SCHRÖDINGER AND HEISENBERG REPRESENTATIONS

The mathematical formulation of the dynamics of a quantum system is not unique. Ultimately we are interested in observables (probability amplitudes)—we can’t measure a wavefunction. An alternative to propagating the wavefunction in time starts by recognizing that a unitary transformation doesn’t change an inner product.

\[
\langle \phi_j | \phi_i \rangle = \langle \phi_j | U^\dagger U | \phi_i \rangle
\]

For an observable:

\[
\langle \phi_j | A | \phi_i \rangle = \langle \langle \phi_j | U^\dagger \rangle A (U | \phi_i \rangle) = \langle \phi_j | U^\dagger A U | \phi_i \rangle
\]

Two approaches to transformation:

1) Transform the eigenvectors: \( |\phi_i\rangle \rightarrow U |\phi_i\rangle \). Leave operators unchanged.

2) Transform the operators: \( A \rightarrow U^\dagger A U \). Leave eigenvectors unchanged.

(1) **Schrödinger Picture**: Everything we have done so far. Operators are stationary. Eigenvectors evolve under \( U(t, t_0) \).

(2) **Heisenberg Picture**: Use unitary property of \( U \) to transform operators so they evolve in time. The wavefunction is stationary. This is a physically appealing picture, because particles move—there is a time-dependence to position and momentum.

**Schrödinger Picture**

We have talked about the time-development of \( |\psi\rangle \), which is governed by

\[
i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle \quad \text{in differential form, or alternatively}
\]

\[
|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle \quad \text{in an integral form.}
\]
Typically for operators: \( \frac{\partial A}{\partial t} = 0 \)

What about observables? Expectation values:

\[
\langle A(t) \rangle = \langle \psi(t) | A | \psi(t) \rangle
\]

\[
i\hbar \frac{\partial}{\partial t} \langle A \rangle = i\hbar \left[ \langle \psi | A | \frac{\partial \psi}{\partial t} \rangle + \langle \psi | \frac{\partial A}{\partial t} | \psi \rangle + \langle \psi | A | \psi \rangle \right]
\]

\[
= \langle \psi | A H | \psi \rangle - \langle \psi | H A | \psi \rangle
\]

\[
= \langle \psi | [A, H] | \psi \rangle
\]

\[
= \langle [A, H] \rangle
\]

If \( A \) is independent of time (as it should be in the Schrödinger picture) and commutes with \( H \), it is referred to as a constant of motion.

**Heisenberg Picture**

Through the expression for the expectation value,

\[
\langle A \rangle = \langle \psi(t) | A | \psi(t) \rangle_S = \langle \psi(t_0) | U_S^\dagger A U_S | \psi(t_0) \rangle_S
\]

\[
= \langle \psi | A(t) | \psi \rangle_H
\]

we choose to define the operator in the Heisenberg picture as:

\[
A_H(t) = U_S^\dagger(t, t_0) A_S U_S(t, t_0)
\]

\[
A_H(t_0) = A_S
\]

Also, since the wavefunction should be time-independent \( \frac{\partial}{\partial t} |\psi_H\rangle = 0 \), we can write

\[
|\psi_S(t)\rangle = U(t, t_0) |\psi_H\rangle
\]

So,

\[
|\psi_H\rangle = U_S^\dagger(t, t_0) |\psi_S(t)\rangle = |\psi_S(t_0)\rangle
\]
In either picture the eigenvalues are preserved:

\[
A |\phi_i\rangle_s = a_i |\phi_i\rangle_s \\
U^\dagger AU^\dagger |\phi_i\rangle_s = a_i U^\dagger |\phi_i\rangle_s \\
A_H |\phi_i\rangle_H = a_i |\phi_i\rangle_H
\]

