Lecture 1

Dynamics and control of open quantum systems

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This lecture covers time-dependent perturbation theory, and several examples. The material here follows closely J. J. Sakurai, *Modern Quantum Mechanics*, Addison-Wesley (1994), for the time-dependent perturbation theory, and Albert Messiah's *Quantum Mechanics*, Dover Publications, 1999, Chapter VIII, for Heisenberg and Dirac picture.

I. HEISENBERG AND DIRAC PICTURES

Let's revisit the second postulate of quantum mechanics and go into more detail regarding the time evolution operator. We have

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle\,, \tag{1}$$

where U is a unitary operator. For Hamiltonian H time-independent, we have $U(t,t_0) = e^{-iH(t-t_0)/\hbar}$. Defining the derivative with respect to time of an operator $O(t)$ as the limit $\lim_{\epsilon\to 0}\frac{O(t+\epsilon)-O(t)}{\epsilon}$, one can show

$$i\hbar\frac{dU(t,t_0)}{dt} = HU(t,t_0). \tag{2}$$

$U(t,t_0)$ solves this first-order ordinary differential equation with initial condition $U(t_0,t_0) = I$. Even if H is time-dependent, and so $U(t,t_0) \neq e^{-iH(t-t_0)/\hbar}$, the equations above can be postulated as the definition of U.

The equations above are equivalent to an integral equation, $U(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} HU(t',t_0)$. Differentiating Eq. (1) with respect to time gives $\frac{d}{dt}|\psi(t)\rangle = \frac{d}{dt}U(t,t_0)\,|\psi(t_0)\rangle$, and using

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Eq. (2), one finds $i\hbar\frac{d}{dt}|\psi(t)\rangle = HU(t,t_0)|\psi(t_0)\rangle = H|\psi(t)\rangle$. So we could have taken Eq. (1) and Eq. (2) as postulates, and only then derived the Schrödinger equation formulation of the second postulate.

Exercises: a) Show that if $U(t,t_0)$ is differentiable with respect to time t and unitary, then $H(t) = i\hbar\left(\frac{d}{dt}U(t)\right)U^\dagger(t)$ is Hermitian. b) If $U(t)$ satisfies $i\hbar\frac{dU}{dt} = HU$, with H Hermitian and time-dependent, then $U^\dagger U$ is time independent, and $i\hbar\frac{d}{dt}(UU^\dagger) = [H, UU^\dagger]$. In particular, if $U(t=t_0)$ is unitary, then it remains so at all times $t \geq t_0$.

So far, we have formulated the postulates of quantum mechanics in the *Schrödinger picture*. There is an equivalent formulation of the second postulate, in what is called the *Heisenberg picture*. We establish below the relationship between these two pictures. For ease of interpretation, we denote quantities pertaining to Schrödinger picture with a subscript S, and those pertaining to Heisenberg picture by a subscript H. Schrödinger picture states, as discussed so far, are time-dependent $|\psi_S(t)\rangle = U(t,t_0)|\psi_S(t_0)\rangle$. We can turn them into time-independent kets by applying the unitary operator $U^\dagger(t,t_0)$. This gives $|\psi_H(t)\rangle \equiv U^\dagger(t,t_0)|\psi_S(t)\rangle = |\psi_S(t_0)\rangle$. As opposed to their counterparts in the Schrödinger picture, states are time-independent in the Heisenberg picture. On the other hand, time-independent observables become time dependent, namely $O_H(t) \equiv U^\dagger(t,t_0)O_S U(t,t_0)$. The previous equation can be written more generally as $O_H(t) \equiv U^\dagger(t,t_0)O_S(t)U(t,t_0)$ to allow for an observable that has an explicit time-dependence in the Schrödinger picture (such as, for example, terms entering the Hamiltonian of an externally-controlled system).

Differentiating the previous equation term by term, using the differential definition of the time-evolution operator Eq. (2), we find $i\hbar\frac{d}{dt}O_H(t) = i\hbar\dot{U}^\dagger(t,t_0)O_S(t)U(t,t_0) + i\hbar U^\dagger(t,t_0)\dot{O}_S(t)U(t,t_0) + i\hbar U^\dagger(t,t_0)O_S(t)\dot{U}(t,t_0) = U^\dagger(t,t_0)[O_S(t),H(t)]U(t,t_0) + i\hbar U^\dagger(t,t_0)\frac{\partial O_S}{\partial t}U(t,t_0)$. For the last term we write $U^\dagger(t,t_0)\frac{\partial O_S}{\partial t}U(t,t_0) = \frac{\partial O_H}{\partial t}$, with the understanding that this is the Heisenberg-picture operator corresponding to the Schrödinger picture operator $\partial O_S(t)/\partial t$. Moreover, letting $H_H(t) = U^\dagger(t,t_0)H(t)U(t,t_0)$, we arrive at the *Heisenberg equation of motion*

$$i\hbar\frac{dO_H(t)}{dt} = [O_H(t), H_H(t)] + i\hbar\frac{\partial O_H}{\partial t}. \tag{3}$$

Exercises: a) Let $H = \frac{\hbar\omega_q}{2}\sigma^z$ and let $\sigma^\pm = \frac{1}{2}(\sigma^x \pm i\sigma^y)$. Find $\sigma_H^\pm(t), \sigma_H^z(t)$. b) If $[O,H]=0$, and O is explicitly time independent, then O_H is time independent.

