SCHRÖDINGER AND HEISENBERG REPRESENTATIONS

The mathematical formulation of the dynamics of a quantum system is not unique. So far we have described the dynamics by propagating the wavefunction, which encodes probability densities. This is known as the Schrödinger representation of quantum mechanics. Ultimately, since we can't measure a wavefunction, we are interested in observables (probability amplitudes associated with Hermetian operators). Looking at a time-evolving expectation value suggests an alternate interpretation of the quantum observable:

$$\begin{aligned}\left\langle \hat{A}(t)\right\rangle &= \langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(0)|U^{\dagger}\hat{A}U|\psi(0)\rangle \\ &= \left(\langle\psi(0)|U^{\dagger}\right)A\left(U|\psi(0)\rangle\right) \\ &= \left\langle\psi(0)\middle|\left(U^{\dagger}AU\right)\middle|\psi(0)\right\rangle\end{aligned} \tag{4.1}$$

The last two expressions here suggest alternate transformation that can describe the dynamics. These have different physical interpretations:

1) Transform the eigenvectors: $|\psi(t)\rangle \to U|\psi\rangle$. Leave operators unchanged.

2) Transform the operators: $\hat{A}(t) \to U^{\dagger}\hat{A}U$. 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.

Let's look at time-evolution in these two pictures:

Schrödinger Picture

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

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle \tag{4.2}$$

in differential form, or alternatively $\left|\psi(t)\right\rangle = U(t,t_0)\left|\psi(t_0)\right\rangle$ in an integral form. In the Schrödinger picture, for operators typically $\frac{\partial A}{\partial t} = 0$. What about observables? For expectation values of operators $\left\langle \hat{A}(t) \right\rangle = \left\langle \psi(t) \middle| \hat{A} \middle| \psi(t) \right\rangle$:

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t}\left\langle \hat{A}(t) \right\rangle &= i\hbar \left[\left\langle \psi \middle| \hat{A} \middle| \frac{\partial \psi}{\partial t} \right\rangle + \left\langle \frac{\partial \psi}{\partial t} \middle| \hat{A} \middle| \psi \right\rangle + \cancel{\left\langle \psi \middle| \frac{\partial \hat{A}}{\partial t} \middle| \psi \right\rangle} \right] \\
&= \left\langle \psi \middle| \hat{A} H \middle| \psi \right\rangle - \left\langle \psi \middle| H \hat{A} \middle| \psi \right\rangle \\
&= \left\langle \psi \middle| \left[\hat{A}, H \right] \middle| \psi \right\rangle \\
&= \left\langle \left[\hat{A}, H \right] \right\rangle
\end{aligned}
\tag{4.3}
$$

Alternatively, written for the density matrix:

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t}\left\langle \hat{A}(t) \right\rangle &= i\hbar \frac{\partial}{\partial t} Tr\left(A\rho\right) \\
&= i\hbar Tr\left(A \frac{\partial}{\partial t} \rho \right) \\
&= Tr\left(A\left[H,\rho\right] \right) \\
&= Tr\left(\left[A,H\right] \rho \right)
\end{aligned}
\tag{4.4}
$$

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

Heisenberg Picture

From eq. (4.1) we can distinguish the Schrödinger picture from Heisenberg operators:

$$
\hat{A}(t) = \left\langle \psi(t) \middle| \hat{A} \middle| \psi(t) \right\rangle_S = \left\langle \psi(t_0) \middle| U^\dagger A U \middle| \psi(t_0) \right\rangle_S = \left\langle \psi \middle| A(t) \middle| \psi \right\rangle_H \tag{4.5}
$$

where the operator is defined as

$$
\begin{aligned}
A_H(t) &= U^\dagger(t,t_0)\, A_S U(t,t_0) \\
A_H(t_0) &= A_S
\end{aligned}
\tag{4.6}
$$

Also, since the wavefunction should be time-independent $\partial|\psi_H\rangle/\partial t = 0$, we can relate the Schrödinger and Heisenberg wavefunctions as

$$|\psi_S(t)\rangle = U(t,t_0)|\psi_H\rangle \tag{4.7}$$

So,
$$|\psi_H\rangle = U^\dagger(t,t_0)|\psi_S(t)\rangle = |\psi_S(t_0)\rangle \tag{4.8}$$

In either picture the eigenvalues are preserved:

$$\begin{aligned} A|\varphi_i\rangle_S &= a_i|\varphi_i\rangle_S \\ U^\dagger A U U^\dagger|\varphi_i\rangle_S &= a_i U^\dagger|\varphi_i\rangle_S \\ A_H|\varphi_i\rangle_H &= a_i|\varphi_i\rangle_H \end{aligned} \tag{4.9}$$

