UNITARY TRANSFORMATIONS AND THE HEISENBERG PICTURE

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Reference: References: Robert D. Klauber, *Student Friendly Quantum Field Theory*, (Sandtrove Press, 2013) - Chapter 2, Problems 2.11 - 2.12.

Most of the quantum mechanics that we've done so far has used the Schrödinger picture, in which a system is described by finding its wave function $\Psi(x,t)$, which depends on spatial position and time. Most operators in the Schrödinger picture are independent of time, so that the time dependence of the solution is contained within the wave function.

There is another way of looking at quantum theory called the Heisenberg picture. The states and operators in the Heisenberg picture are obtained from their counterparts in the Schrödinger picture by means of a *unitary transformation* using the unitary operator U.

Unitary transformations. A unitary transformation in quantum mechanics is obtained by applying an operator U to a state that leaves the square modulus of the state (that is, the probability density) unchanged. In classical mechanics, an orthogonal transformation rotates a 3-d vector without changing its length; in that sense a unitary transformation in quantum mechanics is an analogue of a classical orthogonal transformation, and can be thought of as a rotation of a quantum state vector in Hilbert space.

We can write this condition as

$$\begin{aligned}\langle U\psi|U\psi\rangle &= \left\langle\psi\middle|U^{\dagger}U\psi\right\rangle &(1)\\ &= \langle\psi|\psi\rangle &(2)\end{aligned}$$

From this we see that the hermitian conjugate must also be the inverse of U:

$$U^{\dagger}=U^{-1} \tag{3}$$

Any complex exponential operator $U=e^{iA}$ for some other (hermitian, so that $A^{\dagger}=A$) operator A qualifies as a unitary operator, since

$$\begin{aligned} U^\dagger &= \left(e^{iA}\right)^\dagger = e^{-iA^\dagger} = e^{-iA} && (4)\\ U^\dagger U &= e^{-iA}e^{iA} = 1 && (5)\end{aligned}$$

A unitary transformation can also be thought of as applied to an operator Q rather than the state. The requirement is that the bracket $\langle\psi|Q|\psi\rangle$ is unchanged by the unitary transformation. Transforming the bracket gives (where Q' is the transformed operator)

$$\begin{aligned} \left\langle U\psi\left|Q'\right|U\psi\right\rangle &= \left\langle\psi\left|U^\dagger Q'U\right|\psi\right\rangle && (6)\\ &= \langle\psi|Q|\psi\rangle && (7)\end{aligned}$$

Therefore, the transformed operator can be obtained from

$$\begin{aligned} U^\dagger Q'U &= Q && (8)\\ UU^\dagger Q'UU^\dagger &= UQU^\dagger && (9)\\ Q' &= UQU^\dagger = UQU^{-1} && (10)\end{aligned}$$

The Heisenberg picture. To make the transition to the Heisenberg picture, we first need to recall the expression for the time derivative of the expectation value of some quantum observable Q:

$$\frac{d}{dt}\langle Q\rangle = i\langle[H,Q]\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle \tag{11}$$

where the term $\langle[H,Q]\rangle$ is the expectation value of the commutator of Q with the hamiltonian H and we've used natural units with $\hbar = 1$. This is the situation in the Schrödinger picture, so to make this explicit we can include the states (where a subscript or superscript S indicates 'Schrödinger state' or 'Schrödinger operator').

$$\frac{d}{dt}\langle Q\rangle = \left\langle\psi_S\left|i\left[H,Q^S\right]\right|\psi_S\right\rangle + \left\langle\psi_S\left|\frac{\partial Q^S}{\partial t}\right|\psi_S\right\rangle \tag{12}$$

Usually the Schrödinger operator Q^S is independent of time so that last term is zero.

Now suppose we introduce the unitary transformation

$$U \equiv e^{-iHt} \tag{13}$$

and transform states and operators according to (now the superscript or subscript H indicates 'Heisenberg'):

$$U^{\dagger}|\psi_S\rangle = |\psi_H\rangle \tag{14}$$
$$U^{\dagger}Q^S U = Q^H \tag{15}$$

For a free particle, the wave function is

$$|\psi_S\rangle = e^{-iEt+i\mathbf{p}\cdot\mathbf{x}} \tag{16}$$

where **p** is the momentum. Applying the unitary operator we get, since $|\psi_S\rangle$ is an eigenstate of H:

$$\begin{aligned} e^{iHt}|\psi_S\rangle &= e^{iEt}e^{-iEt+i\mathbf{p}\cdot\mathbf{x}} && (17)\\ &= e^{i\mathbf{p}\cdot\mathbf{x}} && (18)\\ &= |\psi_H\rangle && (19)\end{aligned}$$

