221A Lecture Notes
Time-Dependent Perturbation Theory

1 Introduction

The time-independent perturbation theory is very successful when the system posses a small dimensionless parameter. It allows us to work out corrections to the energy eigenvalues and eigenstates. However, it is not capable of working out consequences of a perturbation that depends on time. Even when the perturbation is time-independent, it is useful to study the time-dependence of the system, for example in scattering or decay processes. Here we would like to see how we can treat a time-dependent perturbation.

2 Interaction Picture

The interaction picture is a half way between the Schrödinger and Heisenberg pictures, and is particularly suited to develop the perturbation theory. It is also called the *Dirac* picture. It tries to discard the "trivial" time-dependence due to the unperturbed Hamiltonian which is by assumption exactly solved and is not of our interest anymore. Taking out the uninteresting time dependence helps us to focus on questions such as the transitions from one H_0 eigenstate to another due to the perturbation. By definition, H_0 does not cause an eigenstate to transform to another, while the perturbation can.

Just like in the time-independent case, the Hamiltonian is split into two pieces, $H = H_0 + V$. The perturbation Hamiltonian may or may not be time-dependent, but the rest of the formalism is the same either case. By assumption, H_0 is solved exactly: we know its eigenvalues and eigenstates. In the Schrödinger picture, the states evolve according to the Schrödinger equation,

$$i\hbar\frac{d}{dt}|\alpha,t\rangle_S = H|\alpha,t\rangle_S, \tag{1}$$

while the observables (operators) don't,

$$i\hbar\frac{d}{dt}O = 0. \tag{2}$$

Because the time evolution due to the unperturbed Hamiltonian H_0 is solved and not of our interest, we try to eliminate the time-dependence due to H_0 out of the state, by defining

$$|\alpha, t\rangle_I = e^{+iH_0 t/\hbar}|\alpha, t\rangle_S. \tag{3}$$

The time-evolution of this state is seen as

$$\begin{aligned} i\hbar\frac{d}{dt}|\alpha, t\rangle_I &= i\hbar\frac{d}{dt}e^{+iH_0 t/\hbar}|\alpha, t\rangle_S \\ &= \left(i\hbar\frac{d}{dt}e^{+iH_0 t/\hbar}\right)|\alpha, t\rangle_S + e^{+iH_0 t/\hbar}\left(i\hbar\frac{d}{dt}|\alpha, t\rangle_S\right) \\ &= -H_0 e^{+iH_0 t/\hbar}|\alpha, t\rangle_S + e^{+iH_0 t/\hbar}(H_0 + V)|\alpha, t\rangle_S \\ &= e^{+iH_0 t/\hbar}V|\alpha, t\rangle_S \\ &= e^{+iH_0 t/\hbar}Ve^{-iH_0 t/\hbar}e^{+iH_0 t/\hbar}|\alpha, t\rangle_S \\ &= V_I|\alpha, t\rangle_I. \end{aligned} \tag{4}$$

As desired, the state does not evolve in the absence of the perturbation, while it does in its presence. The operator for time-evolution is, however, not just the perturbation Hamiltonian, but is

$$V_I(t) = e^{+iH_0 t/\hbar}Ve^{-iH_0 t/\hbar}. \tag{5}$$

This definition is true even when the perturbation depends on time, $V = V(t)$.

Because of the change of the picture, the operators now evolve in time. In order to keep the expectation values of the operators the same as in the Schrödinger picture, we need

$$O_I(t) = e^{+iH_0 t/\hbar}Oe^{-iH_0 t/\hbar}. \tag{6}$$

Therefore the operators follow a Heisenberg-like equation,

$$i\hbar\frac{d}{dt}O_I(t) = [O_I(t), H_0]. \tag{7}$$

Note that the evolution is solely due to H_0, not H or V.

picture	Heisenberg	Interaction	Schrödinger
state ket	no evolution	evolution by V_I	evolution by H
operators	evolution by H	evolution by H_0	no evolution

Table 1: Table 5.2 of Sakurai, which shows the differences among the three pictures.

3 Dyson Series

It is possible to obtain a formal solution to the Schrödinger-like equation in the interaction picture. We introduce the time-evolution operator

$$|\alpha, t\rangle_I = U_I(t)|\alpha, 0\rangle_S, \tag{8}$$

which satisfies

$$i\hbar\frac{d}{dt}U_I(t) = V_I(t)U_I(t). \tag{9}$$

The boundary condition is simply $U_I(0) = 1$. Then we can recast the differential equation into an integral equation,

$$U_I(t) = 1 - \frac{i}{\hbar}\int_0^t V_I(t')U_I(t')dt'. \tag{10}$$

It is easy to verify that this expression satisfies both the differential equation as well as the boundary condition. Now we can solve this integral equation iteratively. At $O(V^0)$, it is simply $U_I(t) = 1$. At $O(V^1)$, we substitute the $O(V^0)$ solution into the r.h.s. of the equation, and find

$$U_I(t) = 1 - \frac{i}{\hbar}\int_0^t V_I(t')dt' + O(V^2). \tag{11}$$

Now that we have U_I up to $O(V^1)$, we substitute this solution into the r.h.s. again to find U_I up to $O(V^2)$,

$$U_I(t) = 1 - \frac{i}{\hbar}\int_0^t dt' V_I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' V_I(t')V_I(t'') + O(V^3). \tag{12}$$

By repeating this process, we find $O(V^n)$ term in $U_I(t)$ to be

$$\left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n V_I(t_1)V_I(t_2)\cdots V_I(t_n). \tag{13}$$

This infinite series expansion of the time-evolution operator in powers of V_I in the interaction picture is called the Dyson series.

It is customary to simplify the expression using the *time-ordered products*.* For instance, two operators $A(t)$ and $B(t)$ have their time-ordered product

$$T(A(t)B(t')) = \begin{cases} A(t)B(t') & t > t' \\ B(t')A(t) & t' > t \end{cases} \tag{14}$$

Using this definition, the second-order piece in $U_I(t)$ can be rewritten as

$$\left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' V_I(t')V_I(t'') = \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^t dt'' T(V_I(t')V_I(t'')). \tag{15}$$

In the original expression, the integration is done over a triangle shown in Fig. 1, while in the latter expression it is integrated over the whole square. Similarly, the $O(V^3)$ term is integrated over the tetrahedron in Fig. 1, which is one sixth= 1/3! of the volume of the cube. It can also be rewritten as

$$\begin{aligned} &\left(\frac{-i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 V_I(t_1)V_I(t_2)V_I(t_3) \\ &\quad = \frac{1}{3!}\left(\frac{-i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^t dt_2 \int_0^t dt_3 T(V_I(t_1)V_I(t_2)V_I(t_3)) \end{aligned} \tag{16}$$

as an integration over the entire cube. The n-th order term becomes

$$\begin{aligned} &\left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n V_I(t_1)V_I(t_2)\cdots V_I(t_n) \\ &= \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n T(V_I(t_1)V_I(t_2)\cdots V_I(t_n)). \end{aligned} \tag{17}$$

Thanks to this new notation of the time-ordered products, the time-evolution operator in the interaction picture can be written simply as

$$U_I(t) = Te^{-i\int_0^t V_I(t')dt'}. \tag{18}$$

This expression is understood in terms of its Taylor expansion, where the n-th order in the expansion has n V_I's which are ordered according to their time arguments.

*This point is mentioned in the footnote on page 326 of Sakurai, but is not elaborated.

