The propagator is a function which is a wave-mechanics equivalent of the time evolution operator $U(t, t_0)$, modulo certain details to be discussed in a moment.

We begin with a summary of some of the important properties of the time evolution operator. This operator is used to advance quantum states in time, so that

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle. \quad (7.1)$$

The time evolution operator satisfies a version of the Schrödinger equation,

$$i\hbar \frac{\partial U}{\partial t} = HU, \quad (7.2)$$

subject to the initial conditions

$$U(t_0, t_0) = 1. \quad (7.3)$$

It also satisfies the composition property,

$$U(t, t_0) = U(t, t_1)U(t_1, t_0). \quad (7.4)$$

Finally, in the special case that the Hamiltonian is independent of time, $\partial H/\partial t = 0$, $U(t, t_0)$ depends only on the time difference $t - t_0$, so we can set $t_0 = 0$ and write simply $U(t)$. This in turn can be expressed in terms of the Hamiltonian, and thence in terms of the energy eigenvalues and eigenstates:

$$U(t) = e^{-iHt/\hbar} = \sum_n e^{-iE_n t/\hbar} |n\rangle\langle n|. \quad (7.5)$$

Here for simplicity we have assumed that the spectrum of $H$ is discrete.

When the properties of $U$ are transformed into wave function language, we obtain the propagator, which for positive times is the kernel of the integral transform representing the wave function equivalent of Eq. (7.1). That is, we write Eq. (7.1) in the form,

$$\psi(x, t) = \int dx_0 K(x, t; x_0, t_0)\psi(x_0, t_0) \quad (t > t_0), \quad (7.6)$$

so that

$$K(x, t; x_0, t_0) = \langle x|U(t, t_0)|x_0\rangle \quad (t > t_0). \quad (7.7)$$
In Eq. (7.6), it is often convenient to think of \( \psi(x_0, t_0) \) as a “cause” and \( \psi(x, t) \) as an “effect,” and since we like to think of causes preceding their effects, we agree to use Eqs. (7.6) and (7.7) only in the case \( t > t_0 \). This restriction is partly motivated by notions of causality, and partly for mathematical reasons, which will become apparent momentarily. In any case, it is conventional to take care of negative times by demanding that \( K \) vanish for \( t < t_0 \), i.e., by replacing Eq. (7.7) by

\[
K(x; t; x_0; t_0) = \Theta(t - t_0) \left( x | U(t, t_0) | x_0 \right).
\] (7.8)

Here \( \Theta \) is the unit (Heaviside) step function, defined by

\[
\Theta(\tau) = \begin{cases} 
0, & \tau < 0, \\
1, & \tau > 0,
\end{cases}
\] (7.9)

which satisfies

\[
\frac{d\Theta(\tau)}{d\tau} = \delta(\tau).
\] (7.10)

Equation (7.8) is the definition of the propagator, \( K(x; t; x_0, t_0) \).

The properties of the propagator are transcriptions of the properties (7.1) to (7.5) of the time evolution operator. We begin by making no assumptions about the Hamiltonian, i.e., we allow it to be time-dependent. First we have the initial condition,

\[
\lim_{t \to t_0^+} K(x, t; x_0, t_0) = \delta(x - x_0),
\] (7.11)

which is essentially the same as Eq. (7.3). Due to the step function in the definition (7.8) of the propagator, we must let \( t \) approach \( t_0 \) from the positive side in this formula.

