1 Propagators

In this section we look at the propagator and how it leads to the Feynman's path integral.

This material is covered in Section 2.6 of Sakurai, and in Chapter 8 of Shankar, which we will follow for the examples.

Recall that for a time-independent Hamiltonian, the Schrödinger picture state evolves as

$$|\psi(t)\rangle = \hat{U}(t,t_0)\,|\psi(t_0)\rangle = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}\,|\psi(t_0)\rangle\,. \tag{1}$$

To see what this does to the wavefunction $\psi(x,t) = \langle x|\psi(t)\rangle$, project onto $\langle x|$ and insert a complete set of position eigenstates on the right,

$$\psi(x,t) = \int dx_0\ \langle x|\,\hat{U}(t,t_0)\,|x_0\rangle\,\langle x_0|\psi(t_0)\rangle \equiv \int dx_0\,K(x,t;x_0,t_0)\,\psi(x_0,t_0). \tag{2}$$

The **propagator** is the time-evolution operator in the position basis,

$$\boxed{K(x,t;x_0,t_0) = \langle x|\,\hat{U}(t,t_0)\,|x_0\rangle = \langle x|\,e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}\,|x_0\rangle\,.} \tag{3}$$

We interpret it as the **amplitude** for a particle that is perfectly localized at x_0 at time t_0 to be found at x at time t. You can think of it as the "kernel" of an integral transform (examples of integrals transforms are Fourier and Laplace transforms). Knowing the function/kernel K is equivalent to solving the Schrödinger equation for any initial condition, since Eq. (2) gives $\psi(x,t)$ for any initial $\psi(x,t_0)$. In fact, we will see that K is the Green's functions of the Schrödinger equation.

Properties of K from the definition.

1. **Initial condition.** Since $\hat{U}(t_0,t_0) = \mathbb{1}$,

$$K(x,t_0;x_0,t_0) = \langle x|x_0\rangle = \delta(x-x_0). \tag{4}$$

2. **Schrödinger equation.** Because $i\hbar\partial_t\hat{U} = \hat{H}\hat{U}$, the propagator satisfies the Schrödinger equation in the variables (x,t) for fixed (x_0,t_0),

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V(x)\right]K(x,t;x_0,t_0) = 0 \quad (t > t_0). \tag{5}$$

   Together with Eq. (4), this shows that K is the solution to the Schrödinger equation with delta function as initial condition at $t = t_0$.

3. **Composition.** From $\hat{U}(t,t_0) = \hat{U}(t,t')\hat{U}(t',t_0)$ and a complete set of states at the intermediate time,

$$K(x,t;x_0,t_0) = \int dx'\,K(x,t;x',t')\,K(x',t';x_0,t_0). \tag{6}$$

   The amplitude to go from x_0 to x is the sum over all intermediate positions x' at any intermediate time t' of the amplitude to go from x_0 to x' times the amplitude to go from x' to x. This property will be the main ingredient for the construction of the path integral formulation of quantum mechanics.

4. **Time reversal.** From $\hat{U}^\dagger(t,t_0) = \hat{U}(t_0,t)$,

$$K^*(x,t;x_0,t_0) = K(x_0,t_0;x,t), \tag{7}$$

the conjugate amplitude is the amplitude for the reverse process.

5. **Energy eigenstates.** If $\hat{H}\,|n\rangle = E_n\,|n\rangle$ with normalized wavefunctions $u_n(x) = \langle x|n\rangle$, inserting a complete set of energy eigenstates we get

$$K(x,t;x_0,t_0) = \sum_n u_n(x)\,u_n^*(x_0)\,e^{-\frac{i}{\hbar}E_n(t-t_0)}. \tag{8}$$

Setting $x = x_0$ and integrating over x, the position dependence drops out

$$G(t) \equiv \int dx\,K(x,t;x,0) = \sum_n \left(\int dx\,|u_n(x)|^2\right) e^{-\frac{i}{\hbar}E_n t} = \sum_n e^{-\frac{i}{\hbar}E_n t}. \tag{9}$$

This function $G(t)$ is just $\mathrm{Tr}\,\hat{U}(t,0)$. Sakurai shows (Section 2.6) that the Fourier-Laplace transform of $G(t)$ has poles at $E = E_n$, so if you know the propagator you know the energy levels. We will use this below to read off the spectrum of the harmonic oscillator.



