Path Integrals Day 2

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1 Derivation of the path integral representation of the propagator

Last time we saw that we could write the propagator as a path integral

$$K = \sum_{\text{paths } \gamma} A[\gamma]\,. \tag{1}$$

Today we will determine $A[\gamma]$ by discretizing the paths. We will see that the path integral (1) for finite time can be written in terms of a product of propagators for infinitesimal time intervals. We will then compute the infinitesimal propagator using perturbation theory and Gaussian integrals (integrals who integrand contains the exponential of a quadratic function such as $\int dx e^{-ax^2+bx+c}$).

2 Discretizing the paths (from day 1 lecture notes)

Let's start by breaking the path into two pieces. If particle number is conserved, then if a particle propagates from position q_i at time t_i to position q_f at time t_f, then it must be somewhere at an intermediate time t_{int}

$$K(q_f, t_f, q_i, t_i) = \int dy K(q_f, t_f, y, t_{\text{int}}) K(y, t_{\text{int}}, q_i, t_i)\,. \tag{2}$$

We can derive this formula by inserting the resolution of the identity as an integral over position eigenstates $\mathbf{1} = \int dy |y\rangle\langle y|$ into the Heisenberg picture expression for the propagator

$$\begin{aligned}
K(q_f, t_f, q_i, t_i) &= \langle q_f| e^{-iH(t_f - t_i)} |q_i\rangle & (3)\\
&= \langle q_f| e^{-iH(t_f - t_{\text{int}})} e^{-iH(t_{\text{int}} - t_i)} |q_i\rangle & (4)\\
&= \langle q_f| e^{-iH(t_f - t_{\text{int}})} \int dy |y\rangle\langle y| e^{-iH(t_{\text{int}} - t_i)} |q_i\rangle & (5)\\
&= \int dy K(q_f, t_f, y, t_{\text{int}}) K(y, t_{\text{int}}, q_i, t_i) & (6)
\end{aligned}$$

Let's repeat the above procedure N times. First we can rewrite the Heisenberg picture expression for the propagator as

$$K(q_f, t_f, q_i, t_i) = \langle q_f| \left(e^{-iH\Delta t}\right)^N |q_i\rangle \tag{7}$$

We can then insert the identity $\int dq_n |q_n\rangle\langle q_n|$ for $n = 1, ..., N-1$ in between each factor of $e^{iH\delta t}$

$$K(q_f, t_f, q_i, t_i) = \langle q_f|e^{-iH\Delta t} \int dq_{N-1}|q_{N-1}\rangle\langle q_{N-1}|e^{-iH\Delta t} \int dq_{N-2}|q_{N-2}\rangle \cdots e^{-iH\Delta t}|q_i\rangle \tag{8}$$

$$= \int dq_1 dq_2 \cdots dq_{N-1} A[\gamma] \,. \tag{9}$$

We see that $A[\gamma]$ is a product of propagators

$$A[\gamma] = K_{q_N, q_{N-1}} \cdots K_{q_1, q_0} \tag{10}$$

where $q_N = q_f$, $q_0 = q_i$, and

$$K_{q_{n-1}, q_n} = K(q_n, n\Delta t, q_{n-1}, (n-1)\Delta t) \,. \tag{11}$$

3 Infinitesimal propagator

To compute the infinitesimal[1] propagator K_{q_{j+1}, q_j} we can expand the infinitesimal time evolution operator $e^{-i\Delta t H/\hbar}$ in a power series:

$$K_{q_{j+1}, q_j} = \langle q_{j+1}|e^{-i\Delta t H/\hbar}|q_j\rangle \tag{12}$$

$$= \langle q_{j+1}| \left[1 - \frac{i\Delta t H}{\hbar} + \frac{1}{2}\left(\frac{i\Delta t H}{\hbar}\right)^2 + \cdots\right] |q_j\rangle \,. \tag{13}$$

The zeroth order term (in $\frac{\Delta t H}{\hbar}$) is a Dirac delta

$$\langle q_{j+1}|q_j\rangle = \delta\left(q_{j+1} - q_j\right) \,. \tag{14}$$

A Dirac delta can also be expressed as the Fourier transform of the identity

$$\delta\left(q_{j+1} - q_j\right) = \int \frac{dp_j}{2\pi} e^{ip_j(q_{j+1} - q_j)} \tag{15}$$

As you will show in an exercise, the first-order term is

$$-i\frac{\Delta t}{\hbar}\langle q_{j+1}|H|q_j\rangle = -i\frac{\Delta t}{\hbar} \int \frac{dp_j}{2\pi\hbar} e^{ip_j(q_{j+1} - q_j)/\hbar} \left(\frac{p_j^2}{2m} + V(q_j)\right) \,. \tag{16}$$

[1] I am calling it the infinitesimal propagator because we are ultimately interested in the limit $\Delta t \to 0$ or $N \to \infty$.