The second property of the propagator is that if we regard \( K(x, t; x_0, t_0) \) as a wave function in the variables \((x, t)\), with \((x_0, t_0)\) being treated as parameters, then \( K \) satisfies the time-dependent Schrödinger equation for positive times. It also satisfies this equation for negative times, trivially so since \( K \) vanishes for \( t < t_0 \). However, exactly at \( t = t_0 \), there is a singular remainder, which causes \( K \) overall to satisfy an inhomogeneous version of the time-dependent Schrödinger equation. Specifically, we have

\[
\left[ H(x, -i\hbar \partial / \partial x, t) - i\hbar \frac{\partial}{\partial t} \right] K(x, t; x_0, t_0) = -i\hbar \delta(x - x_0) \delta(t - t_0).
\] (7.12)

This equation qualifies \( K \) as the Green’s function for the time-dependent Schrödinger equation. In Eq. (7.12), \( H(x, p, t) \) with \( p = -i\hbar \partial / \partial x \) stands for the usual Hamiltonian operator of wave mechanics, in which the variables and derivatives \((x, t)\) refer to the final endpoint.
and endtime in \( K \), not the initial values \((x_0, t_0)\). For example, in the usual 1-dimensional Schrödinger case, we have

\[
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) - i\hbar \frac{\partial}{\partial t} \right] K(x; t; x_0, t_0) = -i\hbar \delta(x - x_0) \delta(t - t_0). \tag{7.13}
\]

To prove Eq. (7.12), we transform the \( x \)-space matrix elements of \( HU \). For clarity we work with the 1-dimensional Schrödinger operator shown in Eq. (7.13), but the calculation works for any Hamiltonian. We have

\[
\langle x|HU(t, t_0)|x_0\rangle \Theta(t - t_0) = \int dx' \langle x|H|x'\rangle \langle x'|U(t, t_0)|x_0\rangle \Theta(t - t_0)
\]

\[
= \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right] K(x; t; x_0, t_0)
\]

\[
= \langle x|i\hbar \frac{\partial U(t, t_0)}{\partial t}|x_0\rangle \Theta(t - t_0)
\]

\[
= i\hbar \frac{\partial}{\partial t} \left[ \langle x|U(t, t_0)|x_0\rangle \Theta(t - t_0) \right] - i\hbar \langle x|U(t, t_0)|x_0\rangle \delta(t - t_0)
\]

\[
= i\hbar \frac{\partial K(x; t; x_0, t_0)}{\partial t} - i\hbar \delta(x - x_0) \delta(t - t_0), \tag{7.14}
\]

where we use Eq. (7.2) in the third equality and Eq. (7.10) in the fourth. In the final equality, we use the fact that since \( \delta(t - t_0) \) vanishes except when \( t = t_0 \), we can replace \( t \) by \( t_0 \) in \( U(t, t_0) \), which produces the identity operator. Thus, Eq. (7.12) is proven. We can see from this derivation the necessity for the step function \( \Theta(t - t_0) \) in the definition of \( K(x; t; x_0, t_0) \), for without it, \( K \) would not be the Green’s function of the time-dependent Schrödinger equation.

Since \( K(x; t; x_0, t_0) \) satisfies the time-dependent Schrödinger equation in \((x, t)\) for positive times, and since it satisfies the initial conditions indicated by Eq. (7.11), we can formulate the following simple rule for computing the propagator:

**Simple Rule:** The propagator \( K(x; t; x_0, t_0) \) for positive times \( t > t_0 \) is the solution \( \psi(x, t) \) of the time-dependent Schrödinger equation satisfying the initial conditions \( \psi(x, t_0) = \delta(x - x_0) \).

In using this rule, however, we should note that the initial “wave function” contemplated here is unphysical, for not only is it not normalizable, but also the complete spatial localization at the initial time implies that the initial wave function contains all momentum components, out to infinite values of momentum. Therefore, thinking in a semiclassical sense, it is no surprise that this function “explodes” as soon as time is turned on.
To conceptualize the propagator, it helps to think of water waves on the surface of a lake instead of matter waves. If we go to such a lake, assumed to be quiet, and poke our finger just once at location \(x_0\) at time \(t_0\), then a pattern of waves \(\psi(x, t)\) will radiate out from our finger in all directions. In accordance with Eq. (7.12), this wave field can be identified with the propagator \(K(x; t; x_0, t_0)\). Notice that it vanishes for negative times (before we poked our finger), and for positive times it satisfies the homogeneous wave equation (with no driving terms), because our finger was in the water only for a single instant at \(t = t_0\). This analogy is not perfect, because real (deep) water waves are governed by a wave equation which is second order in time, and the propagator, as we have presented it, is specific to equations which are first order in time. (In fact, real water waves obey a nonlinear wave equation.) Nevertheless, the analogy is close enough for our purposes.

