TIME-DEPENDENT PROPAGATORS

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One of the postulates of non-relativistic quantum mechanics concerns how states evolve with time. The postulate simply states that in non-relativistic quantum mechanics, a state satisfies the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle \tag{1}$$

where H is the Hamiltonian, which is obtained from the classical Hamiltonian by means of the other postulates of quantum mechanics, namely that we replace all references to the position x by the quantum position operator X with matrix elements (in the x basis) of

$$\left\langle x'\left|X\right|x\right\rangle = \delta\left(x-x'\right) \tag{2}$$

and all references to classical momentum p by the momentum operator P with matrix elements

$$\left\langle x'\left|P\right|x\right\rangle = -i\hbar\delta'\left(x-x'\right) \tag{3}$$

In our earlier examination of the Schrödinger equation, we assumed that the Hamiltonian is independent of time, which allowed us to obtain an explicit expression for the propagator

$$U(t) = e^{-iHt/\hbar} \tag{4}$$

The propagator is applied to the initial state $|\psi(0)\rangle$ to obtain the state at any future time t:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{5}$$

What happens if $H = H(t)$, that is, there is an explicit time dependence in the Hamiltonian? We divide the time interval $[0,t]$ into N small increments $\Delta = t/N$. To first order in Δ, we can integrate 1 by taking the first order term in a Taylor expansion:

$$\left|\psi\left(\Delta\right)\right\rangle = \left|\psi\left(0\right)\right\rangle + \Delta\frac{d}{dt}\left|\psi\left(t\right)\right\rangle\Big|_{t=0} + \mathcal{O}\left(\Delta^{2}\right) \tag{6}$$

$$= \left|\psi\left(0\right)\right\rangle + -\frac{i\Delta}{\hbar}H\left(0\right)\left|\psi\left(0\right)\right\rangle + \mathcal{O}\left(\Delta^{2}\right) \tag{7}$$

$$= \left(1-\frac{i\Delta}{\hbar}H\left(0\right)\right)\left|\psi\left(0\right)\right\rangle + \mathcal{O}\left(\Delta^{2}\right) \tag{8}$$

So far, we've been fairly precise, but now the hand-waving starts. We note that the term multiplying $\left|\psi\left(0\right)\right\rangle$ consists of the first two terms in the expansion of $e^{-i\Delta H(0)/\hbar}$, so we state that to evolve from $t=0$ to $t=\Delta$, we multiply the initial state $\left|\psi\left(0\right)\right\rangle$ by $e^{-i\Delta H(0)/\hbar}$. That is, we propose that

$$\left|\psi\left(\Delta\right)\right\rangle = e^{-i\Delta H(0)/\hbar}\left|\psi\left(0\right)\right\rangle \tag{9}$$

[The reason this is hand-waving is that there are many functions whose first order Taylor expansion matches $\left(1-\frac{i\Delta}{\hbar}H\left(0\right)\right)$, so it seems arbitrary to choose the exponential. I imagine the motivation is that in the time-independent case, the result reduces to 4.]

In any case, if we accept this, then we can iterate the process to evolve to later times. To get to $t=2\Delta$, we have

$$\left|\psi\left(2\Delta\right)\right\rangle = e^{-i\Delta H(\Delta)/\hbar}\left|\psi\left(\Delta\right)\right\rangle \tag{10}$$

$$= e^{-i\Delta H(\Delta)/\hbar}e^{-i\Delta H(0)/\hbar}\left|\psi\left(0\right)\right\rangle \tag{11}$$

The snag here is that we can't, in general, combine the two exponentials into a single exponential by adding the exponents. This is because $H\left(\Delta\right)$ and $H\left(0\right)$ will not, in general, commute, as the Baker-Campbell-Hausdorff formula tells us. For example, the time dependence of $H\left(t\right)$ might be such that at $t=0$, $H\left(0\right)$ is a function of the position operator X only, while at $t=\Delta$, $H\left(\Delta\right)$ becomes a function of the momentum operator P only. Since X and P don't commute, $\left[H\left(0\right),H\left(\Delta\right)\right]\neq0$, so $e^{-i\Delta H(\Delta)/\hbar}e^{-i\Delta H(0)/\hbar}\neq e^{-i\Delta[H(0)+H(\Delta)]/\hbar}$.

This means that the best we can usually do is to write

$$\left|\psi\left(t\right)\right\rangle = \left|\psi\left(N\Delta\right)\right\rangle \tag{12}$$

$$= \prod_{n=0}^{N-1}e^{-i\Delta H(n\Delta)/\hbar}\left|\psi\left(0\right)\right\rangle \tag{13}$$

The propagator then becomes, in the limit

$$U(t) = \lim_{N\to\infty} \prod_{n=0}^{N-1} e^{-i\Delta H(n\Delta)/\hbar} \tag{14}$$

This limit is known as a *time-ordered integral* and is written as

$$T\left\{\exp\left[-\frac{i}{\hbar}\int_0^t H\left(t'\right)dt'\right]\right\} \equiv \lim_{N\to\infty} \prod_{n=0}^{N-1} e^{-i\Delta H(n\Delta)/\hbar} \tag{15}$$

One final note about the propagators. Since each term in the product is the exponential of i times a Hermitian operator, each term is a unitary operator. The product of two unitary operators is still unitary, as we can verify by the calculation:

$$\left(U_1U_2\right)^\dagger\left(U_1U_2\right) = U_2^\dagger U_1^\dagger U_1 U_2 \tag{16}$$
$$= U_2^\dagger U_2 \tag{17}$$
$$= I \tag{18}$$

Therefore, the propagator in the time-dependent case is a unitary operator.

We've defined a propagator as a unitary operator that carries a state from $t = 0$ to some later time t, but we can generalize the notation so that $U(t_2, t_1)$ is a propagator that carries a state from $t = t_1$ to $t = t_2$, that is

$$\left|\psi\left(t_2\right)\right\rangle = U\left(t_2, t_1\right)\left|\psi\left(t_1\right)\right\rangle \tag{19}$$

We can chain propagators together to get

$$\left|\psi\left(t_3\right)\right\rangle = U\left(t_3, t_2\right)\left|\psi\left(t_2\right)\right\rangle \tag{20}$$
$$= U\left(t_3, t_2\right)U\left(t_2, t_1\right)\left|\psi\left(t_1\right)\right\rangle \tag{21}$$
$$= U\left(t_3, t_1\right)\left|\psi\left(t_1\right)\right\rangle \tag{22}$$

Therefore

$$U\left(t_3, t_1\right) = U\left(t_3, t_2\right)U\left(t_2, t_1\right) \tag{23}$$

Since the Hermitian conjugate of a unitary operator is its inverse, we have

$$U^\dagger\left(t_2, t_1\right) = U^{-1}\left(t_2, t_1\right) \tag{24}$$

We can combine this with 23 to get

$$|\psi(t_1)\rangle = I\,|\psi(t_1)\rangle \tag{25}$$
$$= U^{-1}(t_2,t_1)\,U(t_2,t_1)\,|\psi(t_1)\rangle \tag{26}$$
$$= U^{\dagger}(t_2,t_1)\,U(t_2,t_1)\,|\psi(t_1)\rangle \tag{27}$$

Therefore

$$U^{\dagger}(t_2,t_1)\,U(t_2,t_1) = U(t_1,t_1) = I \tag{28}$$
$$U^{\dagger}(t_2,t_1) = U(t_1,t_2) \tag{29}$$

That is, the Hermitian conjugate (or inverse) of a propagator carries a state 'backwards in time' to its starting point.