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

$$\begin{aligned} \frac{\partial A_H}{\partial t} &= \frac{\partial}{\partial t}\left(U^\dagger A_S U\right) = \frac{\partial U^\dagger}{\partial t} A_S U + U^\dagger A_S \frac{\partial U}{\partial t} + U^\dagger \cancel{\frac{\partial A_S}{\partial t}} U \\ &= \frac{i}{\hbar} U^\dagger H A_S U - \frac{i}{\hbar} U^\dagger A_S H U + \cancel{\left(\frac{\partial A}{\partial t}\right)_H} \\ &= \frac{i}{\hbar} H_H A_H - \frac{i}{\hbar} A_H H_H \\ &= \frac{-i}{\hbar}[A,H]_H \end{aligned} \tag{4.10}$$

The result:
$$i\hbar \frac{\partial}{\partial t} A_H = [A,H]_H \tag{4.11}$$

is known as the Heisenberg equation of motion. Here I have written $H_H = U^\dagger H U$. 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.

Particle in a potential

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

$$H = \frac{p^2}{2m} + V(x) \tag{4.12}$$

For which the Heisenberg equation gives:

$$\dot{p} = -\frac{\partial V}{\partial x} \,. \tag{4.13}$$

$$\dot{x} = \frac{p}{m} \tag{4.14}$$

Here, I've made use of

$$\left[\hat{x}^n, \hat{p}\right] = i\hbar n \hat{x}^{n-1} \tag{4.15}$$

$$\left[\hat{x}, \hat{p}^n\right] = i\hbar n \hat{p}^{n-1} \tag{4.16}$$

These equations indicate that the position and momentum operators follow equations of motion identical to the classical variables in Hamilton's equations. These do not involve factors of $\hbar$. Note here that if we integrate eq. (4.14) over a time period *t* we find:

$$\langle x(t) \rangle = \frac{\langle p \rangle t}{m} + \langle x(0) \rangle \tag{4.17}$$

implying that the expectation value for the position of the particle follows the classical motion. These equations also hold for the expectation values for the position and momentum operators (Ehrenfest's Theorem) and indicate the nature of the classical correspondence. In correspondence to Newton's equation, we see

$$m \frac{\partial^2 \langle x \rangle}{\partial t^2} = -\langle \nabla V \rangle \tag{4.18}$$

THE INTERACTION PICTURE

The interaction picture is a hybrid representation that is useful in solving problems with time-dependent Hamiltonians in which we can partition the Hamiltonian as

$$H(t) = H_0 + V(t) \tag{4.19}$$

H_0 is a Hamiltonian for the degrees of freedom we are interested in, which we treat exactly, and can be (although for us generally won't be) a function of time. $V(t)$ is a time-dependent potential which can be complicated. In the interaction picture we will treat each part of the Hamiltonian in a different representation. We will use the eigenstates of H_0 as a basis set to describe the dynamics induced by $V(t)$, assuming that $V(t)$ is small enough that eigenstates of H_0 are a useful basis to describe *H*. If H_0 is not a function of time, then there is simple time-dependence to this part of the Hamiltonian, that we may be able to account for easily.

Setting *V* to zero, we can see that the time evolution of the exact part of the Hamiltonian H_0 is described by

$$\frac{\partial}{\partial t} U_0(t, t_0) = \frac{-i}{\hbar} H_0(t) U_0(t, t_0) \tag{4.20}$$

where, most generally,

$$U_0(t, t_0) = \exp_+ \left[\frac{i}{\hbar} \int_{t_0}^{t} d\tau \, H_0(t) \right] \tag{4.21}$$

but for a time-independent H_0

$$U_0(t, t_0) = e^{-iH_0(t-t_0)/\hbar} \tag{4.22}$$

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

$$|\psi_S(t)\rangle \equiv U_0(t, t_0) |\psi_I(t)\rangle \tag{4.23}$$

or

$$|\psi_I\rangle = U_0^\dagger |\psi_S\rangle \tag{4.24}$$

Effectively the interaction representation defines wavefunctions in such a way that the phase accumulated under $e^{-iH_0 t/\hbar}$ is removed. For small *V*, these are typically high frequency oscillations relative to the slower amplitude changes in coherences induced by *V*.

We are after an equation of motion that describes the time-evolution of the interaction picture wave-functions. We begin by substituting eq. (4.23) into the TDSE:

$$i\hbar \frac{\partial}{\partial t}\left|\psi_S\right\rangle = H\left|\psi_S\right\rangle \tag{4.25}$$

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

$$\frac{\partial U_0}{\partial t}\left|\psi_I\right\rangle + U_0\frac{\partial\left|\psi_I\right\rangle}{\partial t} = \frac{-i}{\hbar}\left(H_0 + V\left(t\right)\right)U_0\left(t,t_0\right)\left|\psi_I\right\rangle \tag{4.26}$$

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

$$\therefore \quad i\hbar\frac{\partial\left|\psi_I\right\rangle}{\partial t} = V_I\left|\psi_I\right\rangle \tag{4.27}$$

where
$$V_I\left(t\right) = U_0^\dagger\left(t,t_0\right)V\left(t\right)\,U_0\left(t,t_0\right) \tag{4.28}$$

$\left|\psi_I\right\rangle$ satisfies the Schrödinger equation with a new Hamiltonian: the interaction picture Hamiltonian, $V_I\left(t\right)$, which is the U_0 unitary transformation of $V(t)$. Note: Matrix elements in $V_I = \left\langle k\right|V_I\left|l\right\rangle = e^{-i\omega_{lk}t}V_{kl}$ where *k* and *l* are eigenstates of H_0.

