

TIME-DEPENDENT PROPAGATORS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

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:

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

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

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

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

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

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

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

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

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

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 Δ , we can integrate 1 by taking the first order term in a Taylor expansion:

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

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

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

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

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

[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

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

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

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

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

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

The propagator then becomes, in the limit

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

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

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

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

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

We can chain propagators together to get

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

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

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

Therefore

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

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

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

We can combine this with 20 to get

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

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

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

Therefore

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

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

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

PINGBACKS

Pingback: Translational invariance and conservation of momentum

Pingback: Time translation and conservation of energy