There is an intermediate picture, called the *interaction*, or *Dirac*, picture. We present it here since our future discussion of perturbation theory will rely on it. We postulated Eq. (2), the differential definition of the time evolution operator $U(t, t_0)$. Suppose you knew an approximate solution to this equation, $U^{(0)}(t, t_0)$. It is convenient to set $U(t, t_0) = U^{(0)}(t, t_0)U'(t, t_0)$, where $U'(t, t_0)$ is also unitary. To piece together a solution $U(t, t_0)$, we are interested in the dynamics of $U'(t, t_0)$. By using Eq. (2), we have

$$i\hbar\frac{d}{dt}U'(t, t_0) = U^{(0)\dagger}(t, t_0)\left[H(t)U^{(0)}(t, t_0) - i\hbar\frac{dU^{(0)}(t, t_0)}{dt}\right]U'(t, t_0), \tag{4}$$

with initial condition $U'(t_0, t_0) = I$. If $U^{(0)}(t, t_0)$ was a good enough approximate solution to Eq. (2), then the term in the bracket almost vanishes, and hence $U'(t, t_0)$ is almost constant. Let's define a new Hamiltonian $H^{(0)}(t) = i\hbar\left[\frac{d}{dt}U^{(0)}(t, t_0)\right]U^{(0)\dagger}(t, t_0)$ such that $i\hbar\frac{d}{dt}U^{(0)}(t, t_0) = H^{(0)}(t)U^{(0)}(t, t_0)$. Then let $H = H^{(0)} + H'$. In accordance with the discussion above, H' is an operator considered as perturbation, and $H^{(0)}$ is an operator whose time-evolution operator is known. Then

$$i\hbar\frac{d}{dt}U'(t, t_0) = H'_I U'(t, t_0), \tag{5}$$

where $H'_I(t) = U^{(0)\dagger}(t, t_0)H'U^{(0)}(t, t_0)$. The task of perturbation theory, as we will discuss in Lecture 3, is to provide strategies to solve the equation above. As for kets and operators, just as in the Heisenberg picture we may write $|\psi_I(t)\rangle = U^{(0)^\dagger}(t, t_0)\,|\psi_S(t)\rangle$, and $O_I(t) = U^{(0)^\dagger}(t, t_0)O_S U^{(0)}(t, t_0)$. Hence, the Schrödinger equation in the interaction picture is $i\hbar\frac{d}{dt}|\psi_I(t)\rangle = H'_I|\psi_I(t)\rangle$, and the equation analogue to the Heisenberg equation of motion is $i\hbar\frac{d}{dt}O_I = [O_I, H_I^{(0)}] + i\hbar\frac{\partial O_I}{\partial t}$.

II. TIME-DEPENDENT PERTURBATION THEORY

Consider a static Hamiltonian with a time-dependent perturbation,

$$H(t) = H_0 + \lambda V(t). \tag{6}$$

We want to find $|\psi(t)\rangle$ that solves the time-dependent Schrödinger equation, expanded over the known eigenbasis $|n\rangle$ of H_0 (note the change of notation from the previous section).

Let's revisit in this notation the interaction picture, introduced previously in Lecture 2. We can define

$$|\psi(t)\rangle_I = e^{iH_0t/\hbar}\,|\psi(t)\rangle_S\,, \tag{7}$$

$$O_I = e^{iH_0t/\hbar}O_S e^{-iH_0t/\hbar}, \tag{8}$$

where we recall that the subscript S appears to distinguish Schrödinger picture operators from interaction-picture operators. Here, using the second equation for the perturbation operator appearing in Eq. (6), we get

$$V_I(t) = e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar}. \tag{9}$$

Then the following Schrödinger-like equation holds for the interaction-picture wavefunction

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle_I = V_I(t)\left|\psi(t)\right\rangle_I, \tag{10}$$

and the following Heisenberg-like equation holds for operators in the interaction picture

$$\frac{dO_I(t)}{dt} = \frac{1}{i\hbar}[O_I(t), H_0]. \tag{11}$$

The problem to find $|\psi(t)\rangle$ reduces to finding its expansion over the eigenbasis of H_0

$$|\psi(t)\rangle = \sum_n c_n(t)\left|n\right\rangle. \tag{12}$$

To do perturbation theory, we shall assume that $c_n(t)$ can be expanded as a series

$$c_n(t) = c_n^{(0)} + c_n^{(1)} + \ldots, \tag{13}$$

where the superscript indicates the order in λ.

