Path Integrals and Ground States

The ground state $|0\rangle$ in a theory described by a hamiltonian H can be found by examining the operator

$$e^{-tH/\hbar} = e^{-\frac{tH}{\hbar}} \sum_{n=0}^{\infty} |n\rangle\langle n|$$

$$= \sum_{n=0}^{\infty} e^{-\frac{tE_n}{\hbar}} |n\rangle\langle n|$$

in which the sum $\sum |n\rangle\langle n|$ is over all e-states of H and so is the identity operator.

So to find the mean value of some observable A in the ground state $|0\rangle$, we may guess a state that has suitable overlap with $|0\rangle$ and then take the limit as $t \to \infty$ of

$$\frac{\langle \psi | e^{-\frac{tH}{\hbar}} A \, e^{-\frac{tH}{\hbar}} | \psi \rangle}{\langle \psi | e^{-\frac{2tH}{\hbar}} | \psi \rangle}$$

$$= \frac{\sum_{n,m=0}^{\infty} \langle \psi | n \rangle\langle n | A | m \rangle\langle m | \psi \rangle \, e^{-t(E_n+E_m)/\hbar}}{\sum_{n=0}^{\infty} \langle \psi | n \rangle\langle n | \psi \rangle \, e^{-2tE_n/\hbar}}.$$

For as $t \to \infty$, the RHS becomes

$$\frac{e^{-2E_0 t/\hbar} \langle \psi|0\rangle\langle 0|A|0\rangle\langle 0|\psi\rangle}{e^{-2E_0 t/\hbar} \langle \psi|0\rangle\langle 0|\psi\rangle} = \langle 0|A|0\rangle.$$

Thus the prescription to find $\langle 0|A|0\rangle$ is

$$\langle 0|A|0\rangle = \lim_{t\to\infty} \frac{\langle \psi| e^{-\frac{tH}{\hbar}} A e^{-tH/\hbar} |\psi\rangle}{\langle \psi| e^{-2Ht/\hbar} |\psi\rangle}.$$

This works best if $|0\rangle$ is nondegenerate, that is, if the ground state is unique, and if $\langle 0|\psi\rangle$ is not too tiny.

This method is the basis of lattice gauge theory.

To apply this method, we do what we did to find the Feynman path integral.

$$\langle x_{j+1}| e^{-\epsilon H/\hbar} |x_j\rangle = \langle x_{j+1}| e^{-\frac{V\epsilon}{2\hbar}} e^{-\frac{p^2}{2m}\frac{\epsilon}{\hbar}} e^{-\frac{V\epsilon}{2\hbar}} |x_j\rangle$$

$$= e^{-\epsilon(V_{j+1}+V_j)/2\hbar} \langle x_{j+1}| \int_{-\infty}^{\infty} dp_j \, e^{-\frac{\epsilon p^2}{2m\hbar}} |p_j\rangle\langle p_j|x_j\rangle$$

$$= e^{-\frac{\epsilon}{2\hbar}\overline{V}_j} \int_{-\infty}^{\infty} dp_j \, e^{-\frac{\epsilon p_j^2}{2m\hbar}} \, e^{i p_j (x_{j+1} - x_j)/\hbar} .$$

We complete the square

$$-\frac{\epsilon p_j^2}{2m\hbar} + i p_j \frac{(x_{j+1} - x_j)}{\hbar} = -\frac{\epsilon}{2m\hbar}(p_j - \alpha)^2 + \beta$$

$$\frac{i p_j (x_{j+1} - x_j)}{\hbar} = \frac{\epsilon}{m\hbar} p_j \alpha$$

$$\epsilon \frac{\alpha^2}{2m\hbar} = \beta$$

So

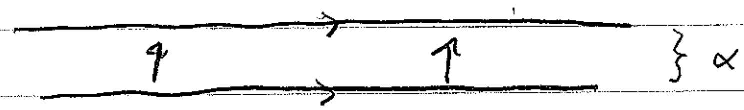
$$\alpha = i m \frac{(x_{j+1} - x_j)}{\epsilon}$$

is an imaginary momentum, and

$$\beta = \frac{\epsilon \alpha^2}{2m\hbar} = -\frac{\epsilon m^2}{2m\hbar}\left(\frac{x_{j+1} - x_j}{\epsilon}\right)^2$$

$$= -\frac{\epsilon m}{2\hbar}\left(\frac{x_{j+1} - x_j}{\epsilon}\right)^2 .$$

We may shift the contour from



the two integrals are the same, and both converge. Thus

$$\langle x_{j+1}| e^{-\epsilon H/\hbar} |x_j\rangle = e^{-\frac{\epsilon \bar{V}_j}{\hbar}} \, e^{-\frac{\epsilon m}{2\hbar}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2}$$

apart from an overall constant which cancels when forming ratios.