The function in Eq. (9) can be rewritten as the partition function of the system in imaginary time, $t \to -i\hbar\beta$, giving

$$Z(\beta) = \sum_n e^{-\beta E_n}, \tag{10}$$

where in statistical mechanics the parameter β is the inverse temperature, $\beta = 1/(k_B T)$. This correspondence between real time and imaginary time is the basis for the connection between quantum mechanics and statistical mechanics, often referred to as the Wick rotation (an analytic continuation to imaginary time). Many problems in thermal quantum field theory, for example, can be solved using this correspondence.



The Laplace-Fourier transform of $G(t)$:

$$\tilde{G}(E) = \frac{-i}{\hbar}\int_0^\infty dt\,e^{\frac{i}{\hbar}Et}G(t) = \frac{-i}{\hbar}\sum_n \int_0^\infty dt\,e^{\frac{i}{\hbar}Et}e^{-\frac{i}{\hbar}E_n t}. \tag{11}$$

We are calling it Laplace-Fourier transform, as it involves both a Laplace-like integral over time and a Fourier-like factor $e^{\frac{i}{\hbar}Et}$. This is a difficult integral, but if we allow for our energy domain to acquire a small positive imaginary part, $E \to E + i\epsilon$, the integral explicitly converges and we obtain

$$\tilde{G}(E) = \frac{-i}{\hbar}\sum_n \int_0^\infty dt\,e^{\frac{i}{\hbar}(E-E_n+i\epsilon)t} = \sum_n \frac{1}{E - E_n + i\epsilon}. \tag{12}$$

where the $i\epsilon$ prescription imposes $\epsilon \to 0^+$ at the end. As we will see later, the positive sign on ϵ ensures the correct *causal* structure of our theory. This prescription will be critical in scattering theory.

Strictly speaking, K is the propagator only for $t > t_0$. The combination $\theta(t-t_0)K(x,t;x_0,t_0)$ is what satisfies the inhomogeneous equation

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{H}_x\right]\theta(t-t_0)K(x,t;x_0,t_0) = i\hbar\,\delta(x-x_0)\,\delta(t-t_0), \tag{13}$$

which is the statement that the propagator is the **Green's function** of the Schrödinger equation (this choice is the *retarded* Green's function). See the Green's function notes for more on this. There is also the *advanced* Green's function, which corresponds to the choice $\theta(t_0-t)K(x,t;x_0,t_0)$ and satisfies the inhomogeneous equation with the opposite time ordering (this is the unphysical choice that propagates signals backward in time). In quantum field theory, you will encounter the Feynman propagator, which is a time-ordered Green's function that combines the retarded and advanced propagators in a way consistent with relativistic causality: particles propagate forward in time while antiparticles propagate backward in time. A major and non-trivial result is that this Feynman propagator correctly preserves causality in relativistic quantum field theory while preventing any superluminal signaling.

1.1 The free particle

The propagator is easy to compute whenever we know the eigenstates of $\hat{H}$. For a free particle, $\hat{H} = \hat{p}^2/2m$, we use momentum eigenstates with Sakurai's normalization (Section 1.7),

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\,e^{\frac{i}{\hbar}px}, \qquad \int dp\;|p\rangle\,\langle p| = \mathbb{1}, \tag{14}$$

and Eq. (8) becomes an integral over p,

$$K_0(x,t;x_0,t_0) = \langle x|\,e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}\left(\int dp\,|p\rangle\,\langle p|\right)|x_0\rangle \tag{15}$$

$$= \int dp\;\langle x|p\rangle\,\langle p|x_0\rangle\;e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t-t_0)} \tag{16}$$

$$= \frac{1}{2\pi\hbar}\int dp\,\exp\left[\frac{i}{\hbar}p(x-x_0) - \frac{i}{\hbar}\frac{p^2}{2m}(t-t_0)\right]. \tag{17}$$

This is a Gaussian integral with an imaginary coefficient.