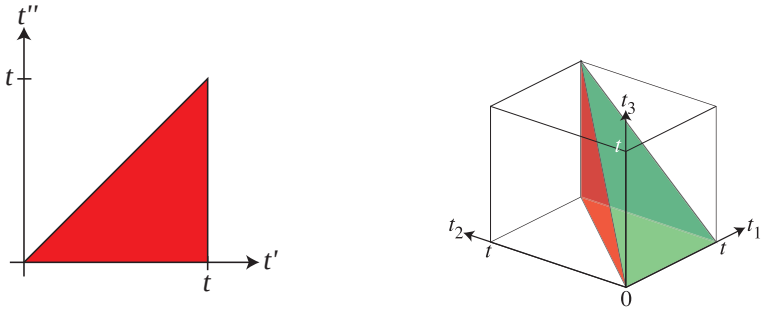

Figure 1: The integrations region of the $O(V^2)$ and $O(V^3)$ terms in the Dyson series.

Actually, the path integral formulation gives this expression right away. Recall that any insertion of observables in the path integral is automatically time ordered,

$$\int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} x(t_n) \cdots x(t_1) = \langle x_f, t_f | T(x(t_n) \cdots x(t_1)) | x_i, t_i \rangle \tag{19}$$

as shown in the lecture notes on the path integral. In this simple example, the time-dependence of the initial and final states is dictated by the Hamiltonian obtained from the action. The inserted operators are Heisenberg operators whose time evolution is dictated also by the same Hamiltonian. In the perturbation theory, we split the action into two pieces,

$$S[x(t)] = \int_{t_i}^{t_f} dt \, (p\dot{q} - H) = \int_{t_i}^{t_f} dt \, (p\dot{q} - H_0 - V) = S_0[x(t)] - \int_{t_i}^{t_f} dt V. \tag{20}$$

Therefore, the path integral is rewritten as

$$\int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} = \int \mathcal{D}x(t) e^{iS_0[x(t)]/\hbar} e^{-i\int_{t_i}^{t_f} V dt/\hbar} = \langle x_f, t_f | T e^{-i\int_{t_i}^{t_f} V dt/\hbar} | x_i, t_i \rangle. \tag{21}$$

In the last expression, the time-evolution of the initial and final states is dictated by the Hamiltonian derived from the action S_0, namely H_0, and the operator also has the time-dependence dictated by H_0, namely $V_I(t)$.

The Dyson series allows us to compute the perturbative expansion up to any arbitrary order.

It is also useful to know that the time-evolution operator in the interaction picture is related to the full time-evolution operator $U(t)$ as

$$U(t) = e^{-iH_0 t/\hbar} U_I(t), \tag{22}$$

where $U(t)$ satisfies

$$i\hbar \frac{d}{dt} U(t) = H U(t). \tag{23}$$

This relationship can be verified as

$$\begin{aligned} i\hbar\frac{d}{dt}e^{-iH_0t/\hbar}U_I(t) &= H_0e^{-iH_0t/\hbar}U_I(t) + e^{-iH_0t/\hbar}V_I(t)U_I(t) \\ &= \left(H_0 + e^{-iH_0t/\hbar}V_I(t)e^{iH_0t/\hbar}\right)e^{-iH_0t/\hbar}U_I(t) \\ &= (H_0+V)e^{iH_0t/\hbar}U_I(t) \\ &= He^{-iH_0t/\hbar}U_I(t), \end{aligned} \tag{24}$$

and the boundary condition $U(0) = U_I(0) = 1$. Eq. (22) clearly shows that the change from the Schrödinger to the interaction picture is done by $e^{-iH_0t/\hbar}$.

4 Transition Probability

Equipped with the interaction picture, we would like to now work out the probability that an H_0 eigenstate $H_0|i\rangle = E_i|i\rangle$ (the $i$nitial state) becomes another H_0 eigenstate $H_0|f\rangle = E_f|f\rangle$ (the $f$inal state) due to the perturbation V. Going back to the Schrödinger picture, the transition amplitude is

$$\mathcal{A}(i \to f, t) = \langle f|U(t)|i\rangle. \tag{25}$$

Using Eq. (22), we find

$$\mathcal{A}(i \to f, t) = \langle f|e^{-iH_0t/\hbar}U_I(t)|i\rangle = e^{-iE_ft/\hbar}\langle f|U_I(t)|i\rangle. \tag{26}$$

Therefore the transition probability can be computed safely in the interaction picture,

$$P(i \to f, t) = |\mathcal{A}(i \to f, t)|^2 = |\langle f|U_I(t)|i\rangle|^2. \tag{27}$$

Note that it is crucial that the state $|f\rangle$ is an eigenstate of H_0 in this derivation; otherwise the amplitude computed in the interaction picture may not be the same as that in the Schrödinger picture.

Therefore all we need to calculate is the matrix element

$$\langle f|U_I(t)|i\rangle \tag{28}$$

which can be worked out with the Dyson series.

4.1 Fermi's Golden Rule(s)

If the perturbation is time-independent $V(t) = V$, *turned on* at $t = 0$, the lowest order term in the expansion of the transition amplitude for $i \neq f$ is

$$\begin{aligned} \frac{-i}{\hbar}\int_0^t dt' \langle f|V_I(t')|i\rangle &= \frac{-i}{\hbar}\int_0^t dt' \langle f|e^{iH_0t'/\hbar}Ve^{-iH_0t'/\hbar}|i\rangle \\ &= \frac{-i}{\hbar}\int_0^t dt' e^{-i(E_i-E_f)t'/\hbar}\langle f|V|i\rangle \\ &= \frac{e^{-i(E_i-E_f)t/\hbar}-1}{E_i-E_f}V_{fi}. \end{aligned} \tag{29}$$

The transition probability is then

$$P(i \to f, t) = 4\frac{\sin^2 \Delta Et/2\hbar}{(\Delta E)^2}|V_{fi}|^2, \tag{30}$$

to the lowest order in perturbation theory. Here, I used the notation $\Delta E = E_i - E_f$.

It is important to understand the time dependence of the probability. I plotted the probability as a function of $\Delta E/\hbar$ at various times in Fig. 2. It is clear that the probability is more and more peaked at $\Delta E = 0$ as the time goes on. The range in ΔE where the probability is sizable decreases as $\Delta E \simeq \hbar/t$.

This is often talked about as a manifestation of the energy-time uncertainty principle, $\Delta E \Delta t \sim \hbar$. Note that this "principle" is not as rigorous as that between the position and the momentum. t is not even an operator! What it means is that the energy may appear not conserved by the amount ΔE within the time interval Δt because you have *turned on* the perturbation: an obvious act of crime that makes the system not invariant under the time translation and hence violate the conservation law of energy. Despite the fact that this "principle" is not rigorous, it comes back repeatedly in many different circumstances.

We are often interested in the behavior when t is large. In particular, we are interested in the *rate* of the transition, namely the transition probability per unit time

$$\Gamma(i \to f) = \lim_{t\to\infty}\frac{P(i \to f, t)}{t} = \lim_{t\to\infty} 4\frac{\sin^2 \Delta Et/2\hbar}{t(\Delta E)^2}|V_{fi}|^2. \tag{31}$$

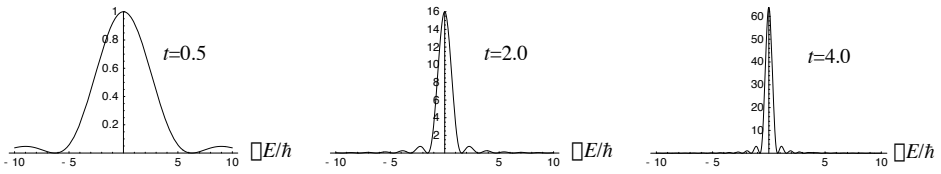

Figure 2: The behavior of the transition probability at various times $t = 0.5$, 2.0, and 4.0 as a function of the energy difference $\Delta E/\hbar$.

