Quantum Dynamics

In this section, I will present some general techniques of solving for the time evolution of quantum systems. Starting from the Schrödinger evolution equation:

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = \mathbf{H}(t)|\Psi(t)\rangle \qquad \#$$

and the time evolution operator $\mathbf{T}(t, t_0)$, which relates the initial state $|\Psi(t_0)\rangle$ to the final state $|\Psi(t)\rangle$ by

$$|\Psi(t)\rangle = \mathbf{T}(t, t_0)|\Psi(t_0)\rangle \qquad \#$$

it follows that the time evolution operator satifies the differential equation and initial condition:

$$i\hbar \frac{d}{dt}\mathbf{T}(t, t_0) = \mathbf{H}(t)\mathbf{T}(t, t_0) \qquad \#$$

$$\mathbf{T}(t_0, t_0) = 1 \qquad \#$$

The evolution for the adjoint space is given by:

$$-i\hbar \frac{d}{dt}\langle\Psi(t)| = \langle\Psi(t)|\mathbf{H}(t) \qquad \#$$

$$i\hbar \frac{d}{dt}\mathbf{T}^\dagger(t, t_0) = -\mathbf{T}^\dagger(t, t_0)\mathbf{H}(t) \qquad \#$$

$$\mathbf{T}^\dagger(t_0, t_0) = 1 \qquad \#$$

I have assumed here that the Hamiltonian is Hermitian, which is usually the case. (Sometimes the Hamiltonian is allowed to be non-Hermitian to represent dissapative systems. When it corresponds to the energy operator of a system, the Hamiltonian is always Hermitian.) Notice that

$$\frac{d}{dt}[\mathbf{T}^\dagger(t, t_0)\mathbf{T}(t, t_0)] = \frac{1}{i\hbar}[-\mathbf{T}^\dagger(t, t_0)\mathbf{H}(t)\mathbf{T}(t, t_0) + \mathbf{T}^\dagger(t, t_0)\mathbf{H}(t)\mathbf{T}(t, t_0)] = 0 \qquad \#$$

which together with the initial conditions implies:

$$\mathbf{T}^\dagger(t, t_0)\mathbf{T}(t, t_0) = \mathbf{1} \qquad \#$$

$$\mathbf{T}^\dagger(t, t_0) = \mathbf{T}^{-1}(t, t_0) = \mathbf{T}(t_0, t) \qquad \#$$

i.e. the time evolution operator is unitary.

Solving for quantum evolution can be reduced to solving the following integral equation:

$$\mathbf{T}(t, t_0) = \mathbf{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt' \mathbf{H}(t')\mathbf{T}(t', t_0) \qquad \#$$

A formal solution to this equation can be constructed by iteration of this equation (starting with $\mathbf{T}^0(t, t_0) = \mathbf{1}$), giving:

$$\mathbf{T}(t, t_0) = \mathbf{1} + \sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n \mathbf{H}(t_1)\ldots\mathbf{H}(t_n) \qquad \#$$

which is known as the Dyson series. One can check that this is indeed a formal solution by simply plugging it back into the integral equation (and renaming the dummy indices: $t' \to t_1$

and $t_n \to t_{n+1}$). The reason for making a distiction between "solution" and "formal solution" is that even though the Dyson series satisfies the integral equation, it must also be a convergent sum (which it is not guaranteed) in order to be considered a well-defined solution.