Putting all the factors together, we get

$$\langle 0| \underline{A(x)} |0\rangle = \frac{\int \mathcal{D}x(t)\; A(x(t))\, e^{-\frac{1}{\hbar}\int_{-\infty}^{\infty} dt \left(\frac{m}{2}\dot{x}^2 + V(x)\right)}}{\int \mathcal{D}x(t)\; e^{-\frac{1}{\hbar}\int_{-\infty}^{\infty} dt \left(\frac{m}{2}\dot{x}^2 + V(x)\right)}} .$$

In particular, if we define

$$X_E(t) = e^{+\frac{tH}{\hbar}}\, x\, e^{-\frac{tH}{\hbar}}$$ then

$$\langle 0| X(t_2)\, X(t_1) |0\rangle = \frac{\int \mathcal{D}x(t)\; x(t_2)\, x(t_1)\, e^{-\frac{1}{\hbar}\int_{-\infty}^{\infty} dt \left[\frac{m}{2}\dot{x}^2 - V(x(t))\right]}}{\int \mathcal{D}x(t)\; e^{-\frac{1}{\hbar}\int_{-\infty}^{\infty} dt \left[\frac{m}{2}\dot{x}^2 - V(x)\right]}}$$

for instance. To derive this formula,

we start from

$$\langle 0|\,x(t_2)\,X(t_1)\,|0\rangle = \frac{\langle\psi| e^{-\frac{TH}{\hbar}} e^{+\frac{t_2 H}{\hbar}} x\, e^{-\frac{t_2 H}{\hbar}} e^{+\frac{t_1 H}{\hbar}} x\, e^{-\frac{t_1 H}{\hbar}} e^{-\frac{TH}{\hbar}} |\psi\rangle}{\langle\psi| e^{-2\frac{TH}{\hbar}} |\psi\rangle}$$

$$= \frac{\langle\psi| e^{-\frac{(T-t_2)H}{\hbar}}\, x\, e^{-\frac{(t_2-t_1)H}{\hbar}}\, x\, e^{-\frac{(T+t_1)H}{\hbar}} |\psi\rangle}{\langle\psi| e^{-2TH/\hbar} |\psi\rangle}$$

and insert factors of $I = \int dx\, |x\rangle\langle x|$ and $I = \int dp\, |p\rangle\langle p|$.

An application: Since for $E_0 = 0$

$$\lim_{t\to\infty} e^{-\frac{tH}{\hbar}} = |0\rangle\langle 0|$$

we have

$$|\psi_0(x)|^2 = \langle x|0\rangle\langle 0|x\rangle = |\langle x|0\rangle|^2$$

$$= N \int_{x(-\infty)=x=x(\infty)} Dx(t)\; e^{-S_E/\hbar}$$

where N is a normalization constant and

$$S_E = \int_{-\infty}^{\infty} dt\; \tfrac{1}{2} m \dot{x}^2 + V(x(t)).$$

The path integral that one uses to find out about ground states is built from

$$Z = \int Dx \, e^{-\frac{1}{\hbar}\int_{-\infty}^{\infty} dt \left[\frac{1}{2} m \dot{x}^2 + V(x(t))\right]}.$$

This Z looks a lot like the partition function Z of statistical mechanics

$$Z = \sum_j e^{-E_j/kT}$$ in which T is the temperature and k is Boltzmann's constant. The main difference is that Z involves a sum over all states j of energy E_j while Z is a sum over all processes of infinite duration. Each process contributes to Z a quantity related to its time-averaged energy $\bar{E}_j$

$$\sim e^{-\mathcal{T}\bar{E}_j/\hbar}$$

where $\mathcal{T}$ is the infinite duration. The correspondence then is

$$\frac{1}{kT} = \frac{\mathcal{T}}{\hbar}$$

which means that the partition function Z

looks like the path integral Z in the old, zero-temperature limit $T \to 0$.