At this point, we can use the identity

$$\lim_{t\to\infty} 4\frac{\sin^2(E_f - E_i)t/2\hbar}{t(E_f - E_i)^2} = 2\pi\delta(E_f - E_i)\frac{1}{\hbar}. \tag{32}$$

To see this, note that the peak becomes more and more prominent ($\propto t$) as the time goes on at $E_i - E_f = 0$, while the rest of the function is suppressed as $1/t$. The area below the peak is given by

$$\int dE_f \; 4\frac{\sin^2(E_f - E_i)t/2\hbar}{t(E_f - E_i)^2} = 2\pi\frac{1}{\hbar}, \tag{33}$$

and hence we find the identity above. Using this identity, we obtain the Fermi's golden rule #2,

$$\Gamma(i \to f) = \frac{2\pi}{\hbar}\delta(E_i - E_f)|V_{fi}|^2. \tag{34}$$

In order to extend the calculation to the next order, $O(V^2)$, we find the term in $\langle f|U_I(t)|i\rangle$ by using the completeness relation $1 = \sum_m |m\rangle\langle m|$ as the sum over all inter*m*ediate states,

$$\begin{aligned}
&\left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' V_I(t')V_I(t'') \\
&= \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \sum_m \langle f|V_I(t')|m\rangle\langle m|V_I(t'')|i\rangle \\
&= \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \sum_m V_{fm} e^{-i(E_m - E_f)t'/\hbar} V_{mi} e^{-i(E_i - E_m)t''/\hbar} \\
&= \frac{-i}{\hbar}\int_0^t dt' \sum_m e^{-i(E_m - E_f)t'/\hbar} \frac{e^{-i(E_i - E_m)t'/\hbar} - 1}{E_i - E_m} V_{fm}V_{mi} \\
&= \sum_m \frac{V_{fm}V_{mi}}{E_i - E_m}\left(\frac{e^{-i(E_i - E_f)t/\hbar} - 1}{E_i - E_f} - \frac{e^{-i(E_m - E_f)t/\hbar} - 1}{E_m - E_f}\right).
\end{aligned} \tag{35}$$

This expression looks asymmetric between the initial and the final states. However, it can be rewritten as

$$
\begin{aligned}
&= \sum_m V_{fm}V_{mi}\left(\frac{e^{-i(E_i-E_f)t/\hbar}-1}{(E_i-E_f)(E_i-E_m)}-\frac{e^{-i(E_m-E_f)t/\hbar}-1}{(E_i-E_m)(E_m-E_f)}\right)\\
&= \sum_m V_{fm}V_{mi}\left(\frac{e^{-i(E_i-E_f)t/\hbar}}{(E_i-E_f)(E_i-E_m)}-\frac{e^{-i(E_m-E_f)t/\hbar}}{(E_i-E_m)(E_m-E_f)}\right.\\
&\qquad\qquad\left.+\frac{1}{(E_i-E_f)(E_m-E_f)}\right)\\
&= e^{-i(E_i-E_f)t/2\hbar}\sum_m V_{fm}V_{mi}\\
&\quad\left[\frac{1}{E_i-E_f}\left(\frac{e^{-i(E_i-E_f)t/2\hbar}}{E_i-E_m}-\frac{e^{i(E_i-E_f)t/2\hbar}}{E_f-E_m}\right)+\frac{e^{-i(2E_m-E_i-E_f)t/2\hbar}}{(E_i-E_m)(E_f-E_m)}\right]
\end{aligned}
\tag{36}
$$

and hence is symmetric under $f \leftrightarrow i$, $V_{fm}V_{mi} \leftrightarrow V_{im}V_{mf}$ apart from the overall phase factor $e^{-i(E_i-E_f)t/2\hbar}$.

Going back to Eq. (35), the first term in the parentheses has the same behavior $\propto t$ when $E_i = E_f$ as the $O(V)$ term when t is large, while the second term does not grow. Therefore, adding to the $O(V)$ term, we find[†]

$$
\Gamma(i\to f,t) = 2\pi\delta(E_i-E_f)\frac{1}{\hbar}\left|V_{fi}+\sum_m\frac{V_{fm}V_{mi}}{E_i-E_m}\right|^2 . \tag{37}
$$

The $O(V^2)$ term is said to be the *virtual* transition, and is clearly important especially when the first-order contribution vanishes $V_{fi} = 0$. The initial state goes to a virtual intermediate state that does not conserve the energy, but comes back to a *real* final state that does conserve energy. Of course, this interpretation fails when $E_m = E_i$. One has to specify a prescription how the pole in the denominator can be avoided. This point will be discussed later.

4.2 Harmonic Perturbation

The harmonic perturbation is a time-dependent perturbation $V(t) = 2V_0\cos\omega t$, where V_0 is in general an operator. For the transition probability at the first

[†]According to the web site `http://www.upscale.utoronto.ca/GeneralInterest/DBailey/SubAtomic/Lectures/LectF14/Lect14.htm` Scott Burt found for us, this formula is the Fermi's golden rule #1 when the first-order contribution vanishes $V_{fi} = 0$. It is curious that the first-order contribution is actually the golden rule #2.

order in perturbation, we go back to Eq. (29) and redo the integral,

$$\begin{aligned}\frac{-i}{\hbar}\int_0^t dt'\langle f|V_I(t')|i\rangle &= \frac{-i}{\hbar}\int_0^t dt'\langle f|e^{iH_0t'/\hbar}V\cos\omega t e^{-iH_0t'/\hbar}|i\rangle \\ &= \frac{-i}{\hbar}\int_0^t dt' e^{-i(E_i-E_f)t'/\hbar}2\cos\omega t\langle f|V_0|i\rangle \\ &= \left(\frac{e^{-i(E_i-E_f+\hbar\omega)t/\hbar}-1}{E_i-E_f+\hbar\omega}+\frac{e^{-i(E_i-E_f-\hbar\omega)t/\hbar}-1}{E_i-E_f-\hbar\omega}\right)V_{fi}. \qquad (38)\end{aligned}$$

Following Eq. (32), the transition rate is

$$\Gamma(i\to f)=\frac{2\pi}{\hbar}(\delta(E_i-E_f+\hbar\omega)+\delta(E_i-E_f-\hbar\omega))|V_{fi}|^2. \qquad (39)$$

Therefore, the "energy conservation" is now changed to $E_f = E_i \pm \hbar\omega$.

It was expected that the energy is strictly not conserved in the presence of a harmonic perturbation, because there is no time-translation invariance. However, there is a discrete time translational invariance by $t \to t + 2\pi/\omega$. Similarly to the discrete spatial translational invariance $x \to x + a$ that led to the Bloch wave, which "conserves the momentum modulo $2\pi\hbar/a$," the energy is "conserved modulo $\hbar\omega$," consistent with the above result. In fact, the second-order contribution can be seen to "conserve" the energy as $E_f = E_i \pm 2\hbar\omega$ or $E_f = E_i$, the third-order term $E_f = E_i \pm 3\hbar\omega$ or $E_f = E_i \pm \hbar\omega$, etc.

Sakurai discusses the photoelectric effect using this formalism. Strictly speaking, the photoelectric effect must be discussed only after properly quantizating the electromagnetic field to obtain "photons." We will not go into this discussion further here.

4.3 Relationship to the Time-independent Case

The Dyson series can be used to work out the results in the time-independent perturbation theory. Even though the formalism explicitly includes time, it can be applied to a case of perturbation with no explicit time dependence.

What we look at is the quantity

$$\langle i^{(0)}|U_I(t)|i^{(0)}\rangle = \langle i^{(0)}|e^{+iH_0t/\hbar}U(t)|i^{(0)}\rangle = e^{iE_i^{(0)}t/\hbar}\sum_m |\langle i^{(0)}|m\rangle_N|^2 e^{-iE_mt/\hbar}, \qquad (40)$$

where $|m\rangle$ is the exact eigenstates of the full Hamiltonian, and $|i^{(0)}\rangle$ the unperturbed state, following Sakurai's notation of the time-independent perturbation theory.[‡] The subscripts $_N$ indicate that the true eigenstates are properly normalized. In particular, the perturbed state $|i\rangle$ has a large overlap with $|i^{(0)}\rangle$,

$$Z_i^{1/2} = \langle i^{(0)}|i\rangle_N. \tag{41}$$

By singling out this contribution to the amplitude,

$$\langle i^{(0)}|U_I(t)|i^{(0)}\rangle = Z_i e^{-i(E_i - E_i^{(0)})t/\hbar} + \sum_m |\langle i^{(0)}|m\rangle_N|^2 e^{-i(E_m - E_i^{(0)})t/\hbar}. \tag{42}$$

It is important to note that the exponent of the first term is $\Delta_i = E_i - E_i^{(0)} = O(V)$ and vanishes in the absence of perturbation.