We can write this in a cleaner looking form by introducing the time-ordered product of operators. For two time-dependant operators $\mathbf{L}_1(t), \mathbf{L}_2(t)$ we define the time ordering as:

$$T\{\mathbf{L}_1(t)\mathbf{L}_2(t')\} = \begin{cases} \mathbf{L}_1(t)\mathbf{L}_2(t') & \text{if } t > t' \\ \mathbf{L}_2(t')\mathbf{L}_1(t) & \text{if } t' > t \end{cases} \qquad \#$$

$$= \theta(t - t')\mathbf{L}_1(t)\mathbf{L}_2(t') + \theta(t' - t)\mathbf{L}_2(t')\mathbf{L}_1(t) \qquad \#$$

where the step function: $\theta(t_i - t_j) = \begin{cases} 1 & \text{for } t_i > t_j \\ 0 & \text{for } t_i < t_j \end{cases}$. The generalization for more than two operators should be clear:

$$T\left\{\prod_{i=1}^{n} \mathbf{L}_i(t_i)\right\} = T\{\mathbf{L}_1(t_1)\dots\mathbf{L}_n(t_n)\}$$

$$= \sum_{\sigma \in S_n} \theta(t_{\sigma(1)} - t_{\sigma(2)})\dots\theta(t_{\sigma(n-1)} - t_{\sigma(n)})\mathbf{L}_1(t_{\sigma(1)})\dots\mathbf{L}_n(t_{\sigma(n)})$$

$$= \sum_{\sigma \in S_n}\left(\prod_{i=1}^{n-1} \theta(t_{\sigma(i)} - t_{\sigma(i+1)}) \prod_{i=1}^{n} \mathbf{L}_i(t_{\sigma(i)})\right)$$

Where the summation is over S_n the permutation group of n objects. (Note that there are $n!$ elements σ in S_n; i.e. there are $n!$ different ways to interchange n objects). This gives:

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \dots \int_{t_0}^{t} dt_n T\{\mathbf{H}(t_1)\dots\mathbf{H}(t_n)\}$$

$$= \sum_{\sigma \in S_n}\left(\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \dots \int_{t_0}^{t} dt_n \left(\prod_{i=1}^{n-1} \theta(t_{\sigma(i)} - t_{\sigma(i+1)}) \prod_{i=1}^{n} \mathbf{H}(t_{\sigma(i)})\right)\right)$$

$$= \sum_{\sigma \in S_n}\left(\int_{t_0}^{t} d(t_{\sigma^{-1}(1)}) \int_{t_0}^{t} d(t_{\sigma^{-1}(2)}) \dots \int_{t_0}^{t} d(t_{\sigma^{-1}(n)}) \left(\prod_{i=1}^{n-1} \theta(t_i - t_{i+1}) \prod_{i=1}^{n} \mathbf{H}(t_i)\right)\right)$$

$$= \sum_{\sigma \in S_n}\left(\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \dots \int_{t_0}^{t} dt_n \left(\prod_{i=1}^{n-1} \theta(t_i - t_{i+1}) \prod_{i=1}^{n} \mathbf{H}(t_i)\right)\right)$$

$$= \sum_{\sigma \in S_n}\left(\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \mathbf{H}(t_1)\dots\mathbf{H}(t_n)\right)$$

$$= n!\left(\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \mathbf{H}(t_1)\dots\mathbf{H}(t_n)\right)$$

which lets us write the time evolution operator as:

$$\mathbf{T}(t, t_0) = \mathbf{1} + \sum_{n=1}^{\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \dots \int_{t_0}^{t} dt_n T\{\mathbf{H}(t_1)\dots\mathbf{H}(t_n)\} \qquad \#$$

$$= T\left\{\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \mathbf{H}(t')\right]\right\} \qquad \#$$

Now we can easily deal with special cases. When the Hamiltonian commutes with itself at different times, we can simply ignore the time-ordering and write the solution of the time evolution operator as:

$$\mathbf{T}(t, t_0) = \exp\left[-\frac{i}{\hbar} \int_{t_0}^{t} dt' \mathbf{H}(t') \right] \qquad \#$$

and when the Hamiltonian is independent of time, we can perform the integral explicitly for all t and write the evolution operator as:

$$\mathbf{T}(t, t_0) = \exp\left[-\frac{i\mathbf{H}}{\hbar} (t - t_0) \right] \qquad \#$$

