Notes for Lecture 12

Prelude to the time-dependent perturbation theory

We begin discussing the two-level problem, before discussing the time-*dependent* perturbation theory. But first, let us ask ourselves the question – why do we need to consider a time-dependent Hamiltonian? It is because basically no system that we are interested in is a really closed system. Practically everything that we study is a system that evolves in time in an interesting way because it interacts with the environment. So, it is essential to consider a time-dependent Hamiltonian.

12.1 Prelude to the two level problem

Below, we will be dealing with a two level problem. Let me say a few words about the generic nature of this problem first. What we are considering is a **quantum mechanical two level system**.

What is a quantum mechanical two level system? An atom can be considered as a two level system, if certain two atomic energy levels are important to consider for a certain type of physics. Is Schrödinger's cat a quantum mechanical two level system? No. Is life and death a quantum mechanical two level system? No. Macroscopic objects in everyday condition are "too noisy" to be describable neatly by two quantum mechanical states. While there is no question that at the base of everything there is quantum mechanics, it does not mean that everything is described by a single wave function that evolves in time in a coherent manner.

However, one can make a special device that involves a macroscopic amount of particles but whose spectrum is discrete enough so that at very low temperature it can be described by a two level quantum mechanics. An example would be a superconducting current loop in a ring. By flux quantization, the current is quantized. However, it can flow in one of the two directions (clockwise or anti-clockwise), defining two discrete quantum states. Researchers have succeeded in creating a state in which the current flows in a superposition of currents in opposite directions. It has been suggested that this current loop can be used as a basis for a quantum computer. This kind of thing is what is closest to what is commonly referred to as the "Schrödinger's cat," but notice that it requires a certain special condition that includes a very low temperature.

Please do not think that literally the life and the death (or "youth" and "age") are describable in the mathematics that we will develop here, while for making certain points it may be useful.

12.2 Two level problem

Let us consider a total Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t) \tag{12.1}$$

where $\hat{H}_1(t)$ represents a coupling between the system ($\hat{H}_0$) and an external agent, and $\hat{H}_0$ is assumed to be time-independent ($\frac{\partial \hat{H}_0}{\partial t} = 0$). The assumption here is that, without $\hat{H}_1$, the system is a closed system. The external agent can be a stream of photons, for example, and $\hat{H}_0$ can represent the Hamiltonian for an atom that interacts with the stream of photons. Lastly, $\hat{H}_1$ generally depends on $\hat{x}$, $\hat{p}$, etc., but this dependence is omitted above, for brevity.

The simplest model to consider is a two level problem, so we shall do that here. Namely, the effective dimension of the Hilbert space is two. This bare bone model retains essential physics for many important problems. Also, you may see that the discussion in this section can be easily generalized to multiple levels, if necessary. Dealing with a two level problem first is a good step towards such a generalization, which we will have to consider later on.

Consider $|0\rangle$ and $|1\rangle$, two eigenstates of $\hat{H}_0$. Their $\hat{H}_0$ eigenvalues are $E_0 \equiv \hbar\omega_0$ and $E_1 \equiv \hbar\omega_1$.

$$\hat{H}_0 |0\rangle = E_0 |0\rangle = \hbar\omega_0 |0\rangle \tag{12.2}$$

$$\hat{H}_0 |1\rangle = E_1 |1\rangle = \hbar\omega_1 |1\rangle \tag{12.3}$$

We shall assume that $E_1 \geq E_0$, while assuming discrete energy spectra[1], so that the states are normalizable to norm 1 (not to a Dirac delta function infinity): $\langle 0 | 0 \rangle = \langle 1 | 1 \rangle = 1$. We define

$$\omega_{1,0} \equiv \omega_N \equiv \omega_1 - \omega_0 \geq 0 \tag{12.4}$$

This corresponds to the "natural frequency" of the system.

We seek the solution of the full Schrödinger equation:

$$\hat{H} |\Psi\rangle = i\hbar \frac{d}{dt} |\Psi\rangle \tag{12.5}$$

Looking ahead to the perturbation, we fashion our solution in the following way.