Gaussian integrals. For $\mathrm{Re}\,\alpha > 0$ and any complex β, completing the square gives

$$\int_{-\infty}^{\infty} dx\,e^{-\alpha x^2+\beta x} = \sqrt{\frac{\pi}{\alpha}}\,e^{\frac{\beta^2}{4\alpha}}, \tag{18}$$

where

$$-\alpha x^2 + \beta x = -\alpha\left(x - \frac{\beta}{2\alpha}\right)^2 + \frac{\beta^2}{4\alpha}. \tag{19}$$

Our integrals here have a purely imaginary α (called Fresnel integrals). They converge only in the "weak sense" that the oscillations cancel. The safe way to think about them is to give α a small positive real part, $\alpha \to \alpha + 0^+$, use Eq. (18), and send this regulator to zero at the end (as we did above with ϵ).

With $\alpha = \frac{i(t-t_0)}{2m\hbar}$ and $\beta = \frac{i(x-x_0)}{\hbar}$, we get $\beta^2/4\alpha = \frac{im(x-x_0)^2}{2\hbar(t-t_0)}$, we find the propagator for the free particle:

$$\boxed{K_0(x,t;x_0,t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\,\exp\left[\frac{i}{\hbar}\frac{m(x-x_0)^2}{2(t-t_0)}\right].} \tag{20}$$

Some points:

- $|K_0|^2 = \frac{m}{2\pi\hbar(t-t_0)}$ is independent of x. This looks counter intuitive, because it says that a particle that starts perfectly localized in space at time t_0 is then equally likely to be found anywhere else a moment later at t. It has to be the case, however, since the uncertainty principle says that a delta function in position contains all momenta, including arbitrarily large ones that can get the particle anywhere in an arbitrarily short time.

- As $t \to t_0$, the Gaussian becomes infinitely narrow and infinitely tall, and you can check with Eq. (18) that $\int dx\, K_0 = 1$ for all t. It therefore reduces to $\delta(x - x_0)$, as it must by Eq. (4).

- The phase is actually quite familiar from classical mechanics. A free particle going from x_0 at t_0 to x at t moves with constant velocity $v = (x - x_0)/(t - t_0)$, and its action is

$$S_{\rm cl} = \int_{t_0}^{t} dt'\, \frac{1}{2} m v^2 = \frac{m(x-x_0)^2}{2(t-t_0)}. \tag{21}$$

  So the free propagator is $K_0 = A(t - t_0)\, e^{\frac{i}{\hbar} S_{\rm cl}}$, with some constant prefactor A that does not depend on the endpoints. This is not a coincidence, as we are azbout to see.

2 The Action and the Path Integral

In the Lagrangian formulation of classical mechanics (see, e.g., Chapter 2 of Shankar), we assign to every conceivable trajectory $x(t')$ between (x_0, t_0) and (x, t) a number called the **action**

$$S[x(t')] = \int_{t_0}^{t} dt'\, L(x, \dot{x}, t) = \int_{t_0}^{t} dt' \left[\frac{1}{2} m\dot{x}^2 - V(x)\right]. \tag{22}$$

Explicitly time-dependent Lagrangians are akin to time-dependent Hamiltonians and lead to energy non-conservation, but can in principle also be considered. We ignore this edge case for now. Hamilton's principle or "principle of least action" says that the trajectory the particle actually follows, $x_{\rm cl}(t')$, is the one for which S is extremized,

$$\delta S = 0,$$

with the endpoints held fixed. Working out the variational calculus in this problem gives the Euler-Lagrange equation:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \tag{23}$$

For Eq. (22) reads $m\ddot{x} = -\partial_x V$, which is just Newton's second law. The action evaluated on the classical path, $S_{\rm cl} \equiv S[x_{\rm cl}]$, is a function of the endpoints only, $S_{\rm cl}(x, t; x_0, t_0)$. This is the same function that appeared in Eq. (21).