In the Heisenberg picture, the time dependence has been removed from the state. So where does the time dependence show up in the Heisenberg picture? Let's go back to 12 and convert it to the Heisenberg picture. We can insert $UU^{\dagger} = U^{\dagger}U = 1$ anywhere since it won't change anything, so we get

$$\frac{d}{dt}\langle Q\rangle = \left\langle \psi_S \left| UU^{\dagger} i\left[H, Q^S\right] UU^{\dagger} \right| \psi_S \right\rangle + \left\langle \psi_S \left| UU^{\dagger} \frac{\partial Q^S}{\partial t} UU^{\dagger} \right| \psi_S \right\rangle \tag{20}$$

$$= \left\langle U^{\dagger}\psi_S \left| U^{\dagger} i\left[H, Q^S\right] U \right| U^{\dagger}\psi_S \right\rangle + \left\langle U^{\dagger}\psi_S \left| U^{\dagger} \frac{\partial Q^S}{\partial t} U \right| U^{\dagger}\psi_S \right\rangle \tag{21}$$

$$= \left\langle \psi_H \left| U^{\dagger} i\left[H, Q^S\right] U \right| \psi_H \right\rangle + \left\langle \psi_H \left| U^{\dagger} \frac{\partial Q^S}{\partial t} U \right| \psi_H \right\rangle \tag{22}$$

From 15, we see that the operators in these two terms are the Heisenberg operators:

$$U^{\dagger} i\left[H, Q^S\right] U = i\left[H, Q^H\right] \tag{23}$$
$$U^{\dagger}\frac{\partial Q^S}{\partial t} U = \frac{\partial Q^H}{\partial t} \tag{24}$$

So in the Heisenberg picture

$$\frac{d}{dt}\langle Q\rangle = \left\langle \psi_H \left| i\left[H, Q^H\right] \right| \psi_H \right\rangle + \left\langle \psi_H \left| \frac{\partial Q^H}{\partial t} \right| \psi_H \right\rangle \tag{25}$$

This has the same form as in the Schrödinger picture 12. The difference is that the time dependence has been shifted from the states to the operators, since the operator U has an explicit time dependence.

Example 1. We have a state

$$|\psi\rangle = C_1 \left|\psi_{E_1}\right\rangle + C_2 \left|\psi_{E_2}\right\rangle \tag{26}$$

where $\left|\psi_{E_1}\right\rangle$ and $\left|\psi_{E_2}\right\rangle$ are eigenstates of the Hamiltonian H and C_1, C_2 are normalization constants. Operating on this state with U, we have

$$U|\psi\rangle = C_1 e^{-iE_1 t} \left|\psi_{E_1}\right\rangle + C_2 e^{-iE_2 t} \left|\psi_{E_2}\right\rangle \tag{27}$$

Example 2. Suppose we have a free particle wave function at some fixed time t_0:

$$|\psi_E\rangle = e^{-i(Et_0 - \mathbf{p}\cdot\mathbf{x})} \tag{28}$$

In the Schrödinger picture, the time-dependent wave function for a free particle is 16. We can get the same wave function by applying the unitary operator $U = e^{-iH(t-t_0)}$ to $|\psi_E\rangle$:

$$\begin{aligned} U|\psi_E\rangle &= e^{-iH(t-t_0)} e^{-i(Et_0 - \mathbf{p}\cdot\mathbf{x})} && (29) \\ &= e^{-i(Et - \mathbf{p}\cdot\mathbf{x})} && (30) \end{aligned}$$

In this sense, U acts as an evolution operator, in that it takes a state at a fixed point in time and turns it into a dynamic state that evolves in time, giving the usual Schrödinger picture wave function. We can turn this state back into the Heisenberg picture by operating with $U^\dagger$:

$$\begin{aligned} U^\dagger e^{-i(Et - \mathbf{p}\cdot\mathbf{x})} &= e^{iH(t-t_0)} e^{-i(Et - \mathbf{p}\cdot\mathbf{x})} && (31) \\ &= e^{-i(Et_0 - \mathbf{p}\cdot\mathbf{x})} && (32) \end{aligned}$$

which is the original time-independent wave function.

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