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

\[
\frac{\partial A_H}{\partial t} = \frac{\partial}{\partial t} \left( U^\dagger A_S U \right) = \frac{\partial U^\dagger}{\partial t} A_S U + U^\dagger A_S \frac{\partial U}{\partial t} + U^\dagger \frac{\partial A_S}{\partial t} U \\
= \frac{i}{\hbar} U^\dagger H A_S U - \frac{i}{\hbar} U^\dagger A_S H U + \left( \frac{\partial A}{\partial t} \right)_H \\
= \frac{i}{\hbar} H_H A_H - \frac{i}{\hbar} A_H H_H \\
= -\frac{i}{\hbar} [A, H]_H
\]

\[i\hbar \frac{\partial}{\partial t} A_H = [A, H]_H \quad \text{Heisenberg Eqn. of Motion}\]

Here \( H_H = U^\dagger H U \). For a time-dependent Hamiltonian, \( U \) and \( H \) need not commute.

Often we want to describe the equations of motion for particles with an arbitrary potential:

\[ H = \frac{p^2}{2m} + V(x) \]

For which we have

\[ \dot{p} = -\frac{\partial V}{\partial x} \quad \text{and} \quad \dot{x} = \frac{p}{m} \quad \ldots \text{using} \quad [x^n, p] = i\hbar n x^{n-1}; [x, p^n] = i\hbar np^{n-1} \]
THE INTERACTION PICTURE

When solving problems with time-dependent Hamiltonians, it is often best to partition the Hamiltonian and treat each part in a different representation. Let’s partition

\[ H(t) = H_0 + V(t) \]

\( H_0 \): Treat exactly—can be (but usually isn’t) a function of time.

\( V(t) \): Expand perturbatively (more complicated).

The time evolution of the exact part of the Hamiltonian is described by

\[ \frac{\partial}{\partial t} U_0(t, t_0) = \frac{i}{\hbar} H_0(t) U_0(t, t_0) \]

where

\[ U_0(t, t_0) = \exp \left[ \frac{i}{\hbar} \int_{t_0}^{t} d\tau H_0(\tau) \right] \Rightarrow e^{-iH_0(t-t_0)/\hbar} \text{ for } H_0 \neq f(t) \]

We define a wavefunction in the interaction picture \( |\psi_I\rangle \) as:

\[ |\psi_s(t)\rangle \equiv U_0(t, t_0)|\psi_I(t)\rangle \]

or \[ |\psi_I\rangle = U_0^\dagger |\psi_s\rangle \]

Substitute into the T.D.S.E.

\[ i\hbar \frac{\partial}{\partial t} |\psi_s\rangle = H |\psi_s\rangle \]
\[
\frac{\partial}{\partial t} U_0(t, t_0)|\psi_i\rangle = -\frac{i}{\hbar} H(t) U_0(t, t_0)|\psi_i\rangle \quad \Rightarrow \quad \frac{\partial}{\partial t} U_0|\psi_i\rangle + U_0 \frac{\partial}{\partial t}|\psi_i\rangle = -\frac{i}{\hbar} \left( H_0 + V(t) \right) U_0(t, t_0)|\psi_i\rangle
\]

\[
-\frac{i}{\hbar} H_0 U_0|\psi_i\rangle + U_0 \frac{\partial}{\partial t}|\psi_i\rangle = -\frac{i}{\hbar} \left( H_0 + V(t) \right) U_0|\psi_i\rangle
\]

\[
\therefore i\hbar \frac{\partial}{\partial t} |\psi_i\rangle = V_1 |\psi_i\rangle
\]

where: \( V_1(t) = U_0^\dagger (t, t_0) V(t) U_0(t, t_0) \)

\( |\psi_i\rangle \) satisfies the Schrödinger equation with a new Hamiltonian: the interaction picture Hamiltonian is the \( U_0 \) unitary transformation of \( V(t) \).

Note: Matrix elements in \( V_1 = \langle k | V_1 | l \rangle = e^{-i\omega_{kl} \tau} \) \( \ldots \) where \( k \) and \( l \) are eigenstates of \( H_0 \).