The zeroth- and first-order terms look like the first two terms in the expansion of the exponential in

$$K_{q_{j+1},q_j} = \int \frac{dp_j}{2\pi\hbar} e^{ip_j(q_{j+1}-q_j)/\hbar} e^{-i\Delta t H(q_j,p_j)/\hbar} . \tag{17}$$

It is not surprising that we end up with an exponential given that we started with an exponential. To more carefully demonstrate that the infinitesimal propagator is given by (17), we would need to compute the higher-order terms.

4 Phase space propagator

Using our result for the infinitesimal propagator, we see that the finite propagator can be written as

$$K = \lim_{N\to\infty} \int dq_1 \cdots dq_{N-1} A[\gamma] \tag{18}$$

$$= \lim_{N\to\infty} \int \prod_{j=1}^{N-1} dq_j \prod_{j=0}^{N-1} \frac{dp_j}{2\pi} \exp\left[i\Delta T \left(\sum_{j=0}^{N-1} p_j \dot{q}_j - H(q_j, p_j) \right) \right] \tag{19}$$

In more compact notation this is

$$K = \int \mathcal{D}q(t)\mathcal{D}p(t) \exp\left[\frac{i}{\hbar} \int_0^T dt \left(p\dot{q} - H(p,q) \right) \right] . \tag{20}$$

This expression is known as the phase-space path integral, and is not quite what we were seeking. Our goal was to find an expression for the propagator as a sum over paths through position space, not phase space.

5 Path integral representation of the propagator

We want to perform the momentum integrals in (20). Fortunately, if the Hamiltonian takes the form

$$H = \frac{p^2}{2m} + V(q) \tag{21}$$

we can perform the momentum integrals analytically since each of the momentum integrals in the infinitesimal propagators (17) is Gaussian. The momentum integrals are

$$\int \frac{dp_j}{2\pi} \exp\left[\frac{i}{\hbar} \Delta t \left(p_j \dot{q}_j - p_j^2/2m \right) \right] = \sqrt{\frac{m\hbar}{2\pi i \Delta t}} e^{\frac{i}{\hbar}\Delta t m {\dot{q}_j}^2/2} \tag{22}$$

Using this result the propagator becomes

$$K = \lim_{N\to\infty} \left(\frac{m\hbar}{2\pi i \Delta t} \right)^{N/2} \int \prod_{j=1}^{N-1} dq_j \exp\left[\frac{i}{\hbar} \Delta T \left(\sum_{j=0}^{N-1} m{\dot{q}_j}^2/2 - V(q_j) \right) \right] \tag{23}$$

or in shorthand notation

$$K = \int \mathcal{D}q(t) \exp\left[iS[q(t)]\right] \, . \tag{24}$$

6 Exercise 1: Conceptual review

- What assumptions did we make in deriving the path integral representation of the propagator?
- What were the key steps in the derivation?
- Explain the final result in words.

7 Exercise 2: First-order term

By inserting the resolution of the identity

$$\mathbf{1} = \int \frac{dp}{2\pi\hbar} |p\rangle\langle p| \tag{25}$$

and using

$$\langle q|p\rangle = e^{ipq/\hbar} \tag{26}$$

show that the first-order term can be expressed as

$$-i\frac{\Delta t}{\hbar}\langle q_{j+1}|H|q_j\rangle = -i\frac{\Delta t}{\hbar}\int \frac{dp_j}{2\pi\hbar} e^{ip_j(q_{j+1}-q_j)/\hbar}\left(\frac{p_j^2}{2m} + V(q_j)\right) . \tag{27}$$

8 Exercise 3: Gaussian integration

Starting from the basic Gaussian integral[2]

$$\int_{-\infty}^{\infty} dx e^{-x^2} = \sqrt{\pi} \tag{28}$$

complete the square and change variables to show that[3]

$$\int_{-\infty}^{\infty} dx e^{-ax^2+bx+c} = \sqrt{\frac{\pi}{a}} \exp\left[\frac{b^2}{4a} + c\right] . \tag{29}$$

[2]Where does this result come from?

[3]Note that one has to be careful if a is complex. Can you justify our use of this equation in the derivation above?