Classically, the action is just an object for generating the equations of motion. Dirac was the first to notice that $e^{\frac{i}{\hbar}S}$ should play a role in quantum mechanics, but the complete reformulation of quantum mechanics in terms of it is thanks to Feynman. He noted that the quantum mechanical propagator is a sum over all paths, each weighted by $e^{\frac{i}{\hbar}S}$. We have a toy derivation of this below, following Sakurai.

Start with the definition Eq. (3) and break the time interval into N slices of duration $\delta t = (t - t_0)/N$. Since $\hat{H}$ is time-independent, $e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} = \left(e^{-\frac{i}{\hbar}\hat{H}\delta t}\right)^N$, and we can insert

a complete set of position eigenstates between each pair of factors (this is the composition property in Eq. (6) applied $N-1$ times),

$$K(x,t;x_0,t_0) = \int dx_1 \int dx_2 \cdots \int dx_{N-1} \prod_{n=1}^{N} \langle x_n | \, e^{-\frac{i}{\hbar}\hat{H}\delta t} \, | x_{n-1} \rangle \,, \qquad x_N \equiv x. \tag{24}$$

Note that the endpoints x_0 and $x_N = x$ are fixed, and we integrate over the $N-1$ intermediate positions $x_1, \ldots, x_{N-1}$. Each sequence $(x_0, x_1, \ldots, x_N)$ is a discretized path from x_0 to x, so Eq. (24) is already a sum over paths.

For small δt, we can split the exponential of $\hat{H} = \hat{p}^2/2m + V(\hat{x})$ into a kinetic and a potential piece,

$$e^{-\frac{i}{\hbar}\delta t\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)} \simeq e^{-\frac{i}{\hbar}\delta t\,\frac{\hat{p}^2}{2m}}\, e^{-\frac{i}{\hbar}\delta t\, V(\hat{x})} + \mathcal{O}(\delta t^2) \tag{25}$$

where the error comes from the commutator $[\hat{p}^2, V(\hat{x})]$ (See, e.g., our solutions to HW 4 for a discussion on exponentials of operators). Note that we can drop the higher order terms because there are $N \sim 1/\delta t$ factors in Eq. (24), so the accumulated error is $\mathcal{O}(N\delta t^2) = \mathcal{O}(\delta t) \to 0$.[1] The potential now acts on the position eigenstate to its right and becomes a number, while the kinetic piece is just the free propagator Eq. (20) over a time δt,

$$\langle x_n | \, e^{-\frac{i}{\hbar}\hat{H}\delta t} \, | x_{n-1} \rangle \simeq e^{-\frac{i}{\hbar}\delta t V(x_{n-1})} \, \langle x_n | \, e^{-\frac{i}{\hbar}\delta t \frac{\hat{p}^2}{2m}} \, | x_{n-1} \rangle \tag{26}$$

$$= \sqrt{\frac{m}{2\pi i\hbar\delta t}} \exp\left\{ \frac{i}{\hbar}\,\delta t \left[\frac{m}{2}\left(\frac{x_n - x_{n-1}}{\delta t}\right)^2 - V(x_{n-1}) \right] \right\}. \tag{27}$$

The quantity $(x_n - x_{n-1})/\delta t$ is the velocity of the discretized path during the n-th slice, so the square bracket is the Lagrangian $L = \frac{1}{2}m\dot{x}^2 - V(x)$ evaluated on that slice. The action accumulated in that slice is then just $L\,\delta t$, or explicitly,

$$S(n, n-1) \equiv \int_{t_{n-1}}^{t_n} dt'\, L \simeq \delta t \left[\frac{m}{2}\left(\frac{x_n - x_{n-1}}{\delta t}\right)^2 - V(x_{n-1}) \right]. \tag{28}$$

Whether we evaluate the potential at x_{n-1}, at x_n, or at the midpoint does not matter at this order.

