

## 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:

$$(1) \quad i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle$$

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

$$(2) \quad \langle x' | X | x \rangle = \delta(x - x')$$

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

$$(3) \quad \langle x' | P | x \rangle = -i\hbar \delta'(x - x')$$

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

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

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

$$(5) \quad |\psi(t)\rangle = U(t) |\psi(0)\rangle$$

What happens if  $H = H(t)$ , 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  $[0, t]$  into  $N$  small increments  $\Delta = t/N$ . To first order in  $\Delta$ , we can integrate 1 by taking the first order term in a Taylor expansion:

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

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

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

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

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

[The reason this is hand-waving is that there are many functions whose first order Taylor expansion matches  $(1 - \frac{i\Delta}{\hbar} H(0))$ , 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

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

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

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

$$(12) \quad |\psi(t)\rangle = |\psi(N\Delta)\rangle$$

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

The propagator then becomes, in the limit

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

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

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

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

$$(16) \quad |\psi(t_2)\rangle = U(t_2, t_1) |\psi(t_1)\rangle$$

We can chain propagators together to get

$$(17) \quad |\psi(t_3)\rangle = U(t_3, t_2) |\psi(t_2)\rangle$$

$$(18) \quad = U(t_3, t_2) U(t_2, t_1) |\psi(t_1)\rangle$$

$$(19) \quad = U(t_3, t_1) |\psi(t_1)\rangle$$

Therefore

$$(20) \quad U(t_3, t_1) = U(t_3, t_2) U(t_2, t_1)$$

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

$$(21) \quad U^\dagger(t_2, t_1) = U^{-1}(t_2, t_1)$$

We can combine this with 20 to get

$$(22) \quad |\psi(t_1)\rangle = I |\psi(t_1)\rangle$$

$$(23) \quad = U^{-1}(t_2, t_1) U(t_2, t_1) |\psi(t_1)\rangle$$

$$(24) \quad = U^\dagger(t_2, t_1) U(t_2, t_1) |\psi(t_1)\rangle$$

Therefore

$$(25) \quad U^\dagger(t_2, t_1)U(t_2, t_1) = U(t_1, t_1) = I$$

$$(26) \quad U^\dagger(t_2, t_1) = U(t_1, t_2)$$

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

#### PINGBACKS

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