First, let us note that the general solution for $|\Psi\rangle$ *without* $\hat{H}_1(t)$ is given by:

$$|\Psi(t)\rangle = C_0 e^{-i\omega_0 t} |0\rangle + C_1 e^{-i\omega_1 t} |1\rangle \tag{12.6}$$

where C_0 and C_1 are time-independent constants.

Let us re-call where this important and basic result comes from. (1) $\hat{H}_0$ is an observable and so it spans the entire Hilbert space. (2) Therefore, $|\Psi(t=0)\rangle$ can be written as $|\Psi(t=0)\rangle = C_0 |0\rangle + C_1 |1\rangle$ (assuming only two levels), where $C_j = \langle j | \Psi(t=0)\rangle$ $(j = 0, 1)$, by the resolution of identity. (3) The time evolution operator, $\hat{\mathcal{U}}(t)$, for $\hat{H}_0$ is given by $\exp\left(-i\hat{H}_0 t/\hbar\right)$, and $|j\rangle$, an eigenstate of $\hat{H}_0$, is also an eigenstate of the time evolution operator, with eigenvalue given by $\exp(-i\omega_j t)$. To summarize

$$\begin{aligned} |\Psi(t)\rangle &= \hat{\mathcal{U}}(t) |\Psi(t=0)\rangle & (12.7)\\ &= \hat{\mathcal{U}}(t) \left(C_0 |0\rangle + C_1 |1\rangle\right) & (12.8)\\ &= C_0 \hat{\mathcal{U}}(t) |0\rangle + C_1 \hat{\mathcal{U}}(t) |1\rangle & (12.9)\\ &= C_0 e^{-i\omega_0 t} |0\rangle + C_1 e^{-i\omega_1 t} |1\rangle & (12.10) \end{aligned}$$

Now, let us consider the full Hamiltonian $\hat{H}(t)$ (Eq. 12.1), which is *not* conserved due to the term $\hat{H}_1(t)$. This fact certainly messes up the above nice derivation. In particular, step (3) is no longer valid. When the Hamiltonian is explicitly dependent

[1] Having said this, the formalism that we develop here *is* useful even for the continuum case. The widely used trick is to consider the space as finite at the beginning ("particle in a big but finite box"), so that every energy spectrum is discrete and every state a bound state. At the end of the calculation of a measurable quantity, however, one can take the volume of the system to go to infinity, and, typically, one obtains results that are applicable to the continuum case. However, the procedure of taking the limit can require much care and appreciation in some cases (however, not so much for problems to be dealt with in this course – so don't worry too much).

on time, the time evolution operator cannot be written in a simple closed form, in general (cf. LN 1). However, note that even for $\hat{H}(t)$, the above steps (1) and (2) are perfectly valid. In particular, at any *fixed* time, any state Ψ can be written as a linear combination of $|0\rangle$ and $|1\rangle$: $|\Psi(t)\rangle = A_0(t)|0\rangle + A_1(t)|1\rangle$. The perturbation idea motivates us to use $A_j(t) = C_j(t)e^{-i\omega_j t}$, and this leads to

$$|\Psi(t)\rangle \;=\; C_0(t)e^{-i\omega_0 t}|0\rangle + \; C_1(t)e^{-i\omega_1 t}|1\rangle \tag{12.11}$$

The *only* difference between this equation and Eq. 12.6 is that C_j is time-dependent here while it is time-independent[2] in Eq. 12.6. However, this is a big difference. Now the "occupancy" for each state $|j\rangle$ can be time-dependent! So, in general, $|j\rangle$ is no longer a stationary state.

If the perturbation is small, then we expect that $C_j(t)$ is mostly time-independent with a small time-dependent term. This is what we mean by the "perturbation idea" above. However, note that the theory that we are doing now is exact within the two level approximation; we are just anticipating the perturbation theory at this point.

