The "Propagator" in Quantum Mechanics

[Notes for the Quant. Mech.-I reading project (Fawad Hassan)]

1 Operators and States

In the operator formulation of quantum mechanics [1] one deals with the position and momentum operators $\widehat{x}$, $\widehat{p}$ satisfying $[\widehat{x}, \widehat{p}] = i\hbar$. These act on the corresponding eigenstates,

$$\begin{array}{llll} \underline{Eigenvalue} & \underline{Orthogonality} & \underline{Completeness} & \\ \widehat{x}|x\rangle = x|x\rangle\,, & \langle x'|x\rangle = \delta(x'-x)\,, & \int dx|x\rangle\langle x| = \mathbf{1}\,, & (1) \\ \widehat{p}|p\rangle = p|p\rangle\,, & \langle p'|p\rangle = \delta(p'-p)\,, & \int dp|p\rangle\langle p| = \mathbf{1}\,. & (2) \end{array}$$

Since $|x\rangle$ and $|p\rangle$ form complete sets of basis states, any arbitrary state vector can be expended in terms of either of them. For example, consider a general quantum state $|\psi(t)\rangle$ at time t. This can be expanded in either basis as,

$$|\psi(t)\rangle = \int dx\, \psi(x,t)|x\rangle\,, \qquad \psi(x,t) = \langle x|\psi(t)\rangle\,, \tag{3}$$

$$|\psi(t)\rangle = \int dp\, \widetilde{\psi}(p,t)|p\rangle\,, \qquad \widetilde{\psi}(p,t) = \langle p|\psi(t)\rangle\,, \tag{4}$$

where $\psi(x,t)$ and $\widetilde{\psi}(p,t)$ are, respectively, the coordinate space and the momentum space wave functions corresponding to projections of the quantum state $|\psi(t)\rangle$ along the coordinate and momentum bases. The modulus of the wave function takes the form,

$$\langle\psi|\psi\rangle = \int dx\, \langle\psi|x\rangle\langle x|\psi\rangle = \int dx\, \psi^*(x)\psi(x)\,.$$

In particular, one can expand $|p\rangle$ in the basis of $|x\rangle$, or vise versa,

$$|p\rangle = \int dx\, u(p,x)\,|x\rangle\,, \qquad u(p,x) = \langle x|p\rangle\,. \tag{5}$$

To determine the expansion coefficients $\langle x|p\rangle$, one uses the well known fact that, on a function $f(x)$, the momentum operator $\widehat{p}$ is represented as $-i\hbar\partial/\partial x$ (as implied by the commutation relation) . Let us make this more precise. The value of $f(x)$ for any x can be regarded as the component of a vector $|f\rangle$ along the basis vector $|x\rangle$:

$$|f\rangle = \int dx\, f(x)|x\rangle\,, \qquad \text{or equivalently,} \qquad f(x) = \langle x|f\rangle\,. \tag{6}$$

[1] Below we will concentrate on systems in 1 dimension. Generalizing the discussion to 3 dimensions is straightforward

Then,

$$\widehat{p}|f\rangle = \int dx\,(-i\hbar\frac{\partial}{\partial x})f(x)|x\rangle\,, \qquad \Rightarrow \qquad \langle x|\widehat{p}|f\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|f\rangle\,. \tag{7}$$

In particular, replacing $|f\rangle$ in the above by $|p\rangle$, we get

$$\langle x|\widehat{p}|p\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle\,. \tag{8}$$

But also $\widehat{p}|p\rangle = p|p\rangle$, leading to the equation $-i\hbar\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle$ which has the solution

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\,e^{\frac{i}{\hbar}px}\,. \tag{9}$$

The normalization is fixed such that

$$\langle p'|p\rangle = \int dx\,\langle p'|x\rangle\langle x|p\rangle = \delta(p'-p)\,,$$

as should be the case.