To continue with the properties of the propagator, we obtain the composition rule by transcribing Eq. (7.4) into the language of wave functions. That is, for \(t > t_1 > t_0\), we have

\[
K(x; t; x_0, t_0) = \int dx_1 \, K(x; t; x_1, t_1)K(x_1; t_1; x_0, t_0).
\]

(7.15)

Notice that the right hand side is independent of \(t_1\).

Finally, in the special case of a time-independent Hamiltonian, the propagator, like the operator \(U(t; t_0)\), depends only on the time difference \(t - t_0\), and we can set \(t_0 = 0\) and write simply \(K(x; x_0; t)\). In this case the propagator can be expressed explicitly in terms of the Hamiltonian and its eigenvalues and eigenfunctions:

\[
K(x; x_0; t) = \Theta(t) \langle x|U(t)|x_0\rangle = \Theta(t) \sum_{nm} \langle x|n\rangle \langle n|e^{-iHt/\hbar}|m\rangle \langle m|x_0\rangle \\
= \Theta(t) \sum_n e^{-iE_n t/\hbar} u_n(x)u_n^*(x_0).
\]

(7.16)

It is possible to obtain explicit expressions for the propagator only in a few cases, notably the free particle and harmonic oscillator. Fortunately, these cases are important in practice. Here we will work out the propagator for the free particle in one dimension. Since both the Hamiltonian \(H = p^2/2m\) and the time evolution operator \(U = e^{-iHt/\hbar}\) are diagonal in the momentum representation, we have

\[
K(x; x_0; t) = \Theta(t) \langle x|U(t)|x_0\rangle = \Theta(t) \int dp \, dp' \langle x|p\rangle \langle p|e^{-iHt/\hbar}|p'\rangle \langle p'|x_0\rangle \\
= \Theta(t) \int \frac{dp}{2\pi\hbar} \exp\left[-\frac{ip^2 t}{2m\hbar} + \frac{ip(x - x_0)}{\hbar}\right] \\
= \Theta(t) \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left[i \frac{m(x - x_0)^2}{\hbar^2} \frac{2t}{2t}\right].
\]

(7.17)
The calculation in higher dimensions is similar; we record here the 3-dimensional result:

\[ K(x, x_0; t) = \Theta(t) \left( \frac{m}{2\pi i\hbar t} \right)^{3/2} \exp \left[ \frac{i m(x - x_0)^2}{\hbar 2t} \right]. \]  
(7.18)

The free particle propagator is obviously a very singular function as \( t \to 0 \) [for this it is sufficient to look at the 1-dimensional formula (7.17)]. The phase factor of course has magnitude unity, but the square root prefactor diverges as \( t^{-1/2} \) for small times. Therefore the propagator diverges at all spatial locations as \( t \to 0 \), regardless how far we are from the initial point \( x_0 \). On the other hand, the propagator, regarded as a function of \( x \) for fixed \( t \), is an oscillatory function, and in a distribution function sense it does vanish as \( t \to 0 \) at all spatial points apart from \( x = x_0 \). For if \( x \neq x_0 \), then it is easy to show that the local wavelength of the spatial oscillations goes to zero as \( t \) for small times, so that any one lobe of the oscillating function \( K \) contains an area which goes to zero as \( t^{1/2} \) as \( t \to 0 \). The diminishing area and diminishing wavelength imply that \( K \) integrated against a smooth test function gives vanishing contribution in regions where \( x \neq x_0 \) as \( t \to 0 \). On the other hand, the one lobe centered on \( x = x_0 \) has a width which goes to zero only as \( t^{1/2} \) as \( t \to 0 \), so this lobe has constant area and vanishing width in the limit. This is precisely the behavior of a \( \delta \)-function, as indicated by Eq. (7.11).