Going back to the Dyson formula for the constant perturbation $V(t) = V$, we evaluate the contributions up to $O(V^2)$ and study the consistency with the time-independent results.

$$\begin{aligned}\langle i^{(0)}|U_I(t)|i^{(0)}\rangle &= 1 + \frac{-i}{\hbar}\int_0^t dt' \langle i^{(0)}|V_I(t')|i^{(0)}\rangle \\ &+ \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \langle i^{(0)}|V_I(t')V_I(t'')|i^{(0)}\rangle + O(V^3).\end{aligned} \tag{43}$$

Compared to the general result Eq. (42), we expect

$$\begin{aligned}\langle i^{(0)}|U_I(t)|i^{(0)}\rangle &= Z_i e^{-i(E_i - E_i^{(0)})t/\hbar} + \sum_{m\neq i} |\langle i^{(0)}|m\rangle_N|^2 e^{-i(E_m - E_i^{(0)})t/\hbar} \\ &= Z_i \left(1 + \frac{-i}{\hbar}(\Delta_i^{(1)} + \Delta_i^{(2)})t + \frac{1}{2!}\left(\frac{-i}{\hbar}\right)^2 (\Delta_i^{(1)}t)^2\right) \\ &\quad + \sum_{m\neq i} |\langle i^{(0)}|m\rangle_N|^2 e^{-i(E_m^{(0)} - E_i^{(0)})t/\hbar} + O(V^3),\end{aligned} \tag{44}$$

where Z_i is evaluated up to $O(V^2)$ (the lowest order), and $\langle i^{(0)}|m\rangle_N$ up to $O(V)$. in the last exponent E_m is replaced by $E_m^{(0)}$ because the difference gives contributions only at $O(V^3)$ (the inner product squared is already $O(V^2)$).

[‡]Note that he dropped the superscript $^{(0)}$ in his discussions on time-dependent perturbation theory. I'm just recovering them.

The $O(V)$ piece in the Dyson series is easy to work out:

$$\begin{aligned}
\frac{-i}{\hbar}\int_0^t dt'\langle i^{(0)}|V_I(t')|i^{(0)}\rangle &= \frac{-i}{\hbar}\int_0^t dt'\langle i^{(0)}|e^{iH_0t'/\hbar}Ve^{-iH_0t'/\hbar}|i^{(0)}\rangle \\
&= \frac{-i}{\hbar}\int_0^t dt'\langle i^{(0)}|e^{iE_i^{(0)}t'/\hbar}Ve^{-iE_i^{(0)}t'/\hbar}|i^{(0)}\rangle \\
&= \frac{-i}{\hbar}\int_0^t dt'\langle i^{(0)}|V|i^{(0)}\rangle \\
&= \frac{-i}{\hbar}V_{ii}t. \qquad (45)
\end{aligned}$$

This agrees with the $O(V)$ piece in Eq. (44), namely $\frac{-i}{\hbar}\Delta_i^{(1)}t$, if

$$\Delta_i^{(1)} = V_{ii}, \qquad (46)$$

consistent with the result in time-independent perturbation theory, Eq. (5.1.37) in Sakurai.

The $O(V^2)$ piece is much richer. We insert the complete set of states $1 = \sum_m |m^{(0)}\rangle\langle m^{(0)}|$ between two V_I's, and separate out the contribution from $m = i$.

$$\begin{aligned}
&\left(\frac{-i}{\hbar}\right)^2\int_0^t dt'\int_0^{t'} dt''\langle i^{(0)}|V_I(t')V_I(t'')|i^{(0)}\rangle \\
&= \left(\frac{-i}{\hbar}\right)^2\int_0^t dt'\int_0^{t'} dt'' \\
&\quad\left[\langle i^{(0)}|V_I(t')|i^{(0)}\rangle\langle i^{(0)}|V_I(t'')|i^{(0)}\rangle + \sum_{m\neq i}\langle i^{(0)}|V_I(t')|m^{(0)}\rangle\langle m^{(0)}|V_I(t'')|i^{(0)}\rangle\right] \\
&= \left(\frac{-i}{\hbar}\right)^2\int_0^t dt'\int_0^{t'} dt''\left[V_{ii}^2 + \sum_{m\neq i}V_{im}e^{-i(E_m^{(0)}-E_i^{(0)})t'/\hbar}V_{mi}e^{-i(E_i^{(0)}-E_m^{(0)})t''/\hbar}\right] \\
&= \left(\frac{-i}{\hbar}\right)^2\int_0^t dt'\left[V_{ii}^2t' + \sum_{m\neq i}|V_{mi}|^2e^{-i(E_m^{(0)}-E_i^{(0)})t'/\hbar}\frac{\hbar}{-i}\frac{e^{-i(E_i^{(0)}-E_m^{(0)})t'/\hbar}-1}{E_i^{(0)}-E_m^{(0)}}\right] \\
&= \left(\frac{-i}{\hbar}\right)^2\frac{1}{2}V_{ii}^2t^2 + \sum_{m\neq i}\frac{|V_{mi}|^2}{E_i^{(0)}-E_m^{(0)}}\left(\frac{-i}{\hbar}t + \frac{e^{-i(E_i^{(0)}-E_m^{(0)})t/\hbar}-1}{E_i^{(0)}-E_m^{(0)}}\right) \\
&= \left(\frac{-i}{\hbar}\right)^2\frac{1}{2}V_{ii}^2t^2 + \frac{-i}{\hbar}\sum_{m\neq i}\frac{|V_{mi}|^2}{E_m^{(0)}-E_i^{(0)}}t + \sum_{m\neq i}\frac{|V_{mi}|^2}{(E_i^{(0)}-E_m^{(0)})^2}e^{-i(E_m^{(0)}-E_i^{(0)})t/\hbar}
\end{aligned}$$

$$-\sum_{m\neq i}\frac{|V_{mi}|^2}{(E_i^{(0)}-E_m^{(0)})^2}. \tag{47}$$

The first term is identified with $\frac{1}{2!}\left(\frac{-i}{\hbar}\right)^2(\Delta_i^{(1)}t)^2$ in Eq. (44). The second term is identified with $\frac{-i}{\hbar}\Delta_i^{(2)}t$ with

$$\Delta_i^{(2)}=\sum_{m\neq i}\frac{|V_{mi}|^2}{E_i^{(0)}-E_m^{(0)}}, \tag{48}$$

again consistent with the time-independent result Sakurai's Eq. (5.1.42). The third term is the contribution of the mixing of other unperturbed states

$$|i\rangle=|i^{(0)}\rangle+\sum_{m\neq i}|m^{(0)}\rangle\frac{V_{mi}}{E_i^{(0)}-E_m^{(0)}}, \tag{49}$$

Sakurai's Eq. (5.1.44). Finally, the last term is the $O(V^2)$ piece in the wave function renormalization,

$$Z_i=1-\sum_{m\neq i}\frac{|V_{mi}|^2}{(E_i^{(0)}-E_m^{(0)})^2}, \tag{50}$$

Sakurai's Eq. (5.1.48b).

In this fashion, we can see that the Dyson formula contains all information we had obtained from the time-independent perturbation theory. Not only that, it is surely applicable to the time-dependent problems and hence is very powerful.

