

## 3.5: Schrödinger and Heisenberg Representations

The mathematical formulation of quantum dynamics that has been presented is not unique. So far, we have described the dynamics by propagating the wavefunction, which encodes probability densities. Ultimately, since we cannot measure a wavefunction, we are interested in observables, which are probability amplitudes associated with Hermitian operators, with time dependence that can be interpreted differently. Consider the expectation value:

$$\langle \hat{A}(t) \rangle = \langle \psi(t) | \hat{A} | \psi(t) \rangle = \langle \psi(0) | U^\dagger \hat{A} U | \psi(0) \rangle \quad (3.5.1)$$

$$= (\langle \psi(0) | U^\dagger) \hat{A} (U | \psi(0) \rangle) \quad (3.5.2)$$

$$= \langle \psi(0) | (U^\dagger \hat{A} U) | \psi(0) \rangle \quad (3.5.3)$$

The last two expressions are written to emphasize alternate “pictures” of the dynamics. Equation 3.5.2 is known as the Schrödinger picture, refers to everything we have done so far. Here we propagate the wavefunction or eigenvectors in time as  $U|\psi\rangle$ . Operators are unchanged because they carry no time-dependence. Alternatively, we can work in the Heisenberg picture (Equation 3.5.3) that uses the unitary property of  $U$  to time-propagate the operators as  $\hat{A}(t) = U^\dagger \hat{A} U$ , but the wavefunction is now stationary. The Heisenberg picture has an appealing physical picture behind it, because particles move. That is, there is a time-dependence to position and momentum.

### Schrödinger Picture

In the Schrödinger picture, the time-development of  $|\psi\rangle$  is governed by the TDSE

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle \quad (3.5.4)$$

or equivalently, the time propagator:

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle \quad (3.5.5)$$

In the Schrödinger picture, operators are typically independent of time,  $\partial A / \partial t = 0$ . What about observables? For expectation values of operators

$$\langle A(t) \rangle = \langle \psi | A | \psi \rangle \quad (3.5.6)$$

$$i\hbar \frac{\partial}{\partial t} \langle \hat{A}(t) \rangle = i\hbar \left[ \left\langle \psi \left| \hat{A} \frac{\partial \psi}{\partial t} \right\rangle + \left\langle \frac{\partial \psi}{\partial t} \left| \hat{A} \right| \psi \right\rangle + \left\langle \psi \left| \frac{\partial \hat{A}}{\partial t} \right| \psi \right\rangle \right] \quad (3.5.7)$$

$$= \langle \psi | \hat{A} H | \psi \rangle - \langle \psi | H \hat{A} | \psi \rangle \quad (3.5.8)$$

$$= \langle [\hat{A}, H] \rangle \quad (3.5.9)$$

If  $\hat{A}$  is independent of time (as we expect in the Schrödinger picture), and if it commutes with  $\hat{H}$ , it is referred to as a *constant of motion*.

### Heisenberg Picture

From Equation 3.5.3, we can distinguish the Schrödinger picture from Heisenberg operators:

$$\hat{A}(t) = \langle \psi(t) | \hat{A} | \psi(t) \rangle_S = \langle \psi(t_0) | U^\dagger \hat{A} U | \psi(t_0) \rangle_S = \langle \psi | \hat{A}(t) | \psi \rangle_H \quad (3.5.10)$$

where the operator is defined as

$$\hat{A}_H(t) = U^\dagger(t, t_0) \hat{A}_S U(t, t_0)$$

$$\hat{A}_H(t_0) = \hat{A}_S$$

Note, the pictures have the same wavefunction at the reference point  $t_0$ . Since the wavefunction should be time-independent,  $\partial |\psi_H\rangle / \partial t = 0$ , we can relate the Schrödinger and Heisenberg wavefunctions as

$$|\psi_S(t)\rangle = U(t, t_0) |\psi_H\rangle \quad (3.5.11)$$

So,

$$|\psi_H\rangle = U^\dagger(t, t_0) |\psi_S(t)\rangle = |\psi_S(t_0)\rangle \quad (3.5.12)$$