Since quantum states are not physically observable objects, it should be conceivable that transformations on the vector space that change the states but leaves certain other properties intact would produce an equally valid formulation for quantum mechanics. Indeed, this is the case, and the properties that need to remain unchanged are the following:
1) the eigenvalue spectra of observable operators
2) the inner products between physical states and (transformed) eigenvectors corresponding to the (original) eigenvalues
Notice that the conservation of these two properties implies that expectation values also remain unchanged by the transformation.
A special class of transformations for which these conditions are inherently satified are the unitary transformations:

$$|\Psi(t)\rangle \rightarrow \mathbf{U}|\Psi(t)\rangle = |\Psi'(t)\rangle \qquad \#$$

$$\langle\Psi(t)| \rightarrow \langle\Psi(t)|\mathbf{U}^\dagger = \langle\Psi(t)|\mathbf{U}^{-1} = \langle\Psi'(t)| \qquad \#$$

$$\mathbf{L}(t) \rightarrow \mathbf{U}\mathbf{L}(t)\mathbf{U}^\dagger = \mathbf{U}\mathbf{L}(t)\mathbf{U}^{-1} = \mathbf{L}'(t) \qquad \#$$

where $\mathbf{U}$ is a unitary operator (i.e. $\mathbf{U}^{-1} = \mathbf{U}^\dagger$), and $\mathbf{L}(t)$ is an arbitrary operator for the system. It is easy to check that the two conditions are preserved:

$$\mathbf{L}'(t)|\lambda_\mathbf{L}'\rangle = \mathbf{U}\mathbf{L}(t)\mathbf{U}^{-1}\mathbf{U}|\lambda_\mathbf{L}\rangle = \mathbf{U}\mathbf{L}(t)|\lambda_\mathbf{L}\rangle = \mathbf{U}\lambda_\mathbf{L}|\lambda_\mathbf{L}\rangle = \lambda_\mathbf{L}\mathbf{U}|\lambda_\mathbf{L}\rangle = \lambda_\mathbf{L}|\lambda_\mathbf{L}'\rangle \qquad \#$$

$$\langle\lambda_\mathbf{L}'|\Psi'(t)\rangle = \langle\lambda_\mathbf{L}|\mathbf{U}^{-1}\mathbf{U}|\Psi(t)\rangle = \langle\lambda_\mathbf{L}|\Psi(t)\rangle \qquad \#$$

The three pictures of quantum dynamics are the Schrödinger picture, the Heisenberg picture, and the Interaction picture (also called the Dirac picture). They are all equivalent vector space formulations of quantum mechanics, based on different "pictures" of how the system is evolving in time, each having its own insights and areas of preferred application. This might lead you to guess (correctly) that these pictures are somehow related to each other through the evolution equations, and that the transformations between the pictures are related to time evolution operators and so would be unitary transformations. I will follow Merzbacher's convention and distinguish the states and operators in the Heisenberg picture by putting a bar over them, and those in the Interaction picture by putting a tilda over them. (States and operators in the Schrödinger picture will be unaltered.) Another common convention is adding a subscript or superscript S, H, or I for states and operators in the Schrödinger, Heisenberg, or Interaction picture respectively. The Schrödinger picture is the

formulation that you are already familiar with, and needs no additional explanation. Since the Heisenberg picture can be thought of as a specific case of the Interaction picture, I will first introduce the Interaction picture.

The Interaction Picture

For the Interaction picture, we begin by splitting the Hamiltonian in to two parts, the model Hamiltonian $\mathbf{H}_0$ and the interaction term $\mathbf{V}$.

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{V} \qquad \#$$

There is no restriction on how the partition of the Hamiltonian must be chosen (except that the two parts should individually be Hermitian), but some choices may largely simplify solving the time evolution. Let the unitary transformation be given by:

$$\mathbf{U}(t) = \mathbf{T}_0(0,t) \qquad \#$$

where $\mathbf{T}_0(0,t)$ satifies the differential equation and initial condition:

$$i\hbar \frac{d}{dt}\mathbf{T}_0(0,t) = -\mathbf{T}_0(0,t)\mathbf{H}_0(t) \qquad \#$$

$$\mathbf{T}_0(0,0) = 1 \qquad \#$$

(i.e. $\mathbf{T}_0$ is the time evolution operator of a Hamiltonian $\mathbf{H}_0(t)$).

