How to Compute the Feynman Propagator

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1 Spectral Approach

Let $H : \mathcal{H} \to \mathcal{H}$ be a time-independent self-adjoint Hamiltonian operator with spectrum $\sigma \subset \mathbb{R}$. Then, the spectral representation of the time evolution operator is

$$U(t) \equiv e^{-iHt/\hbar} = \int_\sigma e^{-i\lambda t/\hbar}\, dP_\lambda$$

where dP_λ is the projection-valued measure on σ such that

$$H = \int_\sigma \lambda\, dP_\lambda.$$

In QM, we may think of dP_λ as $|\lambda\rangle\langle\lambda|\, d\lambda$, where we often refer to $|\lambda\rangle$ as an "eigenket" of H with "eigenvalue" λ. This intuition is correct if each λ lies in a point spectrum. In general, however, it may lie in the continuous spectrum, in which case the ket $|\lambda\rangle$ may not reside in the Hilbert space $\mathcal{H}$ and $|\lambda\rangle\langle\lambda|$ should be interpreted as a shorthand notation for an appropriate projection operator on $\mathcal{H}$; in this case, even though $|\lambda\rangle$ may not lie in $\mathcal{H}$, we can often integrate $\langle x|\lambda\rangle$ multiplied by other functions defined on σ.

Example 1.1. *Free Hamiltonian* $H = \dfrac{p^2}{2m}$, *with* $\sigma = \mathbb{R}$.

$$\begin{aligned}
\langle x|U(t)|y\rangle &= \int_{\mathbb{R}} e^{-ip^2t/2m\hbar}\langle x|p\rangle\langle p|y\rangle\, dp = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \exp\left(-\frac{i}{\hbar}\frac{p^2 t}{2m} + \frac{i}{\hbar}p(x-y)\right) dp \\
&= \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \exp\left[-\frac{it}{2m\hbar}\left(p^2 - \frac{2m}{t}p(x-y) + \frac{m^2(x-y)^2}{t^2} - \frac{m^2(x-y)^2}{t^2}\right)\right] dp \\
&= \exp\left[\frac{im(x-y)^2}{2\hbar t}\right]\frac{1}{2\pi\hbar}\int_{\mathbb{R}} \exp\left[-\frac{it}{2m\hbar}\left(p - \frac{m(x-y)}{t}\right)^2\right] dp \\
&= \sqrt{\frac{m}{2\pi i\hbar\, t}}\,\exp\left[\frac{im(x-y)^2}{2\hbar\, t}\right],
\end{aligned}$$

where the last equality follows from rotating the contour and performing the Gaussian integration (see "Notes on Contour Integration"). To summarize, for a free particle,

$$\boxed{K(x,t;y,t_0) = \sqrt{\frac{m}{2\pi i\hbar\,(t-t_0)}}\,\exp\left[\frac{im(x-y)^2}{2\hbar\,(t-t_0)}\right]}. \tag{1.1}$$

Example 1.2 (1D SHO)**.** *Done in lecture.*

2 Equation of Motion Approach

Let $H = \dfrac{\hat{p}^2}{2m} + V(\hat{x})$ be a 1D Hamiltonian. In the Heisenberg picture, the position x^H and momentum p^H operators evolve as

$$\frac{dx^H}{dt} = \frac{1}{i\hbar}[x^H, H] = \frac{p^H}{m} \quad \text{and} \quad \frac{dp^H}{dt} = -\frac{dV^H}{dx}.$$

For some simple potential $V(x)$, we can integrate these equations of motion and solve for $x^H(t)$ and $p^H(t)$ in terms of the Schrödinger picture $\hat{x}$ and $\hat{p}$ at time $t = 0$. In such a case, we can consider

$$\langle x|x^H(-t)U(t)|y\rangle = \langle x|U(t)\,\hat{x}\,U^\dagger(t)U(t)|y\rangle = y\,K(x,t;y,0), \tag{2.1}$$

which must equal to the expression obtained by substituting the explicit solution $x^H(-t)$ to the equation of motion. This equality will yield a differential equation for the propagator, and solving the differential equation will determine the propagator up to a multiplicative factor that depends on t. The multiplicative factor is then chosen such that $K(x,t;y,0)$ satisfy the Schrödinger's equation in x and t.

Example 2.1. (Free Hamiltonian $H = \dfrac{p^2}{2m}$). *The Heisenberg equation of motion is*

$$x^H(t) = \frac{\hat{p}}{m}\,t + \hat{x}.$$

Hence,

$$\langle x|x^H(-t)U(t)|y\rangle = \langle x|(-\hat{p}\,t/m + \hat{x})U(t)|y\rangle = \left(\frac{i\hbar\,t}{m}\frac{d}{dx} + x\right)K(x,t;y,0).$$

This expression must equal to the right-hand side of (2.1). Thus,

$$\frac{d}{dx}K(x,t;y,0) = \frac{im}{\hbar\,t}(x-y)K(x,t;y,0).$$

We have seen many times in the course that the solution proportional to a Gaussian function:

$$K(x,t;y,0) = C(t)\,\exp\left[\frac{im(x-y)^2}{2\hbar\,t}\right].$$

To determine the remaining function $C(t)$, we require that $K(x,t;y,0)$ satisfies

$$i\hbar\frac{\partial K(x,t;y,0)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 K(x,t;y,0)}{\partial x^2},$$

which becomes

$$\dot{C} = -\frac{C}{2t} \;\Rightarrow\; C(t) = \frac{D}{\sqrt{t}}.$$

Finally, the constant D is determined to be $D = \sqrt{m/2i\hbar}$ by requiring that

$$\lim_{t\to 0} K(x,t;y,0) = \delta(x-y).$$

We have thus reproduced the free particle propagator given in (1.1).