We also can develop a path-integral formula for the density operator ρ for a system in thermal equilibrium at temperature T

$$\rho = \frac{e^{-H/kT}}{\mathrm{Tr}\, e^{-H/kT}}$$

in which the trace is just the partition function

$$Z = \mathrm{Tr}\,\rho = \mathrm{Tr}\, e^{-H/kT}$$
$$= \sum e^{-E_j/kT} = \int dx \, \langle x | e^{-H/kT} | x \rangle .$$

where the sum is over a complete set of states. To get further, we must compute

$$\langle x_{j+1} | e^{-\epsilon H/kT} | x_j \rangle = \langle x_{j+1} | e^{-\frac{V\epsilon}{2kT}} e^{-\frac{\epsilon p^2}{2mkT}} e^{-\frac{V\epsilon}{2kT}} | x_j \rangle$$
$$= e^{-\epsilon \bar{V}_j/kT} \langle x_{j+1} | \int dp_j \, e^{-\epsilon p_j^2/2mkT} | p_j \rangle \langle p_j | x_j \rangle$$
$$= e^{-\epsilon \bar{V}_j/kT} \int \frac{dp_j}{h} \, e^{i p_j (x_{j+1} - x_j)/\hbar - \epsilon p_j^2/2mkT} .$$

Again, we complete the square:

$$-\frac{\epsilon p_j^2}{2mkT} + \frac{i}{\hbar} p_j (x_{j+1} - x_j) = -\frac{\epsilon}{2mkT}(p_j - \alpha)^2 + \beta$$

$$\frac{i}{\hbar}(x_{j+1} - x_j) = \frac{\alpha \epsilon}{mkT} \qquad \beta = \frac{\alpha^2 \epsilon}{2mkT}$$

So $$\alpha = i \frac{mkT}{\hbar} \frac{(x_{j+1} - x_j)}{\epsilon}$$

and
$$\beta = -\epsilon \left[\frac{mkT}{\hbar} \frac{(x_{j+1} - x_j)}{\epsilon} \right]^2 \frac{1}{2mkT}$$

$$\beta = -\epsilon \frac{mkT}{2\hbar^2} \left(\frac{x_{j+1} - x_j}{\epsilon} \right)^2 .$$

So apart from an over-all factor
$$\langle x_{j+1} | e^{-\epsilon H/kT} | x_j \rangle = e^{-\epsilon \bar{V}_j/kT} e^{-\epsilon \frac{mkT}{2\hbar^2} \left(\frac{x_{j+1} - x_j}{\epsilon} \right)^2} .$$

Now let's write the tiny dimensionless ϵ as a tiny time δ divided by $\hbar/kT$, which has units of time

$$\epsilon = \frac{\delta}{(\hbar/kT)} = \frac{\delta kT}{\hbar} .$$

Then

$$\langle x_{j+1}| e^{-\epsilon H/kT} |x_j\rangle = e^{-\frac{\delta}{\hbar}\bar{V}_j - \delta \frac{m}{2}\frac{(kT)^2}{\hbar^3}\left(\frac{x_{j+1}-x_j}{\delta kT/\hbar}\right)^2}$$

$$= e^{-\frac{\delta \bar{V}_j}{\hbar}} e^{-\frac{\delta}{\hbar}\cdot\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\delta}\right)^2}.$$

And so we arrive at

$$Z = \int_{-\infty}^{\infty} dx \, \langle x| e^{-H/kT} |x\rangle$$

$$= \oint Dx \, e^{-\frac{1}{\hbar}\int_0^T dt \left[\frac{1}{2}m\dot{x}^2 + V(x(t))\right]}$$

in which the integral is over all loops from x to x as time runs from 0 to T. What is T? Well, the sum of all the ϵ's must be unity, so the sum of all δ's must be $\hbar/kT$.

$$1 = \sum \epsilon = \frac{kT}{\hbar}\sum \delta$$

So $T = \hbar/kT$, which has units of time. So

$$Z = \oint Dx \, e^{-\frac{1}{\hbar}\int_0^{\hbar/kT} dt \left[\frac{1}{2}m\dot{x}(t)^2 + V(x(t))\right]}.$$

And so the density operator ρ is

$$\rho = \frac{\int Dx \; |x_f\rangle \, e^{-\int_0^{\hbar/kT} \frac{dt}{\hbar}\left[\frac{1}{2} m \dot{x}^2 + V\right]} \langle x_i|}{\oint Dx \; e^{-\int_0^{\hbar/kT} \frac{dt}{\hbar}\left[\frac{1}{2} m \dot{x}^2 + V\right]}} .$$

The paths in the numerator run from x_i to x_f in time $T = \hbar/kT$, while those in the denominator run from x_i to x_i in time T. In the numerator, one integrates over x_i and x_f; in the denominator, one integrates over x_i.

Do not worry if some of the foregoing seemed hard to understand.