4.4 Energy Shift and Decay Width

In the presence of the discrete (*e.g.*, excited bound states of the hydrogen atom) and the continuum states (*e.g.*, the ground state plus a photon), as in the scattering problems (will be discussed in 221B), the sum over the intermediate states cannot exclude the continuum states with the same energy. Then the energy denominator $1/(E_i-E_m)$ diverges; some prescriptions are in order to deal with this singularity. As Sakurai discusses in Section 5.8, one way to deal with it is to gradually turn on the perturbation from the infinite past as $V(t)=Ve^{\eta t}$, whose net result is simply the replacement in Eq. (37),

$$\frac{1}{E_i-E_m}\to\frac{1}{E_i-E_m+i\hbar\eta}\ , \tag{51}$$

where $\eta > 0$ is an infinitesimal positive parameter taken to zero at the end of calculations.

Because we have learned how to relate the Dyson series to the energy shifts $\Delta_i^{(n)}$ at the n-th order in perturbation theory in the previous section, we can immediately apply it to the perturbation $V(t) = Ve^{\eta t}$ to verify Sakurai's results, without resorting to the artificial limit of $t_0 \to -\infty$, recast the result in terms of a differential equation, integrate it again, and extract quantities that are regular in this limit. We simply look for the piece that grows as t in $\langle i^{(0)}|U_I(t)|i^{(0)}\rangle$ under this perturbation. The first order term is the same as the constant perturbation in the limit $\eta \to 0$. We look at the second order piece following Eq. (47),

$$\begin{aligned}
&\left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \langle i^{(0)}|V_I(t')V_I(t'')|i^{(0)}\rangle \\
&= \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \\
&\quad \left[V_{ii}^2 e^{\eta t'} e^{\eta t''} + \sum_{m\neq i} V_{im} e^{\eta t'} e^{-i(E_m^{(0)}-E_i^{(0)})t'/\hbar} V_{mi} e^{\eta t''} e^{-i(E_i^{(0)}-E_m^{(0)})t''/\hbar}\right] \quad (52)
\end{aligned}$$

Clearly we are not interested in the first term. The second term is

$$\frac{-i}{\hbar}\int_0^t dt' \sum_{m\neq i} |V_{mi}|^2 e^{\eta t'} e^{-i(E_m^{(0)}-E_i^{(0)})t'/\hbar} \frac{e^{-i(E_m^{(0)}-E_i^{(0)}+i\hbar\eta)t'/\hbar}-1}{E_i^{(0)}-E_m^{(0)}+i\hbar\eta}. \quad (53)$$

Except for the energy denominator, everything else is regular in the limit $\eta \to 0$ which we take. Therefore

$$\frac{-i}{\hbar}\int_0^t dt' \sum_{m\neq i} |V_{mi}|^2 e^{-i(E_m^{(0)}-E_i^{(0)})t'/\hbar} \frac{e^{-i(E_i^{(0)}-E_m^{(0)})t'/\hbar}-1}{E_i^{(0)}-E_m^{(0)}+i\hbar\eta}. \quad (54)$$

The first term in the numerator cancels the oscillatory factor and gives rise to a term that grows as t,

$$\frac{-i}{\hbar} t \sum_{m\neq i} \frac{|V_{mi}|^2}{E_i^{(0)}-E_m^{(0)}+i\hbar\eta}. \quad (55)$$

As before, we identify this term with $\frac{-i}{\hbar}\Delta_i^{(2)} t$ and we obtain

$$\Delta_i^{(2)} = \sum_{m\neq i} \frac{|V_{mi}|^2}{E_i^{(0)}-E_m^{(0)}+i\hbar\eta}, \quad (56)$$

which is implicit in a combination of Eqs. (5.8.9), (5.8.10), and (5.8.15).

I do not repeat the rest of the discussions in Sakurai. Important points are: (1) the imaginary part of the energy shift corresponds to the *decay rate* of the state, (2) the energy is broadened by the decay rate, and (3) the unitarity relates the total decay rate to the width of the state. We will come back to the meaning of the imaginary energy and the decay width when we discuss the scattering problems in 221B.

5 Two-State System

This note is the derivation of the formula Eq. (5.5.21) in Sakurai. He only gives the result on the probability, while it is essential to see the result in amplitudes in certain cases (like in the NMR discussed in the next section).

5.1 The Exact Solution

The Hamiltonian in matrix notation is

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}, \qquad V(t) = \gamma \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix}. \tag{57}$$

As usual, we define the coefficients $c_i(t)$ by

$$\psi(t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-iE_1 t/\hbar} c_1(t) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-iE_2 t/\hbar} c_2(t) = \begin{pmatrix} e^{-iE_1 t/\hbar} c_1(t) \\ e^{-iE_2 t/\hbar} c_2(t) \end{pmatrix}. \tag{58}$$

The Schrödinger equation is $i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$. We work out each side separately.

$$i\hbar \frac{d}{dt}\psi(t) \;=\; \begin{pmatrix} E_1 e^{-iE_1 t/\hbar} c_1(t) + e^{-iE_1 t/\hbar} i\hbar \dot{c}_1(t) \\ E_2 e^{-iE_2 t/\hbar} c_2(t) + e^{-iE_2 t/\hbar} i\hbar \dot{c}_2(t) \end{pmatrix}. \tag{59}$$

On the other hand,

$$H\psi(t) \;=\; \begin{pmatrix} E_1 e^{-iE_1 t/\hbar} c_1(t) + \gamma e^{i\omega t} e^{-iE_2 t/\hbar} c_2(t) \\ E_2 e^{-iE_2 t/\hbar} c_2(t) + \gamma e^{-i\omega t} e^{-iE_1 t/\hbar} c_1(t) \end{pmatrix}. \tag{60}$$

Equating the above two, we find

$$\begin{pmatrix} e^{-iE_1 t/\hbar} i\hbar \dot{c}_1(t) \\ e^{-iE_2 t/\hbar} i\hbar \dot{c}_2(t) \end{pmatrix} = \begin{pmatrix} \gamma e^{i\omega t} e^{-iE_2 t/\hbar} c_2(t) \\ \gamma e^{-i\omega t} e^{-iE_1 t/\hbar} c_1(t) \end{pmatrix}. \tag{61}$$

We write them in the following form

$$i\hbar\dot{c}_1 = \gamma e^{i(\omega-\omega_{21})t}c_2, \tag{62}$$
$$i\hbar\dot{c}_2 = \gamma e^{-i(\omega-\omega_{21})t}c_1. \tag{63}$$

Here I introduced the notation $\omega_{21} = (E_2 - E_1)/\hbar$.

Now we would like to eliminate c_1 to write down the differential equation for c_2. Using Eq. (63),

$$c_1(t) = \frac{1}{\gamma}e^{i(\omega-\omega_{21})t}i\hbar\dot{c}_2(t), \tag{64}$$

I take $i\hbar\frac{d}{dt}$ of both sides, and the l.h.s. can be rewritten with the Eq. (62),

$$\begin{aligned}\gamma e^{i(\omega-\omega_{21})t}c_2(t) &= i\hbar\dot{c}_1(t) \\ &= \frac{1}{\gamma}e^{i(\omega-\omega_{21})t}\left(-\hbar(\omega-\omega_{21})i\hbar\dot{c}_2(t) + (i\hbar)^2\ddot{c}_2\right).\end{aligned} \tag{65}$$

The equation is simplified to the form

$$\ddot{c}_2 + i(\omega-\omega_{21})\dot{c}_2 + \frac{\gamma^2}{\hbar^2}c_2 = 0. \tag{66}$$

Following the standard technique, we write $c_2 \propto e^{i\alpha t}$ to solve the differential equation. Then the equation becomes

$$-\alpha^2 - (\omega-\omega_{21})\alpha + \frac{\gamma^2}{\hbar^2} = 0. \tag{67}$$