2 Schrodinger Equation and Time Evolution

All the information about a quantum system is contained in its state vector $|\psi(t)\rangle$. The state vector satisfies the Schrodinger equation,

$$\widehat{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle\,, \qquad \text{where} \qquad \widehat{H} = \frac{\widehat{p}^2}{2m} + V(\widehat{x})\,. \tag{10}$$

This reduces to the more familiar form of the equation for the Schrodinger wave function $\psi(x,t) = \langle x|\psi(t)\rangle$ once we note that

$$\langle x|\widehat{p}|\psi(t)\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|\psi(t)\rangle\,, \qquad \text{and} \qquad \langle x|V(\widehat{x})|\psi(t)\rangle = V(x)\langle x|\psi(t)\rangle\,. \tag{11}$$

Then,

$$\langle x|\widehat{H}|\psi(t)\rangle = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\Big)\psi(x,t)\,, \tag{12}$$

and one recovers the familiar form of the Schrodinger equation,

$$H\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)\,, \qquad \text{where} \qquad H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\,. \tag{13}$$

From now on we will mostly concentrate on the form (10) of the equation. For time-independent $\widehat{H}$ (or equivalently, for time-independent $V(\widehat{x})$), the Schrodinger equation has the formal solution,

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\widehat{H}(t-t_0)}|\psi(t_0)\rangle \tag{14}$$

To put it in words, the differential equation (10) describes the infinitesimal time evolution of the system, while the integrated form (14) describes the evolution over a finite time interval $t - t_0$.

It should be mentioned, for the sake of completeness, that if the Hamiltonian depends on time, then the formal solution can be written in terms of the *time-ordered* product,

$$|\psi(t)\rangle = \mathcal{P}(e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt\,\widehat{H}(t-t_0)})|\psi(t_0)\rangle\,. \tag{15}$$

However, we will not be discussing such situations here.

3 The Propagator

In equation (14), $e^{-\frac{i}{\hbar}\widehat{H}(t-t_0)}$ is the *time-evolution operator*. It evolves a state $|\psi(t_0)\rangle$ into a state $|\psi(t)\rangle$ for $t > t_0$. We can also write down an equation for the evolution of the corresponding wave function from $\psi(x_0, t_0)$ to $\psi(x, t)$; again for $t > t_0$: Inserting $\mathbf{1} = \int dx_0 |x_0\rangle\langle x_0|$ next to $|\psi(t_0)\rangle$ in (14) and taking the scalar product with $\langle x|$, we get

$$\begin{aligned}\langle x|\psi(t)\rangle &= \langle x|e^{-\frac{i}{\hbar}\widehat{H}(t-t_0)}\,(\int dx_0\,|x_0\rangle\langle x_0|)|\psi(t_0)\rangle \\ &= \int dx_0\,\langle x|e^{-\frac{i}{\hbar}\widehat{H}(t-t_0)}|x_0\rangle\langle x_0|\psi(t_0)\rangle\,. \end{aligned}\tag{16}$$

The quantity

$$U(x,t;x_0,t_0) = \langle x|e^{-\frac{i}{\hbar}\widehat{H}(t-t_0)}|x_0\rangle \tag{17}$$

is called the *propagator*. It is also customary to define $|x,t\rangle \equiv e^{\frac{i}{\hbar}\widehat{H}t}|x\rangle$ and hence, write $U(x,t;x_0,t_0) = \langle x,t|x_0,t_0\rangle$. Now, in terms of the wave function, the time-evolution of the system takes the form

$$\psi(x,t) = \int dx_0\, U(x,t;x_0,t_0)\,\psi(x_0,t_0)\,. \tag{18}$$

The physical meaning of the propagator is evident from its definition: It is the *probability amplitude* for finding a particle at position x at time t, provided at an earlier time t_0 it was located at position x_0. Thus it tells us how the particle (or the probability amplitude associated with it) "propagates" from x_0, t_0 to x, t. If we simply make a measurement of ψ at point x and time t, we will not be able to tell how the particle got there and hence the integral over all possible initial positions x_0.

