

Time evolution in quantum mechanics

Having focused in the first part of this term on measurement and the representation of states, it's now time to move on to *dynamics*. In fact, the *physical* principles of quantum dynamics are much simpler than those of representation and measurement. But it can take a fair bit of mathematical sophistication to solve the dynamical equations and interpret the results.

Recall that the evolution of an isolated quantum system is given by the Schrödinger Equation (SE),

$$i\hbar \frac{d}{dt} |\Psi\rangle = \mathbf{H} |\Psi\rangle, \quad 1$$

where \mathbf{H} is the system's 'Hamiltonian' operator (observable).

If we fix a basis for the relevant Hilbert space, we can switch from Dirac notation to a vector/matrix representation of the SE. In three dimensions, for example,

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} H_{00} & H_{01} & H_{02} \\ H_{10} & H_{11} & H_{12} \\ H_{20} & H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \end{pmatrix}. \quad 2$$

Hence we recognize that the SE has the form of a *coupled* set of *linear* differential equations in the coefficients c_i . As you should know from elementary linear algebra (and as we shall review below), the eigenspectrum and eigenstates of \mathbf{H} are thus of central importance in understanding time-evolution in quantum mechanics.

Energy eigenstates and the Schrödinger Equation

Suppose we have an N_A -dimensional quantum system H_A with Hamiltonian \mathbf{H} . Since \mathbf{H} is an observable, and therefore a normal operator, there exists a complete orthonormal basis for H_A corresponding to eigenkets of \mathbf{H} :

$$\begin{aligned} \mathbf{H} |j\rangle &= \epsilon_j |j\rangle, \\ \sum_{j=0}^{N_A-1} |j\rangle \langle j| &= \mathbf{1}^A. \end{aligned} \quad 3$$

As the Hamiltonian observable corresponds physically to a system's energy, the $\{|j\rangle\}$ basis is often referred to as the 'energy eigenbasis' or simply the 'energy basis.' Also, the expectation value $\langle \mathbf{H} \rangle$ is usually called the energy of a quantum system (in some given state).

The time-evolution of arbitrary system states $|\Psi\rangle \in H_A$ can easily be computed in the energy basis:

$$\begin{aligned}
 |\Psi(t)\rangle &= \sum_{j=0}^{N_A-1} c_j(t)|j\rangle, \\
 i\hbar \frac{d}{dt} \sum_{j=0}^{N_A-1} c_j(t)|j\rangle &= \mathbf{H} \sum_{j=0}^{N_A-1} c_j(t)|j\rangle \\
 &= \sum_{j=0}^{N_A-1} \epsilon_j c_j(t)|j\rangle.
 \end{aligned} \tag{4}$$

Equating coefficients of $|j\rangle$,

$$i\hbar \frac{d}{dt} c_j(t) = \epsilon_j c_j(t), \tag{5}$$

where the $c_j(t)$ can now be thought of as simple functions of time. Hence,

$$\begin{aligned}
 \frac{dc_j}{c_j} &= -\left(\frac{i\epsilon_j}{\hbar}\right) dt, \\
 \ln \frac{c_j(t)}{c_j(0)} &= -\left(\frac{i\epsilon_j}{\hbar}\right) t \\
 c_j(t) &= c_j(0) \exp[-i\epsilon_j t/\hbar].
 \end{aligned} \tag{6}$$

A quick word about units – since \mathbf{H} is the energy observable its eigenvalues ϵ_j have units of energy, and \hbar has units of [energy×time]. Hence ϵ_j/\hbar is an angular frequency, and we see that the evolution of the coefficients $c_j(t)$ correspond to simple **oscillations in phase**. Hence, quantum dynamics is pretty trivial when viewed in the energy eigenbasis!

Putting it all back together for our arbitrary state $|\Psi\rangle$, if

$$|\Psi(0)\rangle = \sum_{j=0}^{N_A-1} c_j(0)|j\rangle, \tag{7}$$

then

$$|\Psi(t)\rangle = \sum_{j=0}^{N_A-1} c_j(0) \exp(-i\epsilon_j t/\hbar) |j\rangle. \tag{8}$$

Let us not miss the relation of this simple form to the unitary structure of quantum time-evolution. Earlier in the course we derived the time-development operator

$$\begin{aligned}
 \mathbf{T}(t,0) &= \exp\left(-\frac{i\mathbf{H}t}{\hbar}\right), \\
 |\Psi(t)\rangle &= \mathbf{T}(t,0)|\Psi(0)\rangle,
 \end{aligned} \tag{9}$$

where unitarity of $\mathbf{T}(t,0)$ follows from Hermiticity of \mathbf{H} . The energy eigenstates $|j\rangle$ are also eigenstates of $\mathbf{T}(t,0)$ (as we'll see in a minute), but we know that the eigenvalues of a unitary operator must be unimodular. We can simply compute

$$\begin{aligned}
\mathbf{T}(t,0)|j\rangle &= \exp\left(-\frac{i\mathbf{H}t}{\hbar}\right)|j\rangle \\
&= \sum_{k=0}^{\infty} \frac{1}{k!} \left(-\frac{i\mathbf{H}t}{\hbar}\right)^k |j\rangle \\
&= \sum_{k=0}^{\infty} \frac{1}{k!} \left(-\frac{i\epsilon_j t}{\hbar}\right)^k |j\rangle \\
&= \exp(-i\epsilon_j t/\hbar) |j\rangle,
\end{aligned}
\tag{10}$$

and certainly $|\exp(-i\epsilon_j t/\hbar)| = 1$. Hence the simplicity of the oscillating phase factors we get by integrating the Schrödinger Equation in the energy basis is a direct reflection of the fact that quantum evolution for isolated systems corresponds to unitary rotation in Hilbert space.