Let us apply Eq. 12.5 to Eq. 12.11.

$$\begin{aligned} i\hbar\frac{d}{dt}|\Psi(t)\rangle \;&=\; \hat{H}(t)|\Psi(t)\rangle \\ i\hbar\left(\dot{C}_0(t)e^{-i\omega_0 t}|0\rangle + \dot{C}_1(t)e^{-i\omega_1 t}|1\rangle\right) + C_0(t)(\hbar\omega_0)e^{-i\omega_0 t}|0\rangle + C_1(t)(\hbar\omega_1)e^{-i\omega_1 t}|1\rangle \;&=\; \\ \hat{H}_0|\Psi(t)\rangle + \hat{H}_1(t)|\Psi(t)\rangle \end{aligned}$$

Note that in the last equation, the last two terms of the left hand side are equal to $\hat{H}_0|\Psi(t)\rangle$. And, so we get

$$\begin{aligned} i\hbar\left(\dot{C}_0(t)e^{-i\omega_0 t}|0\rangle + \dot{C}_1(t)e^{-i\omega_1 t}|1\rangle\right) \;&=\; \hat{H}_1(t)|\Psi(t)\rangle \\ &=\; C_0(t)e^{-i\omega_0 t}\hat{H}_1|0\rangle + C_1(t)e^{-i\omega_1 t}\hat{H}_1|1\rangle \end{aligned}$$

By multiplying $\langle 0|$ (or $\langle 1|$) from the left, and using the orthonormality condition $\langle i\,|\,j\rangle = \delta_{i,j}$, we get two equations

$$\begin{aligned} i\hbar\dot{C}_0(t)e^{-i\omega_0 t} \;&=\; C_0(t)e^{-i\omega_0 t}\;{}_0\langle\hat{H}_1\rangle_0 + C_1(t)e^{-i\omega_1 t}\;{}_0\langle\hat{H}_1\rangle_1 \\ i\hbar\dot{C}_1(t)e^{-i\omega_1 t} \;&=\; C_0(t)e^{-i\omega_0 t}\;{}_1\langle\hat{H}_1\rangle_0 + C_1(t)e^{-i\omega_1 t}\;{}_1\langle\hat{H}_1\rangle_1 \end{aligned}$$

where

$${}_j\langle\hat{H}_1\rangle_k \;\equiv\; \langle j\,|\hat{H}_1|\,k\rangle \tag{12.12}$$

[2] It is somewhat amusing or catchy to imagine that $|0\rangle$ and $|1\rangle$ correspond to something like life and death, or youth and age, for the sake of making a point why $C_j(t)$ *must* be time-dependent in any real system. However, be warned that what we do here is strictly quantum mechanics, and certainly such arguments will fail the scrutiny, if one really starts to investigate whether the two level quantum mechanics applies to such deep and complicated problems. Please read Section 12.1.

By multiplying the above equations by $\exp(i\omega_0 t)$ (or $\exp(i\omega_1 t)$), then using the definition for $\omega_{1,0}$ (Eq. 12.4), and then dividing by $i\hbar$, we get

$$\left.\begin{aligned} \dot{C}_0(t) &= \frac{C_0(t)}{i\hbar}\,{}_0\big\langle \hat{H}_1(t)\big\rangle_0 + \frac{C_1(t)e^{-i\omega_{1,0}t}}{i\hbar}\,{}_0\big\langle \hat{H}_1(t)\big\rangle_1 \\ \dot{C}_1(t) &= \frac{C_0(t)e^{i\omega_{1,0}t}}{i\hbar}\,{}_1\big\langle \hat{H}_1(t)\big\rangle_0 + \frac{C_1(t)}{i\hbar}\,{}_1\big\langle \hat{H}_1(t)\big\rangle_1 \end{aligned}\right\} \tag{12.13}$$

These are the general equations of motion for the two level system. If only non-diagonal elements of $\hat{H}_1$ are non-zero, as is the case more often than not, this equation is simplified a bit. The textbook makes that assumption. However, this assumption is very unnecessary, and we will *not* make such an assumption.