Then the states and operators in the Interaction picture are related to the states and operators in the Schrödinger picture as follows:

$$\left|\widetilde{\Psi}(t)\right\rangle = \mathbf{U}(t)|\Psi(t)\rangle \qquad \#$$

$$\widetilde{\mathbf{L}}(t) = \mathbf{U}(t)\mathbf{L}(t)\mathbf{U}^\dagger(t) \qquad \#$$

The first consequence of this transformation is that the operators in the Interaction picture satisfy the equation of motion:

$$i\hbar\frac{d}{dt}\widetilde{\mathbf{L}}(t) = i\hbar\frac{d}{dt}[\mathbf{U}(t)\mathbf{L}(t)\mathbf{U}^\dagger(t)] \qquad \#$$

$$= -\mathbf{U}(t)\mathbf{H}_0(t)\mathbf{L}(t)\mathbf{U}^\dagger(t) + i\hbar\mathbf{U}(t)\frac{d\mathbf{L}(t)}{dt}\mathbf{U}^\dagger(t) + \mathbf{U}(t)\mathbf{L}(t)\mathbf{H}_0(t)\mathbf{U}^\dagger(t) \qquad \#$$

$$= -\widetilde{\mathbf{H}}_0(t)\widetilde{\mathbf{L}}(t) + i\hbar\mathbf{U}(t)\frac{\partial\mathbf{L}(t)}{\partial t}\mathbf{U}^\dagger(t) + \widetilde{\mathbf{L}}(t)\widetilde{\mathbf{H}}_0(t) \qquad \#$$

$$= \left[\widetilde{\mathbf{L}}(t),\widetilde{\mathbf{H}}_0(t)\right] + i\hbar\frac{\partial\widetilde{\mathbf{L}}(t)}{\partial t} \qquad \#$$

where $\frac{\partial\widetilde{\mathbf{L}}(t)}{\partial t} = \widetilde{\frac{\partial\mathbf{L}(t)}{\partial t}}$ and the states in the Interaction picture satify the equation of motion:

$$i\hbar\frac{d}{dt}\left|\widetilde{\Psi}(t)\right\rangle = i\hbar\frac{d}{dt}[\mathbf{U}(t)|\Psi(t)\rangle] \qquad \#$$

$$= -\mathbf{U}(t)\mathbf{H}_0(t)|\Psi(t)\rangle + \mathbf{U}(t)\mathbf{H}(t)|\Psi(t)\rangle \qquad \#$$

$$= \mathbf{U}(t)\mathbf{V}(t)|\Psi(t)\rangle \qquad \#$$

$$= \widetilde{\mathbf{V}}(t)\left|\widetilde{\Psi}(t)\right\rangle \qquad \#$$

It follows that the time evolution operator in the Interaction picture satisfies the differential equation and initial condition:

$$ih\frac{d}{dt}\widetilde{\mathbf{T}}(t,t_0) = \widetilde{\mathbf{V}}(t)\widetilde{\mathbf{T}}(t,t_0) \qquad \#$$

$$\widetilde{\mathbf{T}}(t_0,t_0) = 1 \qquad \#$$

for which we can apply the methods of solving the Schrödinger equation presented in the first section. However, we must be careful when applying the transformation to the time evolution operator. Since it can be dependent on two times (unless one is set at zero), the time evolution operator in the Interaction picture is given by the transformation:

$$\widetilde{\mathbf{T}}(t_2,t_1) = \mathbf{U}(t_2)\mathbf{T}(t_2,t_1)\mathbf{U}^\dagger(t_1) \qquad \#$$