Some things to note about the Schrödinger Equation (SE):

1. If $c_j(0) = 0$, then $c_j(t) = 0$ – the **support** of a state does not change under Hamiltonian evolution (energy eigenstates $|j\rangle$ that do not appear in the expansion of $|\Psi(0)\rangle$ never appear in $|\Psi(t)\rangle$ either).
2. In particular, if $|\Psi(0)\rangle = |j\rangle$ then $|\Psi(t)\rangle \propto |j\rangle$. For an isolated system we won't care about the overall phase of the wavefunction, so a system initially prepared in an energy eigenstate essentially 'doesn't evolve' under the SE. This is why these are often referred to as **stationary states** of the SE.
3. We already know that quantum evolution preserves inner products because it is unitary, but it is nice to see this explicitly in the energy basis as well:

$$\begin{aligned}
|\Psi_c(t)\rangle &= \sum_j c_j(0) \exp(-i\epsilon_j t/\hbar) |j\rangle, \\
|\Psi_d(t)\rangle &= \sum_k d_k(0) \exp(-i\epsilon_k t/\hbar) |k\rangle, \\
\langle \Psi_d(t) | \Psi_c(t) \rangle &= \sum_{j,k} d_k^*(0) c_j(0) \exp(-i(\epsilon_j - \epsilon_k)t/\hbar) \langle k | j \rangle \\
&= \sum_j d_j^*(0) c_j(0) \\
&= \langle \Psi_d(0) | \Psi_c(0) \rangle.
\end{aligned}
\tag{11}$$

4. Even though the phase oscillations are simple, they're not completely trivial. Say we have a system with initial state

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \tag{12}$$

where $\mathbf{H}|0\rangle = \epsilon_0|0\rangle$ and $\mathbf{H}|1\rangle = \epsilon_1|1\rangle$. Then

$$|\Psi(t)\rangle \propto \frac{1}{\sqrt{2}}(|0\rangle + \exp(-i(\epsilon_1 - \epsilon_0)t/\hbar)|1\rangle), \tag{13}$$

so as long as $\epsilon_1 \neq \epsilon_0$ there will come a time $t' = \left| \frac{\hbar\pi}{\epsilon_1 - \epsilon_0} \right|$ at which $\exp(-i(\epsilon_1 - \epsilon_0)t'/\hbar) = -1$, i.e., $\langle \Psi(t') | \Psi(0) \rangle = 0$. Hence we see that what evolves nontrivially are the **interferences** between different energy eigenstates.

As a further illustration of the last point, note that *operator moments* can evolve in complex ways under the SE. In general,

$$\begin{aligned}\langle \mathbf{O}_q^m \rangle &= \langle \Psi(t) | \mathbf{O}_q^m | \Psi(t) \rangle \\ &= \sum_{jk} c_j^*(0) c_k(0) \exp(-i(\epsilon_k - \epsilon_j)t/\hbar) \langle j | \mathbf{O}_q^m | k \rangle,\end{aligned}\tag{14}$$

so $\langle \mathbf{O}_q^m \rangle$, as a function of time, appears as a Fourier series with possible components at each of the system's 'Bohr frequencies' $\omega_{jk} \equiv (\epsilon_k - \epsilon_j)/\hbar$. The coefficients in the series are determined by the matrix elements of \mathbf{O}_q^m in the energy basis, and by the initial state of the system.

For example, say we have a three-level system with given orthonormal basis $\{|0\rangle, |1\rangle, |2\rangle\}$ and Hamiltonian operator

$$\mathbf{H} = \hbar\Omega(|1\rangle\langle 1| + 2|2\rangle\langle 2|).\tag{15}$$

The energy eigenvalues are clearly 0, $\hbar\Omega$, and $2\hbar\Omega$, so the Bohr frequencies will be limited to Ω and 2Ω . If we consider the evolving state

$$|\Psi(t)\rangle = \frac{1}{\sqrt{3}}(|0\rangle + \exp(-i\Omega t)|1\rangle + \exp(-2i\Omega t)|2\rangle)\tag{16}$$

