\hbar}\tilde{E}_n}\,\tilde{\psi}_n(x)\,\tilde{\psi}_n^*(x')\quad f(x)$$

$$\sum_m e^{-\frac{(\beta\hbar-\bar{t})}{\hbar}\tilde{E}_m}\,\tilde{\psi}_m(x')\,\psi_m^*(x)$$

If β, $\bar{t} \to \infty$ together then only $n, m = 0$ contributes and we get:

$$\simeq \int dx'\,dx \quad e^{-\beta\tilde{E}_0}\,\tilde{\psi}_0(x)\tilde{\psi}_0^*(x)f(x).\ \tilde{\psi}_0(x')\tilde{\psi}_0^*(x')$$

$$= e^{-\beta\tilde{E}_0}\int\tilde{\psi}_0(x)\tilde{\psi}_0^*(x)f(x)$$

The prefactor cancels the denominator. Thus we have:

$$\delta = \int\tilde{\psi}_0(x)\tilde{\psi}_0^*(x)\left[\tilde{V}(x) - V(x)\right]dx$$

Finally we need to write down:

$$\tilde{E}_0 - \delta = \langle\tilde{H}\rangle_0 - \delta$$

$$= \int\tilde{\psi}_0^*(x)\,\tilde{H}\,\psi_0(x) - \int\tilde{\psi}_0^*(x)\left[\tilde{V}(x) - V(x)\right]\tilde{\psi}_0(x)\,dx$$

$$= \int\tilde{\psi}_0^*(x)\left[\tilde{H} - \tilde{V} + V\right]\psi_0(x)\,dx$$

Now since $H = \frac{p^2}{2m} + V$, $\tilde{H} = \frac{p^2}{2m} + \tilde{V}$,

we have

$$H - V = \tilde{H} - \tilde{V} \quad \text{or}$$

$$\tilde{H} - \tilde{V} + V = H.$$

Thus we finally have

$$E_0 \leq \int dx\, \tilde{\Psi}_0^*(x)\, H\, \tilde{\Psi}_0(x)$$

Here $\tilde{\Psi}_0$ is the ground state wave function of the trial Hamiltonian $\tilde{H}$. However all remaining reference to the trial Hamiltonian has disappeared! The Hamiltonian on the RHS is the true Hamiltonian H, not $\tilde{H}$.

Therefore minimising ~~to~~ the RHS only requires varying $\tilde{\Psi}_0(x)$. Now we can forget about the potential $\tilde{V}$ from which it came, and ~~to~~ vary it as a trial wave function.

Thus we have recovered the Rayleigh-Ritz variational principle!