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Physics 115 - Seminar 6

The Path Integral Method

A propagator is a unitary operator that takes an initial state, such as $|\psi(x',0)\rangle$, to a final state, $|\psi(x,t)\rangle$. We will assume a time-independent Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x}), \tag{1}$$

for which we can write the propagator in the position basis as

$$\begin{aligned} &U(x,x',t) \\ &= \left\langle x \left| \exp\left(-\frac{i}{\hbar}\hat{H}t\right)\right| x' \right\rangle \\ &= \left\langle x \left| \left[\exp\left(-\frac{i}{\hbar}\hat{H}\epsilon\right)\right]^N \right| x' \right\rangle \\ &= \int dx_{N-1}\cdots\int dx_1 \left\langle x_N \left|\exp\left(-\frac{i\epsilon}{\hbar}\hat{H}\right)\right| x_{N-1}\right\rangle \langle x_{N-1}|\cdots|x_1\rangle \left\langle x_1\left|\exp\left(-\frac{i\epsilon}{\hbar}\hat{H}\right)\right| x_0\right\rangle. \end{aligned} \tag{2}$$

where $t = N\epsilon$ and we have inserted $N-1$ complete sets of states. Let's consider one of the braketed terms above. The operator is of the form e^{A+B}, which is not exactly equal to e^Ae^B, since A and B do not commute. However, $e^Ae^B = e^{A+B+[A,B]/2+\cdots}$, and in the limit $\epsilon \to 0$ $(N \to \infty)$, the commutator and higher-order terms will go to zero. Since the position state is an eigenstate of the potential operator, we can pull this term out of the braket, and then the operator containing the kinetic energy can be evaluated by inserting a complete set of momentum states and completing the square.

$$\left\langle x_j \left| \exp\left(-\frac{i\epsilon\hat{H}}{\hbar}\right)\right| x_{j-1}\right\rangle \tag{3}$$

$$= \left\langle x_j \left| \exp\left(-\frac{\hat{p}^2}{2m}\frac{i\epsilon}{\hbar} - \frac{i\epsilon}{\hbar}\hat{V}\right)\right| x_{j-1}\right\rangle \tag{4}$$

$$\approx \left\langle x_j \left| \exp\left(-\frac{\hat{p}^2}{2m}\frac{i\epsilon}{\hbar}\right)\exp\left(-\frac{i\epsilon}{\hbar}\hat{V}\right)\right| x_{j-1}\right\rangle \tag{5}$$

$$= \left\langle x_j \left| \exp\left(-\frac{\hat{p}^2}{2m}\frac{i\epsilon}{\hbar}\right)\right| x_{j-1}\right\rangle e^{-\frac{i\epsilon}{\hbar}V(x_{j-1})} \tag{6}$$

$$= \int_{-\infty}^{\infty} \left\langle x_j \left| \exp\left(-\frac{\hat{p}^2}{2m}\frac{i\epsilon}{\hbar}\right)\right| p\right\rangle \langle p|x_{j-1}\rangle\, dp\; e^{-\frac{i\epsilon}{\hbar}V(x_{j-1})} \tag{7}$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp\left(-\frac{\hat{p}^2}{2m}\frac{i\epsilon}{\hbar}\right)\exp\left(\frac{i(x_j - x_{j-1})}{\hbar}\right) dp\; e^{-\frac{i\epsilon}{\hbar}V(x_{j-1})} \tag{8}$$

$$= \frac{1}{2\pi\hbar}\exp\left(\frac{im}{2\epsilon\hbar}(x_j - x_{j-1})^2\right)\int_{-\infty}^{\infty}\exp\left(-\frac{i\epsilon}{2m\hbar}\left[p - \frac{m}{\epsilon}(x_j - x_{j-1})\right]^2\right) dp\; e^{-\frac{i\epsilon}{\hbar}V(x_{j-1})} \tag{9}$$

$$= \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{1/2}\exp\left(\frac{im}{2\hbar\epsilon}(x_j - x_{j-1})^2 - \frac{i\epsilon}{\hbar}V(x_{j-1})\right). \tag{10}$$

The propagator now becomes

$$U(x_N, x_0, t) = \lim_{\substack{N\to\infty \\ \epsilon\to 0}} \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{N/2} \int dx_{N-1} \cdots \int dx_1 \exp\left[\sum_{j=1}^{N} \left(\frac{im}{2\hbar\epsilon}\left(x_j - x_{j-1}\right)^2 - \frac{i\epsilon}{\hbar} V(x_{j-1})\right)\right]. \quad (11)$$

Comparing to Shankar Eq. (8.4.3) shows that when $V = 0$, this is just the free particle propagator.

We now note Shankar Eq. (8.4.8), which can be rewritten as

$$\int \mathcal{D}[x(t)] = \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{N/2} \lim_{\substack{N\to\infty \\ \epsilon\to 0}} \int dx_{N-1} \cdots \int dx_1. \quad (12)$$

We can thus write the propagator as

$$U(x, x', t) = \int \mathcal{D}[x(t)] \exp\left(\frac{i}{\hbar}\int_0^t \mathcal{L}(x, \dot{x}) dt\right), \quad (13)$$

where the sum over j has become a continuous integral, and we identify $\frac{m}{2}\lim_{\epsilon\to 0}[(x_j - x_{j-1})/\epsilon]^2$ as the kinetic energy. This is known as the *Configuration Space* path integral. Shankar points out that there are many subtleties involved in turning a discrete equation into a continuous one, and that we should remember that the discretized version preceded the continuous one, and not vice versa. However, this form of the path integral can be very useful, as we saw in some of this week's problems.

As Robert will demonstrate in deriving Eq. (21.1.6), we can also express the propagator as

$$U(x, x', t) = \int [\mathcal{D}p\mathcal{D}x] \exp\left[\sum_{i=1}^{N}\left(\frac{-i\epsilon}{2m\hbar}p_n^2 + \frac{i}{\hbar}p_n\left(x_n - x_{n-1}\right) - \frac{i\epsilon}{\hbar}V\left(x_{n-1}\right)\right)\right] \quad (14)$$

$$= \int [\mathcal{D}p\mathcal{D}x] \exp\left[\frac{i\epsilon}{hbar}\sum_{i=1}^{N}\left(\frac{p_n\left(x_n - x_{n-1}\right)}{\epsilon} - \left[\frac{p_n^2}{2m} + V\right]\right)\right]. \quad (15)$$

As before, we turn this discrete sum into a continuous integration over time, giving us the *Phase Space Path Integral*:

$$U(x, x', t) = \int [\mathcal{D}p\mathcal{D}x] \exp\left[\frac{i}{\hbar}\int_0^t \left[p\dot{x} - \mathcal{H}(x, p)\right] dt\right]. \quad (16)$$

Note that the term in the exponential is just the Lagrangian.