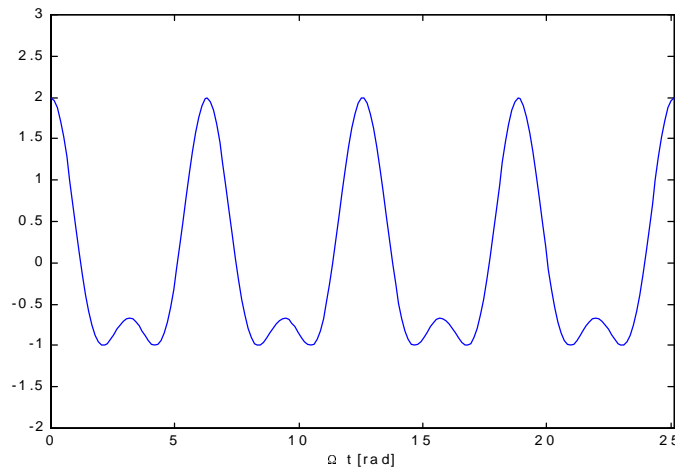
and the observable

$$\mathbf{O}_q = |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 2| + |2\rangle\langle 1| + |0\rangle\langle 2| + |2\rangle\langle 0|,\tag{17}$$

then

$$\begin{aligned}\langle \mathbf{O}_q \rangle &= \frac{1}{3} \left[\begin{array}{c} \exp(-i\Omega t) + \exp(i\Omega t) \\ + \exp(i\Omega t) \exp(-2i\Omega t) + \exp(2i\Omega t) \exp(-i\Omega t) \\ + \exp(-2i\Omega t) + \exp(2i\Omega t) \end{array} \right] \\ &= \frac{2}{3} \cos(\Omega t) + \frac{2}{3} \cos(\Omega t) + \frac{2}{3} \cos(2\Omega t) \\ &= \frac{4}{3} \cos(\Omega t) + \frac{2}{3} \cos(2\Omega t).\end{aligned}\tag{18}$$

Plotting this, we clearly see the influence of the discrete energy eigenspectrum:



Recall that if we have a state $|\Psi(0)\rangle$ expressed as a vector with respect to some arbitrary basis for H_A , and that if we also know the vector representation of the energy eigenstates $|j\rangle$ in this basis, we can easily determine the expansion coefficients according to

$$c_j(0) = \langle j | \Psi(0) \rangle. \quad 19$$

So at some level, ‘solving’ quantum dynamics pretty much boils down to finding the eigenvalues and eigenstates of the Hamiltonian operator! We shall soon see how this approach helps us understand some universal features of two-level quantum systems.

Unfortunately, for the vast majority of interesting physical systems the Hamiltonian operator is too complex to diagonalize explicitly. Hence the utility of approximation methods, many of which we will study in the coming weeks.

A brief digression: open quantum systems

Suppose we have a composite system $H_{AB} = H_A \otimes H_B$ with Hamiltonian \mathbf{H}_{AB} . We know that the overall dynamics is described by the SE

$$i\hbar |\dot{\Psi}_{AB}(t)\rangle = \mathbf{H}_{AB} |\Psi_{AB}(t)\rangle. \quad 20$$

Let’s say, however, that H_A corresponds to a small, ‘compact’ physical system that we are trying to study in the lab, whereas H_B actually represents the degrees of freedom of some environmental reservoir. If we are unable (as is always the case) to completely isolate the system from the environment, then the Hamiltonian will not be factorizable: $\mathbf{H}_{AB} \neq \mathbf{H}_A \otimes \mathbf{H}_B$. Hence, even for pure initial states of the system $|\Psi_A(0)\rangle \in H_A$, the above SE **may** (for some initial states) induce evolution into *entangled* states of the system and environment.

In general we will be unable to perform complete measurements on the joint Hilbert space H_{AB} , because reservoirs are usually infinite-dimensional (hence H_{AB} will be also). So limiting our attention to the system H_A , it appears that we must settle for a density-operator description obtained by tracing over the environmental degrees of freedom:

$$\tilde{\rho}_A(t) = \text{Tr}_B[|\Psi_{AB}(t)\rangle\langle\Psi_{AB}(t)|]. \quad 21$$

From what we have learned about entanglement in previous lectures, we may expect that this type of evolution (formation of entanglements with an unobservable reservoir) will lead to loss of *purity* for the system state. Such phenomena are generally referred to as ‘decoherence.’

Under certain assumptions about the nature of \mathbf{H}_{AB} and of the environment H_B , it is sometimes possible to derive a closed-form evolution equation for the reduced density operator $\tilde{\rho}_A(t)$. In a ‘Master Equation’ of this type, operators and states for H_B do not appear explicitly because they have been analytically traced-out of the equations of motion. This type of approach is particularly useful for understanding things like dissipation and thermal fluctuations in a quantum-mechanical setting, and the overall field of studying these things has come to be known as the theory of open quantum systems.

As we’ll see in the third term, there are very important connections between measurement and dissipation/decoherence. In a sense, these are the dynamical extension of certain well-known connections between information and entropy in thermodynamics. But a detailed investigation of these things will have to wait – at some point next week however we’ll have a look at our first example of a genuine Master Equation, known as the Bloch

Equations for an ensemble of two-level quantum systems.