Another point about the free particle propagator concerns the exponent, which is \( (i/\hbar) \) times the function,

\[ S(x, x_0; t) = \frac{m(x - x_0)^2}{2t}. \]  
(7.19)

This is Hamilton’s principal function of classical mechanics, i.e., it is the integral of the (free particle) Lagrangian along the classical orbit. We will see the reason for the appearance of Hamilton’s principal function in the propagator when we study the Feynman path integral.

It is also possible to work out the propagator for the harmonic oscillator. This is also an important result, but “ordinary” derivations of this propagator involve special function tricks or lengthy algebra. Instead, it is more educational to derive the harmonic oscillator propagator from the Feynman path integral, as we will do later.

Let us now introduce an operator equivalent of the propagator by writing,

\[ \hat{K}(t) = \Theta(t)\hat{U}(t) = \Theta(t)e^{-iHt/\hbar}, \]  
(7.20)

where we work with a time-independent system. Then we have

\[ K(x, x_0; t) = \langle x|\hat{K}(t)|x_0 \rangle. \]  
(7.21)

Here we are using a hat to distinguish the operator \( \hat{K}(t) \) from the propagator \( K(x, x_0; t) \). For other operators this distinction is not necessary, and we will not bother with the hats.
It turns out that the trace of $\hat{K}(t)$, or better, of the time-evolution operator $U(t)$, is of interest. For if we express the trace in terms of energy eigenstates, we have
\[
\text{tr} U(t) = \sum_n \langle n | e^{-iHt/\hbar} | n \rangle = \sum_n e^{-iE_n t/\hbar}. \tag{7.22}
\]
Thus, this trace is a sum of oscillatory contributions, one for each energy level. It is interesting to analytically continue this trace into the complex time plane. In particular, if we evaluate the trace for time values on the negative imaginary axis, we obtain a series of damped exponentials. Let us therefore write
\[
t = -i\hbar\beta, \tag{7.23}
\]
where $\beta$ is a parameter. Then we have
\[
\text{tr} U(-i\hbar\beta) = \sum_n e^{-\beta E_n} = Z(\beta), \tag{7.24}
\]
which we recognize as the partition function of statistical mechanics, in which $\beta$ is related to the temperature by $\beta = 1/kT$. Knowledge of this function suffices to determine (via differentiation) all the equilibrium statistical properties of a system, such as its equation of state, specific heat, etc. Thus we see that there is a close relation (via analytic continuation) between propagators and partition functions, between time and inverse temperature, and between the physical constants $\hbar$ and $k$ (the Boltzmann constant).

We now develop some material which is discussed in Sakurai, but which we will not use for a while in the course.

It is of interest to take the Fourier transform in time of the propagator, because this gives the Green’s function for the time-independent Schrödinger equation. It is generally useful to do this only in the case of a time-independent Hamiltonian, so we will assume $\partial H/\partial t = 0$. We begin by introducing the operator $\hat{G}(E)$,
\[
\hat{G}(E) = \frac{1}{i\hbar} \int_{-\infty}^{+\infty} dt \ e^{iEt/\hbar} \hat{K}(t), \tag{7.25}
\]
and its $x$-space matrix elements,
\[
G(x, x_0; E) = \langle x | \hat{G}(E) | x_0 \rangle = \frac{1}{i\hbar} \int_{-\infty}^{+\infty} dt \ e^{iEt/\hbar} K(x, x_0; t). \tag{7.26}
\]
We will call $G(x, x_0; E)$ the energy-dependent Green’s function, for reasons which will become apparent in a moment. Because of the functions $\Theta(t)$ in the definitions of $\hat{K}(t)$ or $K(x, x_0; t)$, the lower limit ($-\infty$) in the two integrals in Eqs. (7.25) and (7.26) can be replaced by zero (or any negative number). In the following discussion, it is important to
remember that the quantity $E$ which appears in the energy-dependent Green’s function is a free parameter, which we can set to any value we like, as long as the formulas are meaningful. In particular, $E$ is not necessarily an energy eigenvalue of the system. In fact, in a moment we will see the necessity of allowing $E$ to be complex.