This is a simple quadratic equation you can solve,

$$\alpha_\pm = \frac{1}{2}\left[-(\omega-\omega_{21}) \pm \sqrt{(\omega-\omega_{21})^2 + 4\frac{\gamma^2}{\hbar^2}}\right]. \tag{68}$$

In general, c_2 is given by a linear combination of $e^{i\alpha_\pm t}$,

$$c_2(t) = A_+e^{i\alpha_+ t} + A_-e^{i\alpha_- t}. \tag{69}$$

Correspondingly, c_1 is given by Eq. (64)

$$c_1(t) = \frac{1}{\gamma}e^{i(\omega-\omega_{21})t}i\hbar\dot{c}_2(t) = \frac{\hbar}{\gamma}e^{i(\omega-\omega_{21})t}(A_+\alpha_+e^{i\alpha_+ t} + A_-\alpha_-e^{i\alpha_- t}). \tag{70}$$

Now we impose the boundary condition

$$c_1(0) = 1, \qquad c_2(0) = 0. \tag{71}$$

The corresponding conditions on the coefficients are

$$A_+ + A_- = 0, \tag{72}$$

$$-\frac{\hbar}{\gamma}(A_+\alpha_+ + A_-\alpha_-) = 1. \tag{73}$$

We find

$$A_+ = -A_- = \frac{\gamma/\hbar}{\sqrt{(\omega-\omega_{21})^2 + 4\gamma^2/\hbar^2}}. \tag{74}$$

The end result then is

$$\begin{aligned} c_1(t) &= e^{i\frac{1}{2}(\omega-\omega_{21})t}\left\{\frac{-i(\omega-\omega_{21})}{\sqrt{(\omega-\omega_{21})^2+4\gamma^2/\hbar^2}}\sin\frac{1}{2}\sqrt{(\omega-\omega_{21})^2+4\gamma^2/\hbar^2}\ t\right. \\ &\quad \left. + \cos\frac{1}{2}\sqrt{(\omega-\omega_{21})^2+4\gamma^2/\hbar^2}\ t\right\} \end{aligned} \tag{75}$$

$$c_2(t) = -ie^{-i\frac{1}{2}(\omega-\omega_{21})t}\frac{2\gamma/\hbar}{\sqrt{(\omega-\omega_{21})^2+4\gamma^2/\hbar^2}}\sin\frac{1}{2}\sqrt{(\omega-\omega_{21})^2+4\gamma^2/\hbar^2}\ t. \tag{76}$$

The probability for the state 1 to evolve to state 2 is

$$|c_2|^2 = \frac{4\gamma^2/\hbar^2}{(\omega-\omega_{21})^2+4\gamma^2/\hbar^2}\sin^2\frac{1}{2}\sqrt{(\omega-\omega_{21})^2+4\gamma^2/\hbar^2}\ t. \tag{77}$$

This is the important equation Eq. (5.5.21a) in Sakurai.

In many cases, were are interested in the situation where γ is small. Then for most values of ω, $|c_2|^2 \sim 4\gamma^2/\hbar^2(\omega-\omega_{21})^2 \ll 1$ and hence the transition is negligible. However for a narrow range of $|\omega-\omega_{21}| \simeq \gamma/\hbar$, the probability is non-negligible. In particular, the probability oscillates between zero and unity *on resonance* $\omega = \omega_{21}$.

On the other hand, in many cases we are also interested in the phase information beyond the probabilities. On the resonance $\omega = \omega_{21}$, $c_i(t)$ simplify drastically to

$$\begin{aligned} c_1(t) &= \cos\frac{\gamma}{\hbar}t \\ c_2(t) &= -i\sin\frac{\gamma}{\hbar}t \end{aligned} \tag{78}$$

5.2 Nuclear Magnetic Resonance

The Nuclear Magnetic Resonance (NMR) uses the exact solution obtained in the previous section to study the composition of a material in a completely non-destructive fashion. Because of this feature, it is used in the Magnetic Resonance Imaging (MRI) in medicine to take picture of the slices of your body. Even though I'm no expert on this imaging technique, I can at least describe the basic concepts behind it.

Consider nuclear spins in a strong magnetic field. For the sake of clarify, let us assume that we are talking about hydrogen atoms and protons as their nuclei. The magnetic moment interaction is nothing but

$$H_0 = -g_p \frac{e}{2m_p c} \vec{S}_p \cdot \vec{B} = -2.79 \times 2 \frac{e}{2m_p c} S_{zp} B_z, \tag{79}$$

assuming $\vec{B} = (0, 0, B_z)$. For spin up and down states, this Hamiltonian gives the two state system as in Eq. (57). To find the numerical value, we use $\mu_N = \frac{e\hbar}{2m_p c} = 3.152 \times 10^{-14}$MeV/T, and we obtain

$$H_0 = 8.79 \times 10^{-8}\text{eV} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{B}{\text{T}}. \tag{80}$$

The resonance frequency is therefore

$$\nu_r = \frac{\omega_r}{2\pi} = \frac{E_2 - E_1}{2\pi\hbar} = 42.5 \text{ MHz } \frac{B}{\text{T}}, \tag{81}$$

in the radio range for a magnetic field in the multi-tesla range.

We apply a time-varying magnetic field in the x-direction,

$$V = -g_p \frac{e}{2m_p c} S_{xp} B_x \cos\omega t, \tag{82}$$

where I ignored the space-dependence because it has a longer wave length than the body parts in the radio range and the magnetic field can be regarded approximately constant. Typically B_x is much smaller than B_z and hence γ in the resonance is narrow; therefore practically the only interest is when ω satisfies the resonance condition exactly. We decompose $\cos\omega t = \frac{1}{2}(e^{+i\omega t} + e^{-i\omega t})$, and only one term satisfies the resonance condition. Therefore we can ignore the wrong frequency component and keep only the resonant term in V. Then the Hamiltonian has precisely the form in Eq. (57).

On resonance, we can use the amplitudes given in Eq. (78). The spin state goes around a full circle,

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \to \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \to \begin{pmatrix} 0 \\ -i \end{pmatrix} \to \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ -i \end{pmatrix} \to \begin{pmatrix} -1 \\ 0 \end{pmatrix}. \tag{83}$$

The second state is the spin pointing along the negative y-axis, the third along the negative z-axis, the fourth along the positive y-axis, and the last state is back along the positive z-axis (even though the 2π rotation gives an overall minus sign of the state because of the half-odd spin). On the other hand, *off resonance*, the spin barely moves at all.

For the use of imaging, we would like to pick up a *slice* of your, say, brain. This is achieved by creating a slight gradient in the B_z field. If, for instance, $B_z(z)$ depends slowly as a function of z, only the slice of z which satisfies the resonance condition makes the nuclear spins rotate.

The temperature of a human body is not cold enough to *freeze* the nuclear spins. In the strong magnetic field, however, the spins are not completely random; there is a slight preference for the proton spins to be along the magnetic field. The measurements can be done with enough sensitivity to pick up the small difference in the populations of different spin states. For the rest of the discussions, I assume that all spins are initially along the magnetic field for simplicity.

The way the MRI works is that you apply the oscillatory magnetic field (radio wave) just for the duration that the spin is rotated from the positive z-axis to the negative y-axis, the so-called "90° pulse." In most parts of the brain (or whatever), the resonance condition is not satisfied and the spins are still along the z-direction. Only in the slice where the resonance condition is satisfied, the spins rotate to point along the negative y-axis. Then you turn off the radio.

The spins along the negative y-axis start to precess around the z-axis because of B_z. Because *all* of them in this slice precess together, there is a macroscopic size of a magnetic moment that precesses and produce an oscillating dipole magnetic field that can be detected by a coil thanks to the induced electricity.