We can now define a time-evolution operator in the interaction picture:

\[
|\psi_1(t)\rangle = U_1(t, t_0)|\psi_1(t_0)\rangle
\]

where \( U_1(t, t_0) = \exp \left[ -\frac{i}{\hbar} \int_{t_0}^t d\tau V_1(\tau) \right] \)

\[
|\psi_s(t)\rangle = U_0(t, t_0)|\psi_1(t)\rangle
\]

\[
= U_0(t, t_0)U_1(t, t_0)|\psi_1(t_0)\rangle
\]

\[
= U_0(t, t_0)U_1(t, t_0)|\psi_1(t_0)\rangle
\]

\[
\therefore U(t, t_0) = U_0(t, t_0)U_1(t, t_0) \quad \text{Order matters!}
\]

\[
U(t, t_0) = U_0(t, t_0) \exp \left[ -\frac{i}{\hbar} \int_{t_0}^t d\tau V_1(\tau) \right]
\]

which is defined as
\[ U(t, t_0) = U_0(t, t_0) + \sum_{n=1}^{\infty} \left( \frac{-i}{\hbar} \right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n U_0(t, t_{n-1}) V(t_{n-1}) U_0(t_{n-1}, t_0) \]

where we have used the composition property of \( U(t, t_0) \). The same positive time-ordering applies. Note that the interactions \( V(\tau_i) \) are not in the interaction representation here. Rather we have expanded

\[ V_i(t) = U_0^\dagger(t, t_0) V(t) U_0(t, t_0) \]

and collected terms.

For transitions between two eigenstates of \( H_0 \), \( l \) and \( k \): The system evolves in eigenstates of \( H_0 \) during the different time periods, with the time-dependent interactions \( V \) driving the transitions between these states. The time-ordered exponential accounts for all possible intermediate pathways.

Also:

\[ U^\dagger(t, t_0) = U_0^\dagger(t, t_0) U_0^\dagger(t, t_0) = \exp \left[ \frac{-i}{\hbar} \int_{t_0}^{t} \mathrm{d}\tau \, V(t) \right] \exp \left[ \frac{-i}{\hbar} \int_{t_0}^{t} \mathrm{d}\tau \, H_0(t) \right] \]

or \( e^{iH(t-t_0)/\hbar} \) for \( H \neq f(t) \)

The expectation value of an operator is:

\[ \langle A(t) \rangle = \langle \psi(t) | A | \psi(t) \rangle = \langle \psi(t_0) | U^\dagger(t, t_0) A U(t, t_0) | \psi(t_0) \rangle = \langle \psi(t_0) | U_0^\dagger U_0 A U_0 U_0^\dagger | \psi(t_0) \rangle = \langle \psi(t_0) | A_I \psi(t_0) \rangle \]

\[ A_I \equiv U_0^\dagger A S U_0 \]

Differentiating \( A_I \) gives:
\[
\frac{\partial}{\partial t} A_i = \frac{i}{\hbar} [H_0, A_i]
\]

also,
\[
\frac{\partial}{\partial t} |\psi_i\rangle = -\frac{i}{\hbar} V_i(t) |\psi_i\rangle
\]

Notice that the interaction representation is a partition between the Schrödinger and Heisenberg representations. Wavefunctions evolve under \( V_i \), while operators evolve under \( H_0 \).

For \( H_0 = 0 \), \( V(t) = H \) \( \Rightarrow \) \( \frac{\partial A}{\partial t} = 0; \) \( \frac{\partial}{\partial t} |\psi_s\rangle = -\frac{i}{\hbar} H |\psi_s\rangle \) \text{ Schrödinger} \n
For \( H_0 = H \), \( V(t) = 0 \) \( \Rightarrow \) \( \frac{\partial A}{\partial t} = \frac{i}{\hbar} [H, A]; \) \( \frac{\partial |\psi\rangle}{\partial t} = 0 \) \text{ Heisenberg}