The energy-dependent Green’s function can be expressed in terms of energy eigenvalues and eigenfunctions. For simplicity we will work with the case of a discrete spectrum. First we work with the operator $\hat{G}(E)$. We invoke the operator equivalent of Eq. (7.16),

$$\hat{K}(t) = \Theta(t) \sum_n e^{-iE_n t/\hbar} |n\rangle\langle n|,$$

which we substitute into Eq. (7.25). This leads to integrals of the form,

$$\frac{1}{i\hbar} \int_0^\infty dt e^{i(E-E_n)t/\hbar},$$

which do not converge for real values of $E$. [Nevertheless, one can see that if the lower limit were extended to $-\infty$, the result would be essentially $\delta(E - E_n)$.] If, however, we promote $E$ into a complex variable, then the integral will converge for $E$ values in the upper half plane. Notationally it is perhaps more convenient to keep $E$ as a real quantity, but to replace it wherever it occurs by $E + i\epsilon$, where sometimes we want to think of $\epsilon$ as small, since we sometimes want to work close to the real energy axis. In this notation, the integrals become

$$\frac{1}{i\hbar} \int_0^\infty dt e^{i(E+i\epsilon-E_n)t/\hbar} = \frac{1}{E + i\epsilon - E_n},$$

and the operator $\hat{G}(E + i\epsilon)$ becomes

$$\hat{G}(E + i\epsilon) = \sum_n \frac{|n\rangle\langle n|}{E + i\epsilon - E_n}.$$  

(7.30)

In view of our definition of functions of operators, we see that $\hat{G}$ can also be written,

$$\hat{G}(E + i\epsilon) = \frac{1}{E + i\epsilon - H}.$$  

(7.31)

The operator on the right hand side is called the resolvent of $H$. The wave function equivalent of Eq. (7.30) is

$$G(x, x_0; E + i\epsilon) = \sum_n \frac{u_n(x)u_n^*(x_0)}{E + i\epsilon - E_n}.$$  

(7.32)

Finally, if we take the trace of Eq. (7.30), we obtain

$$\text{tr} \hat{G}(E + i\epsilon) = \int dx G(x, x; E + i\epsilon) = \sum_n \frac{1}{E + i\epsilon - E_n},$$  

(7.33)
a formula which Sakurai discusses briefly.

One reason $G(x, x_0; E + i\epsilon)$ (or its trace) is interesting is that its analytic structure, as a function of the complex energy $E$, captures the information contained in the eigenvalues and eigenfunctions of the Hamiltonian (the trace only contains information about the eigenvalues). That is, Eqs. (7.30), (7.32) and (7.33) show that $\hat{G}(E + i\epsilon)$ or its trace possesses poles in the complex energy $E + i\epsilon$ at energy eigenvalues, so that $\hat{G}(E + i\epsilon)$ or $G(x, x_0; E + i\epsilon)$ diverges as $E \to E_n$ and $\epsilon \to 0$. Furthermore, Eq. (7.32) shows that the residue of the pole of $G(x, x_0; E + i\epsilon)$ at $E_n$ is just the quantity $u_n(x)u_n^*(x_0)$, i.e., for fixed $x_0$ it is proportional to the eigenfunction $u_n(x)$. Furthermore, the order of the degeneracy of the energy level is the order of the pole.

