TIME-DEPENDENT PROPAGATORS

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 4.3.

The fourth postulate 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:

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = H\left|\psi\right\rangle \tag{0.1}$$

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

$$\left\langle x'\left|X\right|x\right\rangle = \delta\left(x-x'\right) \tag{0.2}$$

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

$$\left\langle x'\left|P\right|x\right\rangle = -i\hbar\delta'\left(x-x'\right) \tag{0.3}$$

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

$$U\left(t\right) = e^{-iHt/\hbar} \tag{0.4}$$

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

$$\left|\psi\left(t\right)\right\rangle = U\left(t\right)\left|\psi\left(0\right)\right\rangle \tag{0.5}$$

What happens if $H = H\left(t\right)$, that is, there is an explicit time dependence in the Hamiltonian? The approach taken by Shankar is a bit hand-wavy, but goes as follows. We divide the time interval $\left[0,t\right]$ into N small increments $\Delta = t/N$. To first order in Δ, we can integrate 0.1 by taking the first order term in a Taylor expansion:

$$|\psi(\Delta)\rangle = |\psi(0)\rangle + \Delta \frac{d}{dt}|\psi(t)\rangle\Big|_{t=0} + \mathscr{O}\left(\Delta^2\right) \tag{0.6}$$

$$= |\psi(0)\rangle + -\frac{i\Delta}{\hbar}H(0)|\psi(0)\rangle + \mathscr{O}\left(\Delta^2\right) \tag{0.7}$$

$$= \left(1 - \frac{i\Delta}{\hbar}H(0)\right)|\psi(0)\rangle + \mathscr{O}\left(\Delta^2\right) \tag{0.8}$$

So far, we've been fairly precise, but now the hand-waving starts. We note that the term multiplying $|\psi(0)\rangle$ 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 $|\psi(0)\rangle$ by $e^{-i\Delta H(0)/\hbar}$. That is, we propose that

$$|\psi(\Delta)\rangle = e^{-i\Delta H(0)/\hbar}|\psi(0)\rangle \tag{0.9}$$

[The reason this is hand-waving is that there are many functions whose first order Taylor expansion matches $\left(1 - \frac{i\Delta}{\hbar}H(0)\right)$, so it seems arbitrary to choose the exponential. I imagine the motivation is that in the time-independent case, the result reduces to 0.4.]

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

$$|\psi(2\Delta)\rangle = e^{-i\Delta H(\Delta)/\hbar}|\psi(\Delta)\rangle \tag{0.10}$$

$$= e^{-i\Delta H(\Delta)/\hbar}e^{-i\Delta H(0)/\hbar}|\psi(0)\rangle \tag{0.11}$$

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 $H(\Delta)$ and $H(0)$ will not, in general, commute, as the Baker-Campbell-Hausdorff formula tells us. For example, the time dependence of $H(t)$ might be such that at $t=0$, $H(0)$ is a function of the position operator X only, while at $t=\Delta$, $H(\Delta)$ becomes a function of the momentum operator P only. Since X and P don't commute, $[H(0), H(\Delta)] \neq 0$, 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

$$|\psi(t)\rangle = |\psi(N\Delta)\rangle \tag{0.12}$$

$$= \prod_{n=0}^{N-1} e^{-i\Delta H(n\Delta)/\hbar}|\psi(0)\rangle \tag{0.13}$$

The propagator then becomes, in the limit

$$U(t)=\lim_{N\to\infty}\prod_{n=0}^{N-1}e^{-i\Delta H(n\Delta)/\hbar} \tag{0.14}$$

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

$$T\left\{\exp\left[-\frac{i}{\hbar}\int_0^t H\left(t'\right)dt'\right]\right\}\equiv\lim_{N\to\infty}\prod_{n=0}^{N-1}e^{-i\Delta H(n\Delta)/\hbar} \tag{0.15}$$

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. Further, since the product of two unitary operators is still unitary, 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

$$|\psi(t_2)\rangle=U(t_2,t_1)|\psi(t_1)\rangle \tag{0.16}$$

We can chain propagators together to get

$$\begin{aligned}|\psi(t_3)\rangle&=U(t_3,t_2)|\psi(t_2)\rangle &(0.17)\\&=U(t_3,t_2)U(t_2,t_1)|\psi(t_1)\rangle &(0.18)\\&=U(t_3,t_1)|\psi(t_1)\rangle &(0.19)\end{aligned}$$

Therefore

$$U(t_3,t_1)=U(t_3,t_2)U(t_2,t_1) \tag{0.20}$$

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

$$U^\dagger(t_2,t_1)=U^{-1}(t_2,t_1) \tag{0.21}$$

We can combine this with 0.20 to get

$$\begin{aligned}|\psi(t_1)\rangle&=I|\psi(t_1)\rangle &(0.22)\\&=U^{-1}(t_2,t_1)U(t_2,t_1)|\psi(t_1)\rangle &(0.23)\\&=U^\dagger(t_2,t_1)U(t_2,t_1)|\psi(t_1)\rangle &(0.24)\end{aligned}$$

Therefore

$$U^{\dagger}(t_2,t_1)\,U(t_2,t_1) = U(t_1,t_1)=I \quad (0.25)$$

$$U^{\dagger}(t_2,t_1) = U(t_1,t_2) \quad (0.26)$$

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

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