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

$$\left|\psi_I\left(t\right)\right\rangle = U_I\left(t,t_0\right)\left|\psi_I\left(t_0\right)\right\rangle \tag{4.29}$$

where
$$U_I\left(t,t_0\right) = \exp_+\left[\frac{-i}{\hbar}\int_{t_0}^{t}d\tau\,V_I\left(\tau\right)\right]. \tag{4.30}$$

Now we see that

$$\begin{aligned}\left|\psi_S\left(t\right)\right\rangle &= U_0\left(t,t_0\right)\left|\psi_I\left(t\right)\right\rangle \\ &= U_0\left(t,t_0\right)U_I\left(t,t_0\right)\left|\psi_I\left(t_0\right)\right\rangle \\ &= U_0\left(t,t_0\right)U_I\left(t,t_0\right)\left|\psi_S\left(t_0\right)\right\rangle\end{aligned} \tag{4.31}$$

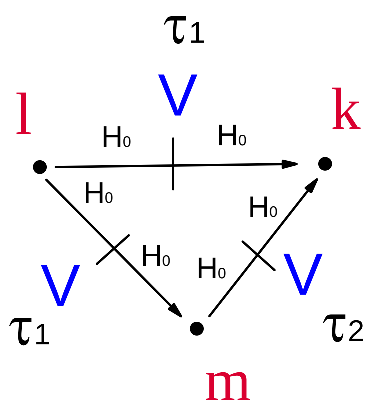
$$\therefore \quad U\left(t,t_0\right) = U_0\left(t,t_0\right)U_I\left(t,t_0\right) \tag{4.32}$$

Using the time ordered exponential in eq. (4.30), U can be written as

$$U(t,t_0) = U_0(t,t_0) + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1} \ldots \int_{t_0}^{\tau_2} d\tau_1\, U_0(t,\tau_n)V(\tau_n)U_0(\tau_n,\tau_{n-1})\ldots U_0(\tau_2,\tau_1)V(\tau_1)U_0(\tau_1,t_0) \tag{4.33}$$

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 used the definition in eq. (4.28) 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, the time evolution of conjugate wavefunction in the interaction picture is expressed as

$$U^{\dagger}(t,t_0) = U_I^{\dagger}(t,t_0)\,U_0^{\dagger}(t,t_0) = \exp_{-}\left[\frac{+i}{\hbar}\int_{t_0}^{t} d\tau\, V_I(\tau)\right]\exp_{-}\left[\frac{+i}{\hbar}\int_{t_0}^{t} d\tau\, H_0(\tau)\right] \tag{4.34}$$

or $U_0^{\dagger} = e^{iH(t-t_0)/\hbar}$ when H_0 is independent of time.

The expectation value of an operator is:

$$\begin{aligned}\langle A(t)\rangle &= \langle \psi(t)|A|\psi(t)\rangle \\ &= \langle \psi(t_0)|U^{\dagger}(t,t_0)\,A\,U(t,t_0)|\psi(t_0)\rangle \\ &= \langle \psi(t_0)|U_I^{\dagger}U_0^{\dagger}AU_0U_I|\psi(t_0)\rangle \\ &= \langle \psi_I(t)|A_I|\psi_I(t)\rangle\end{aligned} \tag{4.35}$$

where
$$A_I \equiv U_0^{\dagger}\, A_S\, U_0 \tag{4.36}$$

Differentiating A_I gives:

$$\frac{\partial}{\partial t}A_I = \frac{i}{\hbar}\left[H_0, A_I\right] \tag{4.37}$$

also,
$$\frac{\partial}{\partial t}\left|\psi_I\right\rangle = \frac{-i}{\hbar}V_I\left(t\right)\left|\psi_I\right\rangle \tag{4.38}$$

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.

$$\begin{array}{lllll} \text{For } H_0 = 0, V\left(t\right) = H & \Rightarrow & \dfrac{\partial A}{\partial t} = 0; & \dfrac{\partial}{\partial t}\left|\psi_S\right\rangle = \dfrac{-i}{\hbar}H\left|\psi_S\right\rangle & \text{Schrödinger} \\ \text{For } H_0 = H, V\left(t\right) = 0 & \Rightarrow & \dfrac{\partial A}{\partial t} = \dfrac{i}{\hbar}\left[H, A\right]; & \dfrac{\partial \psi}{\partial t} = 0 & \text{Heisenberg} \end{array} \tag{4.39}$$