To obtain x and y information on the picked z-slice, you combine "phase encoding gradient" and "frequency encoding gradient." After you turn off the radio, the first step is to provide a slight gradient in B_z along the x direction. Within the z-slice (elsewhere spins are ligned up with z), spins start along the y direction, and start to precess. Now that $B_z(x)$ depends

slightly on x, the amount of precession angle θ is a function of x, $\theta(x)$. This is the "phase encoding." Next, you turn off the gradient along the x-axis, and turn on a gradient along the y-axis. Spins precess around the z-axis with different frequencies $\omega(y)$. This is the "frequency encoding." At the end of the day, the spin precession goes like $\cos(\omega(y)t+\theta(x))$, keeping both x and y information within the specified z-slice. By Fourier transform, you recover y information, and the phase in each Fourier component gives x information. This way, you recover full three-dimensional information. (Of course, $\theta(x)$ is prediodic and the information gets ambiguous. By doing it several times with different gradients for phase encoding, you can resolve the ambiguity.)

For the study of the chemical composition, however, the most important pieces of information are the "relaxations." The purely quantum mechanical motion of spins is disturbed by their interaction with the environment, which leads to the *relaxation* of the oscillatory signal. There are two components to the relaxation. One of them ("spin-spin relaxation") is that the spins that originally precess together begin to *dephase*, namely some of them go slower than the rest, and the magnetic moments do not exactly add up any more. Even though each spins are still rotating, the macroscopic magnetic moment gets reduced exponentially over a time scale called T_2. The relaxation can occur due to the spin-exchange reactions (two spins may interact to go from $|\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\rangle$, etc) or the chemical exchange (two atoms get swapped between two molecules). The other (slower) relaxation is that the z-component of the spins goes back to its equilibrium population. During the spin precession (especially after dephasing) the spins are more or less randomized without a net magnetic moment along the z-axis, but after the interaction of spins with the environment ("spin-lattice relaxation"), they reach the population in the thermal equilibrium over a time scale called T_1. Two relation times T_1 and T_2 tell us the environment the spins live in, giving us information about the chemical composition of the material, either water, fat, a kind of tumor, etc.

I consulted web sites "The Basics of MRI" by J.P. Hornak, `http://www.cis.rit.edu/htbooks/mri/`, and numerous other web sites I don't remember anymore (sorry!).

6 Sudden and Adiabatic Approximations

A type of time-dependent Hamiltonian of interest is

$$H = \begin{cases} H_1 & t < t_1 \\ H(t) & t_1 < t < t_2 \\ H_2 & t > t_2 \end{cases} \tag{84}$$

Namely, the Hamiltonian changes from H_1 to H_2 over a time interval $\tau = t_2 - t_1$. Assuming that the initial state was an eigenstate of the original Hamiltonian H_1, we would like to know what kind of state we have at $t = t_2$ beyond which the system evolves according to the Hamiltonian H_2.

There are two extreme cases of interest. One is when the change is *sudden*, namely when τ is small. The other is when the change is *slow*, namely when τ is large. We discuss each case separately, and then interesting examples.

6.1 Sudden Approximation

When the Hamiltonian is changed *suddenly*, the state cannot catch up with the change and basically remains unchanged. This is the basis of the sudden approximation.

Under this approximation, the initial state at $t = t_1$

$$H_1|i_1\rangle = E_{i_1}|i_1\rangle \tag{85}$$

is used unchanged at $t = t_2$,

$$|\psi(t_2)\rangle = |i_1\rangle. \tag{86}$$

Beyond this point, the state evolves according to the Hamiltonian H_2, which can be worked out by its eigenstates and eigenvalues,

$$|\psi(t)\rangle = e^{-iH_2(t-t_2)/\hbar}|i_1\rangle = \sum_f e^{-iE_{f_2}(t-t_2)/\hbar}|f_2\rangle\langle f_2|i_1\rangle. \tag{87}$$

The sudden approximation is expected to be good if the time scale of the change τ is much smaller than the typical energy splittings ΔE among the energy levels

$$\tau \ll \frac{\hbar}{\Delta E}. \tag{88}$$

This is because the appreciable change in the state is possible only when different terms in a linear combination acquire substantially different phases,

$$e^{-iHt/\hbar}\sum_n c_n|n\rangle = e^{-iE_it/\hbar}\sum_n c_n|n\rangle e^{-i(E_n-E_i)t/\hbar}, \tag{89}$$

requiring $t \gtrsim \hbar/(E_n - E_i)$. In other words, the *response time* of a state is given by the energy-time uncertainty principle $\Delta t \sim \hbar/\Delta E$, and the quick change of the Hamiltonian within $\tau \ll \Delta t$ does not change the state appreciably.

For instance, the beta decay of the tritium $^3\mathrm{H} \to {}^3\mathrm{He} + e^- + \bar{\nu}_e$ changes the nuclear charge $Z = 1$ *suddenly* to $Z = 2$. The average kinetic energy of the beta electron is $K = \frac{1}{2}mv^2 = 5.7\mathrm{keV}$, and hence the velocity of the electron is $\sqrt{2K/m} = 0.15c$. The electron escapes the atom within time of approximately $\tau = a_B/(0.15c) = 0.529\text{Å}/(0.15c) = 1.2 \times 10^{-18}\mathrm{sec}$. In comparison, the smallest energy difference that involves the ground state is $\Delta E = E_{n=2} - E_{n=1} = 10$ eV, and hence the relevant time scale is $\hbar/\Delta E = 6.4 \times 10^{-17}\mathrm{sec}$. Therefore, $\tau \ll \hbar/\Delta E$ and the sudden approximation is justified. In most other beta decays, the kinetic energy of the beta electron is much larger (MeV scale) and the approximation is even better.

6.2 Adiabatic Approximation

When the Hamiltonian is changed *slowly*, the state does not realize that it is subject to a time-dependent Hamiltonian, and simply tracks the *instantaneous eigenstates*. This is the basis of the adiabatic approximation.

Under this approximation, you first solve the eigenvalue problem of the Hamiltonian at each t,

$$H(t)|i\rangle_t = E_i(t)|i\rangle_t. \tag{90}$$

The eigenstates are called the *instantaneous eigenstates* because they diagonalize the Hamiltonian at each instance. Note that the subscript $_t$ indicates that it is the eigenstate at the instance t, as opposed to the true time dependence of the state $|i(t)\rangle$. The adiabatic approximation gives

$$|i(t)\rangle = e^{-i\int_{t_1}^t dt' E_i(t')} e^{i\phi(t)}|i\rangle_t, \tag{91}$$

namely that the actual time evolution of the state tracks the instantaneous eigenstates. The *dynamical phase* is the integral of the instantaneous energy eigenvalues $E_i(t)$ over the period. In addition, there may be the *geometrical phase* $\phi(t)$, which we will discuss later.

Since this is the opposite of the sudden approximation, the adiabatic approximation is expected to be good if the time scale of the change τ is much smaller than the response time,

$$\tau \ll \Delta t \sim \frac{\hbar}{\Delta E}. \tag{92}$$

The formalism defines the rotating axis representation. It basically defines a new picture where the basis kets are the instantaneous Hamiltonian eigenstates. For detailed discussions of the applicability of the adiabatic approximation, see, *e.g.*, "Quantum Mechanics," by Albert Messiah, Amsterdam, North-Holland Pub. Co. (1961).