Now we can address the question of how to partition the original Hamiltonian. An obvious choice is to pick $\mathbf{H}_0$ as the part of the Hamiltonian that corresponds to a system that we already know how to evolve, and then $\mathbf{V}$ represents a sort of interaction within this system (hence the name). This is particularly useful when it leaves the interaction term $\mathbf{V}$ as being small enough so that when using the Dyson series:

$$\widetilde{\mathbf{T}}(t,t_0) = \mathbf{1} + \sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n \widetilde{\mathbf{V}}(t_1)\ldots\widetilde{\mathbf{V}}(t_n) \qquad \#$$

the first few terms will give a good approximation to the solution. This method is one of the approachs used to solve problems in quantum field theory for example. You will later (3rd term) see another application of this is found in time-dependent perturbation theory, for which the approximation:

$$\widetilde{\mathbf{T}}(t,t_0) \approx \mathbf{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt' \widetilde{\mathbf{V}}(t')$$

is used to find transition probabilities between energy eigenstates of $\mathbf{H}_0$.

Of course, there are systems for which picking $\mathbf{H}_0$ as the entire familiar part of the Hamiltonian is not the best choice. In the 11/21/01 and 12/3/01 lectures, we had the Hamiltonian:

$$\mathbf{H}(t) = -\gamma[B_0\mathbf{S}_z + b_1(\cos(\omega t)\mathbf{S}_x + \sin(\omega t)\mathbf{S}_y)] \qquad \#$$

$$= \frac{\hbar}{2}[\omega_L\boldsymbol{\sigma}_z - \gamma b_1(\cos(\omega t)\boldsymbol{\sigma}_x + \sin(\omega t)\boldsymbol{\sigma}_y)] \qquad \#$$

If we pick

$$\mathbf{H}_0 = \frac{\hbar\omega_L}{2}\boldsymbol{\sigma}_z \qquad \#$$

$$\mathbf{V}(t) = -\frac{\hbar\gamma b_1}{2}[(\cos(\omega t)\boldsymbol{\sigma}_x + \sin(\omega t)\boldsymbol{\sigma}_y)] = -\frac{\hbar\gamma b_1}{2}\begin{pmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{pmatrix} \qquad \#$$

$$\mathbf{U}(t) = \exp\left[i\frac{\hbar\omega_L}{2}\boldsymbol{\sigma}_z t\right] = \begin{pmatrix} e^{i\hbar\omega_L t/2} & 0 \\ 0 & e^{-i\hbar\omega_L t/2} \end{pmatrix} \qquad \#$$

then we get an interaction term in the Interaction picture given by:

$$\widetilde{\mathbf{V}}(t) = -\frac{\hbar\gamma b_1}{2}\begin{pmatrix} 0 & e^{-i(\omega-\omega_L)t} \\ e^{i(\omega-\omega_L)t} & 0 \end{pmatrix} \qquad \#$$

which does not even commute with itself at different times (i.e. the worst case to solve). Instead, if we pick:

$$\mathbf{H}_0 = \frac{\hbar\omega}{2}\boldsymbol{\sigma}_z \qquad \#$$

$$\mathbf{V}(t) = \frac{\hbar}{2}[(\omega_L - \omega)\boldsymbol{\sigma}_z - \gamma b_1(\cos(\omega t)\boldsymbol{\sigma}_x + \sin(\omega t)\boldsymbol{\sigma}_y)] \qquad \#$$

$$\mathbf{U}(t) = \exp\left[i\frac{\hbar\omega}{2}\boldsymbol{\sigma}_z t\right] = \begin{pmatrix} e^{i\hbar\omega t/2} & 0 \\ 0 & e^{-i\hbar\omega t/2} \end{pmatrix} \qquad \#$$

it looks messy at first, but we get an interaction term that is constant in the Interaction picture:

