# Quantum Mechanics

*Robert C. Roleda*
*Physics Department*

## Interaction Picture

De La Salle University

# Time Evolution Operator

In the Schrödinger formulation of quantum mechanics, wave functions contain all essential information about the state of the system, and it is through wave functions that all predictions about observables are made. The dynamics of the wave function is described by the Schrödinger Equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$$

where $H$ is the Hamiltonian that defines the system.

If the system is initially in a state $\psi(x,0)$, then at a later time $t$, the Schrödinger Equation gives

$$\psi(x,t) = e^{-i\hat{H}t/\hbar}\,\psi(x,0)$$

The $\hat{H}$ operates on the initial state $\psi(x,0)$, and

$$U(t) = e^{-i\hat{H}t/\hbar}$$

is called the time evolution operator.

# Schrödinger v Heisenberg Picture

In the Heisenberg formulation of quantum mechanics, operators are paramount. One does not even need to know the expression of eigenstates. Knowing how the operators act on the states is sufficient to predict values of observables.

The key that connects the Schrödinger and the Heisenberg pictures is that two formulations can be deemed equivalent if their predictions about observables are the same. Thus, for any observable $A$,

$$\langle A \rangle_S = \langle A \rangle_H$$

where the subscripts refer to the two formulations. In the Schrödinger formulation,

$$\langle A \rangle_S = \langle \psi(x,t)|A|\psi(x,t) \rangle$$

If we let $\psi(x,0) = \alpha(x)$, then

$$\langle A \rangle_S = \langle \alpha | U^\dagger A U | \alpha \rangle$$

In the Heisenberg formulation, it is convenient to represent the operators using a fixed basis. Thus, time-dependence lies exclusively with the operators

$$\langle A \rangle_H = \langle \alpha | A(t) | \alpha \rangle$$

# Evolution of Operators

Equating the last two expressions, we have

$$A_H(t) = U^\dagger A_S U$$

where the subscripts $H, S$ are introduced to label the two pictures.

In the Schrödinger picture, wave functions evolve, while operators are fixed. In the Heisenberg picture, wave functions are fixed while operators evolve. The evolution of the operators may be obtained by finding the derivative

$$\frac{dA_H}{dt} = \frac{dU^\dagger}{dt} A_S U + U^\dagger A_S \frac{dU}{dt}$$

Since

$$U(t) = e^{-i\hat{H}t/\hbar}$$

we have

$$\frac{dA_H}{dt} = \frac{iH}{\hbar} U^\dagger A_S U - U^\dagger A_S \frac{iH}{\hbar} U = -\frac{1}{i\hbar}(HA_H - A_H H) = \frac{1}{i\hbar}[A_H, H]$$

# Interaction Picture

Let us consider systems with time-dependent potentials $V(t)$. In such cases, we may separate out the time-independent and the time-dependent parts

$$H = H_0 + V(t)$$

where $H_0$ contains parts of the potential that are time-independent.

We now introduce a third picture by defining

$$\psi_I(x,t) = e^{i\hat{H}_0 t/\hbar}\psi_S(x,t)$$

where the subscript $I$ stands for the interaction picture (this is sometimes called the Dirac picture). The two pictures are equivalent if

$$\langle A\rangle_S = \langle A\rangle_I$$

Thus.

$$\langle\psi_S(x,t)|A_S|\psi_S(x,t)\rangle = \left\langle\psi_I(x,t)\middle|e^{i\hat{H}_0 t/\hbar}A_S e^{-i\hat{H}_0 t/\hbar}\middle|\psi_I(x,t)\right\rangle = \langle\psi_I(x,t)|A_I|\psi_I(x,t)\rangle$$

and

$$A_I = e^{i\hat{H}_0 t/\hbar}A_S e^{-i\hat{H}_0 t/\hbar}$$

# Evolution of Wave Functions

The time evolution of the wave function in this picture is

$$i\hbar\frac{\partial\psi_I(x,t)}{\partial t} = -H_0 e^{\frac{i\hat{H}_0 t}{\hbar}}\psi_S + e^{\frac{i\hat{H}_0 t}{\hbar}}\, i\hbar\frac{\partial\psi_S}{\partial t} = -H_0 e^{\frac{i\hat{H}_0 t}{\hbar}}\psi_S + e^{\frac{i\hat{H}_0 t}{\hbar}}\big(H_0 + V(t)\big)\psi_S$$

$$= e^{\frac{i\hat{H}_0 t}{\hbar}} V(t)\psi_S = e^{\frac{i\hat{H}_0 t}{\hbar}} V(t) e^{-\frac{i\hat{H}_0 t}{\hbar}}\psi_I$$

Now,

$$e^{\frac{i\hat{H}_0 t}{\hbar}} V(t) e^{-\frac{i\hat{H}_0 t}{\hbar}} = V_I$$

Thus,

$$i\hbar\frac{\partial\psi_I(x,t)}{\partial t} = V_I\psi_I(x,t)$$

# Evolution of Operators

The time evolution of operator on the other hand, is given by

$$\frac{dA_I}{dt} = \frac{i}{\hbar} H_0 e^{\frac{iH_0 t}{\hbar}} A_S e^{-\frac{iH_0 t}{\hbar}} - \frac{i}{\hbar} e^{\frac{iH_0 t}{\hbar}} A_S H_0 e^{-\frac{iH_0 t}{\hbar}} = -\frac{1}{i\hbar}[H_0 A_I - A_I H_0]$$

Thus,

$$\frac{dA_I}{dt} = \frac{1}{i\hbar}[A_I, H_0]$$

We then think of the Interaction picture as a hybrid picture, whereby the time evolution of the wave function is governed by the time-dependent interaction potential, while the evolution of operators is governed by the time-independent Hamiltonian.

# Eigenket Expansion

Taking the eigenkets of $H_0$ as basis for expansion

$$H_0|n\rangle = E_n|n\rangle$$

and

$$|\psi(t)\rangle_I = \sum_n c_n(t)\,|n\rangle$$

we have

$$i\hbar\frac{\partial\langle n|\psi\rangle_I}{\partial t} = \langle n|V_I|\psi\rangle_I = \sum_m \langle n|V_I|m\rangle\langle m|\psi\rangle_I$$

Now,

$$\langle n|V_I|m\rangle = \left\langle n\middle|e^{iH_0t/\hbar}\,V(t)e^{-iH_0t/\hbar}\middle|m\right\rangle = \langle n|\,V(t)|m\rangle e^{i(E_n-E_m)t/\hbar}$$

# Evolution of Expansion Coefficients

If we write

$$V_{nm} = \langle n|\, V(t)|m\rangle$$

$$E_n - E_m = \hbar\omega_{nm}$$

And noting that

$$\langle n|\psi\rangle_I = c_n(t)$$

Then

$$i\hbar\frac{dc_n}{dt} = \sum_m V_{nm}e^{i\omega_{nm}t}c_m$$