The physical reason for these divergences in the energy-dependent Green’s function can be seen again in terms of waves on a lake. Instead of poking our finger once into the lake, consider driving it up and down at frequency $\omega$ (to be identified in the quantum mechanical analog with the Einstein frequency $E/\hbar$), and imagine doing this for all times from $-\infty$ to $+\infty$. The frequency $\omega$ need not be an eigenfrequency of the lake. Indeed, if it is not an eigenfrequency, then the waves radiated from our finger will go out, reflect off the shore, and be out of phase with themselves on returning. Therefore, while the lake will respond at the driving frequency $\omega$, that it, the disturbance will have the form $\psi(x, x_0; \omega)e^{-i\omega t}$, this disturbance (i.e., its spatially dependent part) will not be an eigenfunction of the lake. As we will see momentarily, the function $\psi(x, x_0; \omega)$ can be identified in the quantum mechanical analog with $G(x, x_0; E)$. On the other hand, if we do drive the lake at an eigenfrequency, $\omega = \omega_n$, then the reflecting waves will reinforce each other, and, in the absence of damping, the response of the lake will be infinite (after an infinite amount of time). Of course, real lakes have damping, so in fact the ultimate response will be finite, i.e., it will be a state in which the energy lost by damping is balanced by the energy coming in from the driving source. This is a way of saying that the eigenfrequencies $\omega_n$ of real lakes have negative imaginary parts. If we somehow let the damping go to zero, these eigenfrequencies move onto the real axis, like the energy eigenvalues of the quantum mechanical system. In view of this picture, it should be no surprise that $G(x, x_0; E)$ has singularities at $E = E_n$. Furthermore, it is easy to see why the residues of the poles are proportional to the energy eigenfunctions, for if we drive the lake at a frequency very near to an eigenfrequency $\omega_n$, then we expect the large response to be dominated by the $n$-th eigenfunction $u_n(x)$.

Finally, let us demonstrate that $G(x, x_0; E)$ actually is the Green’s function for the time-independent Schrödinger equation. In the following we change notation and write $E$ for what was formerly $E + i\epsilon$, so that $E$ is now a possibly complex number. Again, for clarity
we will work with the 1-dimensional Schrödinger operator shown in Eq. (7.13), although
the demonstration actually works for any Hamiltonian. First we rewrite Eq. (7.13) for the
case of a time-independent system,
\[
\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) - i\hbar \frac{\partial}{\partial t}\right] K(x, x_0; t) = -i\hbar \delta(x - x_0) \delta(t).
\] (7.34)
Then we apply the Schrödinger Hamiltonian to both sides of Eq. (7.26) and use Eq. (7.34),
to obtain
\[
\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] G(x, x_0; E) = \int_{-\infty}^{+\infty} dt \ e^{iEt/\hbar} \left[ \frac{\partial K(x, x_0; t)}{\partial t} - \delta(x - x_0) \delta(t) \right]
\]
\[
= e^{iEt/\hbar} K(x, x_0; t) \bigg|_{-\infty}^{+\infty} - \frac{iE}{\hbar} \int_{0}^{+\infty} dt \ e^{iEt/\hbar} K(x_0, x; t) - \delta(x - x_0),
\] (7.35)
or, in other words,
\[
[H(x) - E] G(x, x_0; E) = -\delta(x - x_0),
\] (7.36)
where the notation $H(x)$ means that the Hamiltonian only acts on the variable $x$ (not on
$x_0$). Thus, we see that the energy-dependent Green’s function satisfies the time-independent
Schrödinger equation at all spatial points except $x = x_0$, for any value of $E$ (not only energy
eigenvalues).

A usual application of Green’s functions is in solving inhomogeneous equations. Therefore $K(x, t; x_0, t_0)$ is useful for solving the inhomogeneous time-dependent Schrödinger equation, and $G(x, x_0; E)$ for solving the inhomogeneous time-independent Schrödinger equation.
You may wonder why we are interested in the inhomogeneous Schrödinger equations, since
the physics seems to give us only the homogeneous versions. The reason is that such inho-
mogeneous equations occur in perturbation theory, as we will see later.