The time evolution operator $U_I(t, t_0)$ in the interaction picture is defined as

$$\left|\psi(t)\right\rangle_I = U_I(t, t_0)\left|\psi(t_0)\right\rangle_I, \tag{14}$$

which together with the Schrödinger equation gives the following equation of motion for the time evolution operator

$$i\hbar\frac{d}{dt}U_I(t, t_0) = V_I(t)U_I(t, t_0), \tag{15}$$

with initial condition $U_I(t_0, t_0) = I$. This ordinary differential equation can be brought to integral form

$$U_I(t, t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')U_I(t', t_0)dt'. \tag{16}$$

The main result of this section, the Dyson series, is derived by iteratively plugging in the left-hand side of this equation into its right-hand side

$$
\begin{aligned}
U_I(t,t_0) &= I - \frac{i}{\hbar}\int_{t_0}^{t} dt' V_I(t')\left[1 - \frac{i}{\hbar}\int_{t_0}^{t'} dt'' V_I(t'')U_I(t'',t_0)\right] \\
&= I - \frac{i}{\hbar}\int_{t_0}^{t} dt' V_I(t') \\
&\quad + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' V_I(t')V_I(t'') \\
&\quad + \dots \\
&\quad + \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \dots \int_{t_0}^{t^{(n-1)}} dt^{(n)} V_I(t')V_I(t'')\dots V_I(t^{(n)}) \\
&\quad + \dots
\end{aligned}
\tag{17}
$$

The Dyson series allows us to evaluate *transition probabilities.*

Transition probabilities

Note that

$$
|\psi(t)\rangle_I = U_I(t,t_0)\,|i\rangle = \sum_n |n\rangle\,\langle n|\,U_I(t,t_0)\,|i\rangle \equiv \sum_n |n\rangle\, c_n(t) \tag{18}
$$

So the coefficient $c_n(t)$ in the expansion of the wavefunction in the interaction picture corresponds to a matrix element of the time evolution operator in the interaction picture. Moreover, this is easily related to matrix elements of the time evolution operator in the Schrödinger picture, that is

$$
\langle n|\,U_I(t,t_0)\,|i\rangle = e^{i(E_n t - E_i t_0)/\hbar}\,\langle n|\,|U(t,t_0)\,|i\rangle\,, \tag{19}
$$

since by definition $U_I(t,t_0) = e^{iH_0t/\hbar}U(t,t_0)e^{-iH_0t_0/\hbar}$. Here, $\langle n|\,U(t,t_0)\,|i\rangle$ is interpreted as the transition amplitude for a transition into state $|n\rangle$ at time t if the system was prepared in state $|i\rangle$ at time t_0. Then $|\,\langle n|\,U(t,t_0)\,|i\rangle\,|^2$ is interpreted as the *transition probability.* Note that the transition probability is the same whether evaluated in the Schrödinger picture or in the interaction picture, as the two amplitudes differ only by a phase factor *when* $|n\rangle$ *and* $|i\rangle$ *are energy eigenstates of* H_0.

Then the probability to measure the system in state $|n\rangle$ at time t, having prepared the system in state $|i\rangle$ at time t_0, is

$$|c_n(t)|^2 = |\langle n| U_I(t,t_0) |i\rangle|^2 = |c_n^{(0)}(t) + c_n^{(1)}(t) + \ldots|^2, \tag{20}$$

where the first two terms are given by

$$\begin{aligned}
c_n^{(0)}(t) &= \delta_{ni}, \\
c_n^{(1)}(t) &= -\frac{i}{\hbar}\int_{t_0}^{t} dt' \,\langle n| V_I(t') |i\rangle \\
&\equiv -\frac{i}{\hbar}\int_{t_0}^{t} dt' e^{i\omega_{ni}t'} V_{ni}(t') \\
c_n^{(2)}(t) &= \left(\frac{-i}{\hbar}\right)^2 \sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' e^{i\omega_{nm}t'} V_{nm}(t') e^{i\omega_{mi}t''} V_{mi}(t''),
\end{aligned} \tag{21}$$

with $\omega_{ni} = \Delta_{ni}/\hbar$ and $\Delta_{ni} = E_n - E_i$, analogous to the notation in the previous section. Then the transition probability is $P(i \to n) = |c_n^{(1)}(t) + c_n^{(2)}(t) + \ldots|^2$.