Putting Eq. (27) back into Eq. (24), the product of exponentials becomes the exponential of the sum, and the sum of the $S(n, n-1)$ is the action of the whole discretized path, $S[x] = \sum_n S(n, n-1)$. Therefore

$$K(x,t;x_0,t_0) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} \int dx_1 \cdots \int dx_{N-1} \, \exp\left\{ \frac{i}{\hbar} \sum_{n=1}^{N} S(n, n-1) \right\}, \tag{29}$$

with $S(n, n-1)$ given by Eq. (28). Following Sakurai, we hide the prefactor and the $N-1$ integrals in the symbol $\int \mathcal{D}[x(t')]$, and write the **Feynman path integral**

$$\boxed{K(x,t;x_0,t_0) = \int_{x(t_0)=x_0}^{x(t)=x} \mathcal{D}[x(t')] \, \exp\left\{ \frac{i}{\hbar} S[x(t')] \right\},} \tag{30}$$

with $S[x(t')]$ the action of Eq. (22). In words: the amplitude to go from (x_0, t_0) to (x, t) is the sum over every path connecting the two points, each path contributing a phase equal to its classical action in units of $\hbar$.

A few remarks, mostly following Shankar's Section 8.2.

[1] This is a more general fact known as the Trotter product formula, $e^{\hat{A}+\hat{B}} = \lim_{N\to\infty}\left(e^{\hat{A}/N} e^{\hat{B}/N}\right)^N$, which holds even when $[\hat{A}, \hat{B}] \neq 0$.

- Note that for each path we have $|e^{\frac{i}{\hbar}S}| = 1$. So, the classical path is not singled out by a larger weight, but rather by a phase that varies more slowly compared to its neighbors, leading to constructive interference (stationary phase).
- For a macroscopic system, $S \gg \hbar$ and the phase $S/\hbar$ varies wildly from one path to its neighbors. Contributions from a generic path and from the paths around it cancel out, except near the path where S is stationary, $\delta S = 0$, where all nearby paths have the same phase and add up coherently. Hamilton's principle is thus the stationary-phase approximation to Eq. (30). In quantum mechanics, paths whose action differs from S_{cl} by less than about $\hbar$ still contribute coherently, and that is what you would refer to as "quantum effects".
- If V depends on time, the derivation goes through unchanged, with $V(x_{n-1}, t_{n-1})$ in each slice. The path integral automatically orders the operators in time, which is why it is so convenient in field theory.



Using the short-time propagator Eq. (27) in Eq. (2) for a single slice,

$$\psi(x, t+\delta t) = \sqrt{\frac{m}{2\pi i\hbar\delta t}} \int d\eta\, e^{\frac{i}{\hbar}\frac{m\eta^2}{2\delta t}}\, e^{-\frac{i}{\hbar}\delta t V(x)}\, \psi(x-\eta, t), \qquad \eta \equiv x - x_0. \tag{31}$$

I evaluated the potential at x rather than at x_0, which makes no difference at this order. The Gaussian has width $\sqrt{\hbar\delta t/m}$, so expand $\psi(x-\eta, t)$ to second order in η and $e^{-\frac{i}{\hbar}\delta t V}$ to first order in δt. Using Eq. (18), one can show that the Gaussian average of η vanishes and that of η^2 is $i\hbar\delta t/m$, leading to

$$\psi(x, t+\delta t) - \psi(x,t) = \frac{\delta t}{i\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t) + \mathcal{O}(\delta t^2), \tag{32}$$

which is just the Schrödinger equation. The Schrödinger equation is encoded in the infinitesimal time evolution of the path integral, and the full propagator obtained by summing over all paths will automatically satisfy it.