The extent that the adiabatic approximation is violated can be expressed by the "hopping probability," namely the probability for one instantaneous eigenstate to "hop" to another instantaneous eigenstate. There are exact solutions for many examples of the type

$$H = \begin{pmatrix} \beta_1 t & V \\ V & \beta_2 t \end{pmatrix}. \tag{93}$$

In the infinite past, V is negligible and the Hamiltonian eigenstates are simply upper or lower components. At $t = 0$, however, the diagonal elements vanish and the two states mix maximally. Because of the no level crossing theorem, the two states always remain non-degenerate; however they may come quite close, violating the condition $\tau \ll \hbar/\Delta E$. When $A(t)$ is linear in time, it is called the Landau–Zener model (L.D. Landau, *Phys. Z. Sowjetunion* **2** 46 (1932); C. Zener, *Proc. R. Soc.* **A 137** 696 (1932)). The hopping probability was found to be

$$P_h = e^{-2\pi V^2/\hbar|\beta_1 - \beta_2|}. \tag{94}$$

The time scale for which the off-diagonal term V is important is approximately $\tau = V/|\beta_1 - \beta_2|$, while the minimum difference between two instantaneous energy eigenvalues is $\Delta E = 2V$. Therefore we expect the hopping probability is suppressed when $\tau \gg \hbar/\Delta E$. Indeed the negative exponent is approximately $\tau \Delta E/\hbar \gg 1$.

The neutrinos generated by the fusion process in the Sun's core propagate through the entire mass of the Sun. Because the electron neutrino has the potential energy due to its interaction with the electrons in the plasma, they experience the time-dependent Hamiltonian of this type. For the high-energy component of the neutrinos $E \gtrsim 1$MeV, the transition is adiabatic, while the

low-energy component $E \lesssim 0.1$MeV it is sudden. This energy dependence explains why different experiments had measured different fluxes of solar neutrinos, albeit all of them had been much less than predicted.

The adiabatic approximation crucially relies on the assumption that one can continuously connect instantaneous eigenstates over a period uniquely. In particular, a degeneracy of energy levels invalidates the approximation. Assuming that the energy levels maintain non-degeneracy, one still needs to connect the instantaneous eigenstates from one time to next. Therefore, it defines a complex line bundle over the space of parameters in the Hamiltonian whose section is the instantaneous eigenstates $|i\rangle_t$. A complex line bundle requires a connection ("vector potential" in a generalized sense) $\langle i|_t \frac{d}{dt}|i\rangle_t$ which is used to relate the phase convention of the state at different times. Therefore the phase $\phi(t)$ is related to the geometry of the fiber bundle, hence the name the "geometrical phase" or the "topological phase." M.V. Berry was the first one to realize this point clearly, published in "*Quantal phase factors accompanying adiabatic changes*," *Proc. R. Soc. Lond.* **A 392**, 45 (1984). In particular, when the space of parameters in the Hamiltonian is singular, as in the example of the rotating magnetic field we will discuss in the next section, the line bundle is twisted with non-zero Chern class. In such a case, the geometric phase cannot be eliminated and has experimental consequences, *e.g.*, in T. Bitter and D. Dubbers, "*Manifestation of Berry's topological phase in neutron spin rotation*," *Phys. Rev. Lett.*, **59**, 251 (1987). See Supplement I in Sakurai for more on this point.

6.3 Example

A good example is the spin in the time-dependent magnetic field. Consider the magnetic field

$$\vec{B} = (B_x, B_y, B_z) = B(\sin\theta\cos\omega t, \sin\theta\sin\omega t, \cos\theta). \tag{95}$$

The magnitude of the magnetic field is constant, while the direction rotates around the z-axis.

The Hamiltonian is

$$\begin{aligned} H = -\vec{\mu}\cdot\vec{B} &= -\mu B \begin{pmatrix} \cos\theta & \sin\theta e^{-i\omega t} \\ \sin\theta e^{i\omega t} & -\cos\theta \end{pmatrix} \\ &= \mu B_z \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} - \mu B_\perp \begin{pmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{pmatrix}. \end{aligned} \tag{96}$$

Here, I used $B_z = B\cos\theta$, $B_\perp = B\sin\theta$. This Hamiltonian is the same as the exactly solvable Hamiltonian Eq. (57) upon replacements $\omega \to -\omega$,

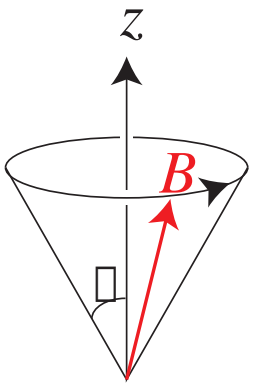

Figure 3: Time-dependent magnetic field of Eq. (95).

$E_1 \to -\mu B_z$, $E_2 \to \mu B_z$, $\gamma \to -\mu B_\perp$. The frequencies in Eq. (68) are

$$\alpha_\pm = \frac{1}{2\hbar}\left[(\hbar\omega + 2\mu B_z) \pm \sqrt{(\hbar\omega + 2\mu B_z)^2 + 4\mu^2 B_\perp^2}\right]. \tag{97}$$

The solution with $A_- = 0$ in Eqs. (69,70) gives

$$\psi(t) = A_+ \begin{pmatrix} \frac{\hbar}{\gamma}\alpha_+ e^{-i\omega t} \\ 1 \end{pmatrix} e^{-i(\mu B_z - \hbar\alpha_+)t/\hbar}. \tag{98}$$

First we consider the *fast* change of the Hamiltonian, $\omega \gg \omega_{21} = 2\mu B_z/\hbar$. The Hamiltonian changes by a finite amount within the time period $\tau \sim 1/\omega$. Neglecting corrections suppressed by $\mu B/\hbar\omega$, $\alpha_+ \simeq \omega$ and

$$\psi(t) = \begin{pmatrix} e^{-i\omega t} \\ 0 \end{pmatrix} e^{i\omega t}, \tag{99}$$

and the time-dependence cancels. Namely the state hardly *moves* over the time interval $\tau \sim 1/\omega$.

Now we consider the *slow* change of the Hamiltonian, $\omega \ll \omega_{21} = 2\mu B_z/\hbar$. The phase is given by

$$\begin{aligned} \mu B_z - \hbar\alpha_+ &= -\frac{1}{2}\left[\hbar\omega + \sqrt{(\hbar\omega + 2\mu B_z)^2 + 4\mu^2 B_\perp^2}\right] \\ &= -\mu B - \frac{1}{2}\hbar\omega(1 + \cos\theta) + O(\hbar\omega)^2. \end{aligned} \tag{100}$$

We had to consider $O(\hbar\omega)$ terms because the phase factor is multiplied by t and we regard $\omega t \sim O(1)$ to account for a finite change in the Hamiltonian. On the other hand, when $O(\omega)$ corrections is not enhanced by $t \sim 1/\omega$, we can safely ignore them. Therefore, up to this order, the exact solution in Eq. (98) becomes

$$\begin{aligned} \psi(t) &= A_+ \begin{pmatrix} -\frac{(B+B_z)}{B_\perp} e^{-i\omega t} \\ 1 \end{pmatrix} e^{-i(\mu B_z - \hbar\alpha_+)t/\hbar} \\ &= \begin{pmatrix} -\cos\frac{\theta}{2} e^{-i\omega t} \\ \sin\frac{\theta}{2} \end{pmatrix} e^{i\mu Bt/\hbar} e^{i(1+\cos\theta)\omega t/2}. \end{aligned} \tag{101}$$

In the last step, we chose A_+ to properly normalize the state. The state is always the *instantaneous eigenstate* of the Hamiltonian with the eigenvalue $E = -\mu B$.

The last phase factor is the Berry's phase. When the magnetic field rotates around the z-axis once, $\omega t = 2\pi$, and the phase is $e^{i\pi(1+\cos\theta)} = e^{im\Omega}$, where $m = 1/2$ is the magnetic quantum number $S_z = m\hbar$, and Ω is the area swept by the magnetic field $\Omega = \int_{-1}^{\cos\theta} d\cos\theta' \int_0^{2\pi} d\phi = 2\pi(1+\cos\theta)$.

The Berry's phase is non-trivial in this case because the line bundle is singular at the origin $\vec{B} = 0$ where the states with different m become degenerate. In order to consistently define the complex line bundle, the origin must be removed from the base space, and hence the base space is topologically equivalent to $S^2 \times \mathbb{R}$. This base manifold supports first Chern class c_1. The complex line bundle is in fact twisted.