Example 2.2 (1D SHO)**.** *Exercise.*

3 Path Integral Approach

We would like to compute the propagator $K(x,t;y,t_0)$ by applying the formula

$$K(x,t;y,t_0) = \lim_{N\to\infty} \int \cdots \int dx_1 \cdots dx_N \prod_{n=0}^{N} K(x_{n+1},t_{n+1};x_n,t_n) \tag{3.1}$$

where $x_{N+1} = x, x_0 = y, t_n = t_0 + n\Delta t$, and $\Delta t = (t-t_0)/(N+1)$. In the limit $\Delta t << 1$, Feynman proposed to express

$$K(x_{n+1},t_{n+1};x_n,t_n) \propto \exp\left(\frac{i}{\hbar}\int_{t_n}^{t_{n+1}} L(x,\dot{x})\,dt\right) \approx \exp\left[\frac{i\Delta t}{\hbar} L\left(\frac{x_n+x_{n+1}}{2}, \frac{x_{n+1}-x_n}{\Delta t}\right)\right].$$

where L is the Lagrangian and the proportionality factor is chosen so that

$$\lim_{t_{n+1}\to t_n} K(x_{n+1},t_{n+1};x_n,t_n) = \delta(x_{n+1}-x_n).$$

When the potential does not depend on $\dot{x}$ or time, the normalization factor depends only on the kinetic energy term, and the incremental propagator is

$$K(x_{n+1},t_{n+1};x_n,t_n) = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \exp\left[\frac{i\Delta t}{\hbar} L\left(\frac{x_n+x_{n+1}}{2}, \frac{x_{n+1}-x_n}{\Delta t}\right)\right]. \tag{3.2}$$

In some simple cases, you can plug (3.2) into (3.1), perform the integrals, and then take the limit $N \to \infty$.

Example 3.1 (Free Particle)**.** $L = \frac{1}{2}m\dot{x}^2$. *Partitioning the time $t-t_0$ into $N+1$ intervals as above, we get*

$$K(x,t;y,t_0) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N+1}{2}} \int \cdots \int dx_1 \cdots dx_N \exp\left[-\frac{m}{2i\hbar\Delta t}\sum_{n=0}^{N}(x_{n+1}-x_n)^2\right].$$

We now note the following useful formula:

$$\frac{1}{\sqrt{2\pi\sigma^2}}\int_{\mathbb{R}} e^{-\frac{(x-z)^2}{2\sigma^2}-\frac{(z-y)^2}{2n\sigma^2}}\,dz = e^{-\frac{(x-y)^2}{2(n+1)\sigma^2}}\sqrt{\frac{n}{n+1}}.$$

Using this formula, the propagator becomes

$$K(x,t;y,t_0) = \lim_{N\to\infty} \sqrt{\frac{m}{2\pi i\hbar(N+1)\Delta t}} \exp\left[\frac{im(x-y)^2}{2\hbar(N+1)\Delta t}\right] = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}} \exp\left[\frac{im(x-y)^2}{2\hbar(t-t_0)}\right].$$

3.1 Stationary Phase Approximation

As discussed in class, the leading order semi-classical approximation ($\hbar \ll 1$) of the propagator using stationary phase approximation is given by

$$K(x,t;y,t_0) = \sum_j \frac{e^{-i\nu_j\pi/2}}{\sqrt{2\pi i\hbar}} \left|\frac{\partial^2 S_j}{\partial x \partial y}\right|^{1/2} \exp\left(\frac{i}{\hbar} S_j(x,y,t,t_0)\right)$$

where the sum is over all classical paths that are critical points of the action, S_j is Hamilton's principal function for the j-th classical path x_j connecting (y,t_0) to (x,t), and ν_j is the number of negative eigenvalues of the operator

$$T_j = -\frac{m}{2}\frac{d^2}{d\tau^2} - \frac{1}{2}V''(x_j(\tau))$$

associated with the second-order Taylor expansion of the Lagrangian around the j-th classical x_j.

Example 3.2 (Free Particle)**.** *In homework, you will show that for the unique path connecting (y,t_0) to (x,t),*

$$S(x,y,t,t_0) = \frac{m(x-y)^2}{2(t-t_0)}.$$

From this, we get

$$\left|\frac{\partial^2 S}{\partial x \partial y}\right|^{1/2} = \sqrt{\frac{m}{t-t_0}}.$$

Finally, the operator

$$T = -\frac{m}{2}\frac{d^2}{d\tau^2}$$

is positive semi-definite and has no negative eigenvalues. Thus, we have

$$K(x,t;y,t_0) = \frac{1}{\sqrt{2\pi i\hbar}}\sqrt{\frac{m}{t-t_0}} \exp\left(\frac{i}{\hbar}\frac{m(x-y)^2}{2(t-t_0)}\right),$$

agreeing with the previous calculations.

REMARK 3.1. *This stationary phase approximation is exact when $V = a+bx+cx^2$, because Taylor expanding the Lagrangian to second order in the stationary phase approximation is exact in this case.*