As expected for a unitary transformation, in either picture the eigenvalues are preserved:

$$\hat{A}|\varphi_i\rangle_S = a_i|\varphi_i\rangle_S \quad (3.5.13)$$

$$U^\dagger \hat{A} U U^\dagger |\varphi_i\rangle_S = a_i U^\dagger |\varphi_i\rangle_S \quad (3.5.14)$$

$$\hat{A}_H |\varphi_i\rangle_H = a_i |\varphi_i\rangle_H \quad (3.5.15)$$

The time evolution of the operators in the Heisenberg picture is:

$$\begin{aligned} \frac{\partial \hat{A}_H}{\partial t} &= \frac{\partial}{\partial t} (U^\dagger \hat{A}_S U) = \frac{\partial U^\dagger}{\partial t} \hat{A}_S U + U^\dagger \hat{A}_S \frac{\partial U}{\partial t} + U^\dagger \frac{\partial \hat{A}_S}{\partial t} U \\ &= \frac{i}{\hbar} U^\dagger H \hat{A}_S U - \frac{i}{\hbar} U^\dagger \hat{A}_S H U + \left( \frac{\partial \hat{A}_S}{\partial t} \right)_H \\ &= \frac{i}{\hbar} H_H \hat{A}_H - \frac{i}{\hbar} \hat{A}_H H_H \\ &= -\frac{i}{\hbar} [\hat{A}, H]_H \end{aligned}$$

The result

$$i\hbar \frac{\partial}{\partial t} \hat{A}_H = [\hat{A}, H]_H \quad (3.5.16)$$

is known as the *Heisenberg equation of motion*. Here I have written the odd looking  $H_H = U^\dagger H U$ . This is mainly to remind one about the time-dependence of  $\hat{H}$ . Generally speaking, for a time-independent Hamiltonian  $U = e^{-iHt/\hbar}$ ,  $U$  and  $H$  commute, and  $H_H = H$ . For a time-dependent Hamiltonian,  $U$  and  $H$  need **not** commute.

### Classical equivalence for particle in a potential

The Heisenberg equation is commonly applied to a particle in an arbitrary potential. Consider a particle with an arbitrary one-dimensional potential

$$H = \frac{p^2}{2m} + V(x) \quad (3.5.17)$$

For this Hamiltonian, the Heisenberg equation gives the time-dependence of the momentum and position as

$$\dot{p} = -\frac{\partial V}{\partial x} \quad (3.5.18)$$

$$\dot{x} = \frac{p}{m} \quad (3.5.19)$$

Here, I have made use of

$$[\hat{x}^n, \hat{p}] = i\hbar n \hat{x}^{n-1} \quad (3.5.20)$$

$$[\hat{x}, \hat{p}^n] = i\hbar n \hat{p}^{n-1} \quad (3.5.21)$$

Curiously, the factors of  $\hbar$  have vanished in Equations 3.5.18 and 3.5.19, and quantum mechanics does not seem to be present. Instead, these equations indicate that the position and momentum operators follow the same equations of motion as Hamilton's equations for the classical variables. If we integrate Equation 3.5.19 over a time period  $t$  we find that the expectation value for the position of the particle follows the classical motion.

$$\langle x(t) \rangle = \frac{\langle p \rangle t}{m} + \langle x(0) \rangle \quad (3.5.22)$$

We can also use the time derivative of Equation 3.5.19 to obtain an equation that mirrors Newton's second law of motion,  $F = ma$ :

$$m \frac{\partial^2 \langle x \rangle}{\partial t^2} = -\langle \nabla V \rangle \quad (3.5.23)$$

These observations underlie *Ehrenfest's Theorem*, a statement of the classical correspondence of quantum mechanics, which states that the expectation values for the position and momentum operators will follow the classical equations of motion.

## Readings

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