$$\widetilde{\mathbf{V}} = \frac{\hbar}{2}[(\omega_L - \omega)\boldsymbol{\sigma}_z - \gamma b_1\boldsymbol{\sigma}_x] = \frac{\hbar}{2}\begin{pmatrix} (\omega_L - \omega) & -\gamma b_1 \\ -\gamma b_1 & -(\omega_L - \omega) \end{pmatrix} \qquad \#$$

which is the easiest case to solve for time evolution (i.e. exponentiate a diagonalizable 2x2 matrix). This particular transformation is exactly what was carried out in those two lectures when we applied the transformation to the rotating frame. To make this claim explicitly clear, the translation between the notation used in those lectures and the notation used here is given by: $\mathbf{O}_z \leftrightarrow \mathbf{U}(t), |\Psi'(t)\rangle \leftrightarrow \left|\widetilde{\Psi}(t)\right\rangle, \mathbf{H}' \leftrightarrow \widetilde{\mathbf{V}}$

The Heisenberg Picture

Obviously, the special case of the Interaction picture where we pick $\mathbf{H}_0 = 0$ simply returns the Schrödinger picture. On the other extreme, when $\mathbf{H}_0 = \mathbf{H}$ we get what is known as the Heisenberg picture. Repeating the above steps with:

$$\mathbf{U}(t) = \mathbf{T}(0,t) \qquad \#$$

we get the results:

$$|\overline{\Psi}(t)\rangle = \mathbf{U}(t)|\Psi(t)\rangle = |\Psi(0)\rangle \qquad \#$$

$$i\hbar\frac{d}{dt}\overline{\mathbf{L}}(t) = \left[\overline{\mathbf{L}}(t), \overline{\mathbf{H}}(t)\right] + i\hbar\frac{\partial\overline{\mathbf{L}}(t)}{\partial t} \qquad \#$$

(remember the bar indicates being in the Heisenberg picture). Hence, the special aspect of the Heisenberg picture is that the states themselves do not evolve in time; all the time evolution is carried out in the operators. This makes the Heisenberg picture particularly useful when dealing with constants of motion.

Of important significance is the correlation between "dynamical variables" in classical mechanics and in the Heisenberg picture of quantum mechanics. In particular, for any dynamical variable

$$\overline{\mathbf{F}}(\overline{\mathbf{q}}, \overline{\mathbf{p}}, t) \equiv F(\overline{\mathbf{q}}(t), \overline{\mathbf{p}}(t), t) \qquad \#$$

(where the non-bold $F(q,p,t)$ is a classical function of the canonical variables and time). Comparing the quantum evolution:

$$\frac{d}{dt}\overline{\mathbf{F}}(\overline{\mathbf{q}},\overline{\mathbf{p}},t) = \frac{1}{i\hbar}\left[\overline{\mathbf{F}}(\overline{\mathbf{q}},\overline{\mathbf{p}},t),\overline{\mathbf{H}}(t)\right] + \frac{\partial\overline{\mathbf{F}}(\overline{\mathbf{q}},\overline{\mathbf{p}},t)}{\partial t} \qquad \#$$

to the analogous classical equation of motion:

$$\frac{d}{dt}F(q,p,t) = [F(q,p,t),H(t)]_{P.B.} + \frac{\partial F(q,p,t)}{\partial t} \qquad \#$$

where Poisson brackets are defined as

$$[u,v]_{P.B.} = \sum_i \frac{\partial u}{\partial q_i}\frac{\partial v}{\partial p_i} - \frac{\partial v}{\partial q_i}\frac{\partial u}{\partial p_i} \qquad \#$$

led Dirac to discover the correspondence between the Poisson brackets in classical mechanics and the commutator in quantum mechanics:

$$[F,G]_{P.B.} \rightarrow \frac{1}{i\hbar}\left[\overline{\mathbf{F}},\overline{\mathbf{G}}\right] \qquad \#$$

(There are some subtleties involved in this correspondence concerning ordering of non-commuting operators, but I will not get into that here.)