3.1 Some properties of the propagator

Two properties of the propagator are evident from its definition. First, in the limit, $t - t_0 \to 0$,

$$\lim_{t\to t_0} U(x,t;x_0,t_0) = \langle x|x_0\rangle = \delta(x-x_0)\,. \tag{19}$$

To see the second property, choose an intermediate time t' between t_0 and t and regard the time evolution as, first, from t_0 to t' and then from t' and t. Then, insert $\mathbf{1}$ in terms of a complete set of position states at time t',

$$\begin{aligned} U(x,t;x_0,t_0) &= \langle x|e^{-\frac{i}{\hbar}\widehat{H}(t-t')}e^{-\frac{i}{\hbar}\widehat{H}(t'-t_0)}|x_0\rangle \\ &= \langle x|e^{-\frac{i}{\hbar}\widehat{H}(t-t')}(\int dx'\,|x'\rangle\langle x'|)e^{-\frac{i}{\hbar}\widehat{H}(t'-t_0)}|x_0\rangle \\ &= \int dx'\,U(x,t;x',t')\,U(x',t';x_0,t_0)\,. \end{aligned} \tag{20}$$

The physical meaning of this equation is self-evident.

3.2 Evaluation of the Propagator

The propagator contains information about the time-evolution of quantum systems and hence its computation is an important problem in quantum mechanics. Below, we set out to express the propagator in terms of more familiar quantities that arise in elementary quantum mechanics:

We have been considering the Schrodinger equation (10) for systems with a time independent Hamiltonian. For such systems, in the operator formalism, one first solves the time-independent Schrodinger equation (or the energy eigenvalue problem),

$$\widehat{H}|E_n\rangle = E_n|E_n\rangle\,, \quad \text{where} \quad \langle E_m|E_n\rangle = \delta_{mn}\,, \quad \sum_n |E_n\rangle\langle E_n| = \mathbf{1}\,. \tag{21}$$

The energy eigenstates $|E_n\rangle$ form a complete, orthonormal set. The symbol $\sum_n$ denotes either a discrete sum or an integral over continuous energies, as the case may be. Note that the components of $|E_n\rangle$ in the coordinate basis are the energy eigen functions $\psi_n(x)$,

$$|E_n\rangle = \int dx\,\psi_n(x)|x\rangle\,, \qquad \psi_n(x) = \langle x|E_n\rangle\,, \tag{22}$$

in terms of which the time-independent Schrodinger equation takes the more familiar form,

$$\Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\Big)\psi_n(x) = E_n\,\psi_n(x)\,. \tag{23}$$

For example, remember that for the harmonic oscillator potential, the solutions are given in terms of Hermite polynomials and for the hydrogen atom problem (in 3 dimensions) they are given in terms of spherical harmonics and Laguerre functions. For a free particle, the solution is simply $e^{ipx/\hbar}$. Having determined the energy eigenvalues and eigenstates, the solution to the time-dependent Schrodinger equation (10) can be expanded as

$$|\psi(t)\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}|E_n\rangle\,, \qquad \text{or} \qquad \psi(x,t) = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}\psi_n(x)\,. \tag{24}$$

Here c_n are constants that can be determined by the initial conditions.

It is desirable to express the propagator in terms of the quantities encountered above. After inserting the completeness relation for $|E_n\rangle$ in the expression for $U(x,t;x_0,t_0)$, one gets,

$$
\begin{aligned}
U(x,t;x_0,t_0) &= \langle x|e^{-\frac{i}{\hbar}\widehat{H}(t-t_0)}(\sum_n |E_n\rangle\langle E_n|)|x_0\rangle \\
&= \sum_n \langle x|E_n\rangle e^{-\frac{i}{\hbar}E_n(t-t_0)}\langle E_n|x_0\rangle \\
&= \sum_n \psi_n(x)\psi_n^*(x_0)e^{-\frac{i}{\hbar}E_n(t-t_0)} \qquad (25)
\end{aligned}
$$

This expresses the propagator in terms of the familiar quantities that one encounters in elementary quantum mechanics.Thus knowing the energy eigenvalues and eigen functions, the propagator can be evaluated; at least in principle. In practice this method of computing the propagator is not always the most convenient one.

We will see later that the propagator has a representation in term of a path integral,

$$
U(x,t;x_0,t_0) = \int \mathcal{D}x\, e^{i/\hbar S[x(t)]} \qquad (26)
$$

In the path integral formulation of quantum mechanics, this is taken as the starting point and U is treated as the fundamental object. Information about the energy eigenvalues and eigen function can then be extracted from U (this will be explained later).