MIT Department of Chemistry
5.74, Spring 2004: Introductory Quantum Mechanics II
Instructor: Prof. Andrei Tokmakoff

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.

$$\langle \varphi_j | \varphi_i \rangle = \langle \varphi_j | U^\dagger U | \varphi_i \rangle$$

For an observable:

$$\langle \varphi_j | A | \varphi_i \rangle = \left(\langle \varphi_j | U^\dagger \right) A \left(U | \varphi_i \rangle \right) = \langle \varphi_j | U^\dagger A U | \varphi_i \rangle$$

Two approaches to transformation:

1) Transform the eigenvectors: $|\varphi_i\rangle \rightarrow U|\varphi_i\rangle$. 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

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$$ in differential form, or alternatively

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$$ in an integral form.

Typically for operators: $\frac{\partial A}{\partial t} = 0$

What about observables? Expectation values:

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

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

or...

$$= i\hbar\frac{\partial}{\partial t}\mathrm{Tr}(A\rho)$$
$$= i\hbar\mathrm{Tr}\left(A\frac{\partial}{\partial t}\rho\right)$$
$$= \mathrm{Tr}(A[H,\rho])$$
$$= \mathrm{Tr}([A,H]\rho)$$

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,

$$\langle A\rangle = \langle \psi(t)|A|\psi(t)\rangle_S = \langle \psi(t_0)|U^\dagger\,A\,U|\psi(t_0)\rangle_S$$
$$= \langle \psi|A(t)|\psi\rangle_H$$

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

$$A_H(t) = U^\dagger(t,t_0)A_S U(t,t_0)$$
$$A_H(t_0) = A_S$$

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,

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

In either picture the eigenvalues are preserved:

$$
\begin{aligned}
A\,|\varphi_i\rangle_S &= a_i\,|\varphi_i\rangle_S \\
U^\dagger A U U^\dagger\,|\varphi_i\rangle_S &= a_i U^\dagger\,|\varphi_i\rangle_S \\
A_H\,|\varphi_i\rangle_H &= a_i\,|\varphi_i\rangle_H
\end{aligned}
$$

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

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

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

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

$$
\dot{p} = -\frac{\partial V}{\partial x} \text{ and } \dot{x} = \frac{p}{m} \qquad \ldots\text{using } \left[x^n, p\right] = i\hbar n x^{n-1}; \left[x, p^n\right] = i\hbar n p^{n-1}
$$

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

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

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

$$|\psi_S(t)\rangle \equiv U_0(t,t_0)|\psi_I(t)\rangle$$

$$\text{or} \qquad |\psi_I\rangle = U_0^\dagger |\psi_S\rangle$$

Substitute into the T.D.S.E. $\qquad i\hbar\frac{\partial}{\partial t}|\psi_S\rangle = H|\psi_S\rangle$

$$\frac{\partial}{\partial t} U_0(t,t_0)|\psi_I\rangle = \frac{-i}{\hbar} H(t)\, U_0(t,t_0)|\psi_I\rangle$$

$$\frac{\partial U_0}{\partial t}|\psi_I\rangle + U_0 \frac{\partial|\psi_I\rangle}{\partial t} = \frac{-i}{\hbar}\left(H_0 + V(t)\right) U_0(t,t_0)|\psi_I\rangle$$

$$\cancel{\frac{-i}{\hbar} H_0 U_0|\psi_I\rangle} + U_0 \frac{\partial|\psi_I\rangle}{\partial t} = \frac{-i}{\hbar}\left(\cancel{H_0} + V(t)\right) U_0|\psi_I\rangle$$

$$\therefore\quad i\hbar \frac{\partial|\psi_I\rangle}{\partial t} = V_I|\psi_I\rangle$$

$$\text{where: } V_I(t) = U_0^\dagger(t,t_0)\, V(t)\, U_0(t,t_0)$$

$|\psi_I\rangle$ 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 $V_I = \langle k|V_I|l\rangle = e^{-i\omega_{lk}t}V_{kl}$ …where k and l are eigenstates of H_0.

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

$$|\psi_I(t)\rangle = U_I(t,t_0)|\psi_I(t_0)\rangle$$

$$\text{where } U_I(t,t_0) = \exp_+\left[\frac{-i}{\hbar}\int_{t_0}^{t} d\tau\, V_I(\tau)\right]$$

$$\begin{aligned}|\psi_S(t)\rangle &= U_0(t,t_0)|\psi_I(t)\rangle \\ &= U_0(t,t_0)U_I(t,t_0)|\psi_I(t_0)\rangle \\ &= U_0(t,t_0)U_I(t,t_0)|\psi_S(t_0)\rangle \\ \therefore\quad U(t,t_0) &= U_0(t,t_0)U_I(t,t_0) \qquad \text{Order matters!}\end{aligned}$$

$$U(t,t_0) = U_0(t,t_0)\exp_+\left[\frac{-i}{\hbar}\int_{t_0}^{t} d\tau\, V_I(\tau)\right]$$

which is defined as

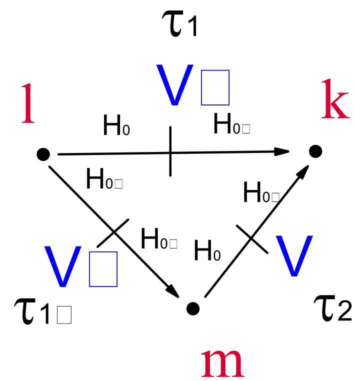
$$U(t,t_0) = U_0(t,t_0) + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1} \ldots \int_{t_0}^{\tau_2} d\tau_1\, U_0(t,\tau_n) V(\tau_n) U_0(\tau_n,\tau_{n-1}) \ldots U_0(\tau_2,\tau_1) V(\tau_1) U_0(\tau_1,t_0)$$

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:

$$U^\dagger(t,t_0) = U_I^\dagger(t,t_0)\, U_0^\dagger(t,t_0) = \exp_-\left[\frac{+i}{\hbar}\int_{t_0}^{t} d\tau\, V_I(\tau)\right] \exp_-\left[\frac{+i}{\hbar}\int_{t_0}^{t} d\tau\, H_0(\tau)\right]$$

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

The expectation value of an operator is:

$$\begin{aligned}
\langle A(t)\rangle &= \langle \psi(t)|A|\psi(t)\rangle \\
&= \langle \psi(t_0)|U^\dagger(t,t_0) A\, U(t,t_0)|\psi(t_0)\rangle \\
&= \langle \psi(t_0)|U_I^\dagger U_0^\dagger A U_0 U_I|\psi(t_0)\rangle \\
&= \langle \psi_I(t)|A_I|\psi_I(t)\rangle \\
A_I &\equiv U_0^\dagger\, A_S\, U_0
\end{aligned}$$

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 $H_0 = 0, V(t) = H \Rightarrow \frac{\partial A}{\partial t} = 0; \quad \frac{\partial}{\partial t}|\psi_S\rangle = \frac{-i}{\hbar} H|\psi_S\rangle$ Schrödinger

For $H_0 = H, V(t) = 0 \Rightarrow \frac{\partial A}{\partial t} = \frac{i}{\hbar}[H, A]; \quad \frac{\partial \psi}{\partial t} = 0$ Heisenberg