III. TIME-DEPENDENT PERTURBATION THEORY. EXAMPLES

A. Constant perturbation, turned on at $t = 0$

Consider the following time-dependent perturbation. It is a constant perturbation operator V that is turned on at $t = 0$

$$V(t) = \begin{cases} 0, & \text{for } t < 0 \\ V \ \ (\text{independent of } t), & \text{for } t \geq 0 \end{cases} \tag{22}$$

Assume that the system is prepared in one of the eigenstates of H_0, $|i\rangle$, at $t = 0$. Then using Eq. (21) we have

$$\begin{aligned}
c_n^{(0)} &= c_n^{(0)}(0) = \delta_{in}, \\
c_n^{(1)} &= \frac{-i}{\hbar} V_{ni} \int_0^t e^{i\omega_{ni}t'} dt' = \frac{V_{ni}}{E_n - E_i}\left(1 - e^{i\omega_{ni}t}\right),
\end{aligned} \tag{23}$$

This gives the following for the transition probability defined above, obtained to lowest nontrivial order in the small perturbation

$$\left|c_n^{(1)}\right|^2 = \frac{|V_{ni}|^2}{|E_n - E_i|^2}(2 - 2\cos\omega_{ni}t) = \frac{4\,|V_{ni}|^2}{|E_n - E_i|^2}\sin^2\left[\frac{(E_n - E_i)\,t}{2\hbar}\right]. \tag{24}$$

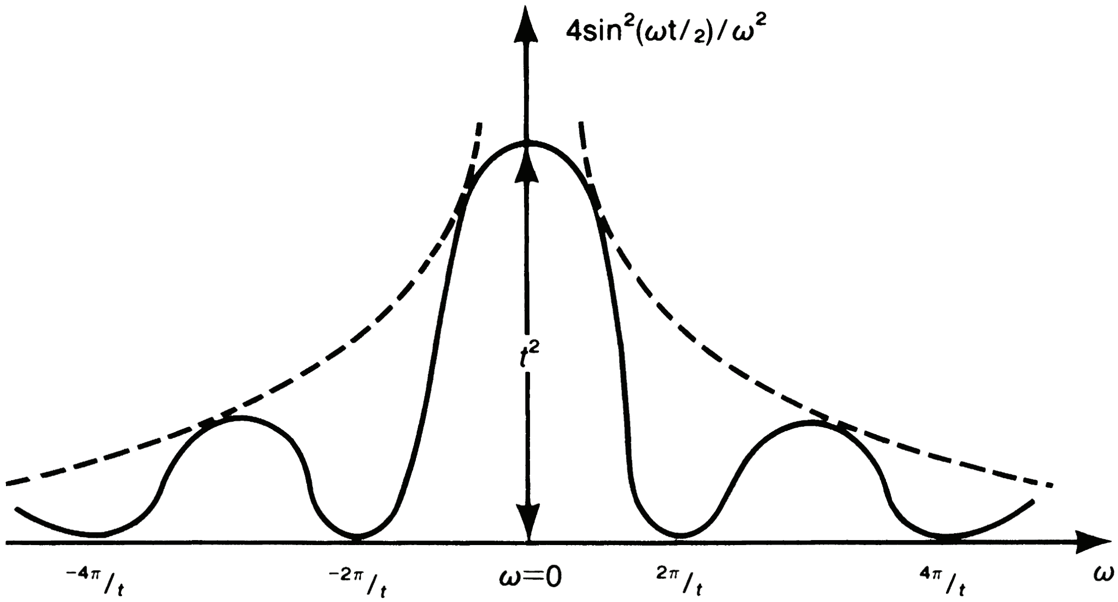

FIG. 1. Plot of $\propto 4\sin^2[\omega t/2]/\omega^2$ as a function of ω at constant time t after the perturbation Eq. (22) has been turned on. Reproduced from J. J. Sakurai, *Modern Quantum Mechanics*, Addison-Wesley 1994, page 330.

We are now interested in analyzing the frequency and time dependence of the transition probability from $i \to n$, Eq. (24). In a physical system, the energy spectrum of H_0, the set $\{E_n | n = 0, 1, 2, \ldots\}$, may have a large number of states of nearby energies, say around a given energy E_n; in some instances we can talk about a *continuum of states* around the energy E_n, and it then makes sense to rewrite the transition probability Eq. (24) in terms of the transition energy ω, defined as

$$\omega \equiv \frac{E_n - E_i}{\hbar}, \tag{25}$$

in which case the transition probability is $\propto 4\sin^2[\omega t/2]/\omega^2$, with the proportionality constant determined by the square of the matrix element of the perturbation. We plot this transition probability in Fig. 1. The transition probability is peaked for states whose energy is nearby E_i, i.e. $\omega = (E_n - E_i)/\hbar \approx 0$. The height of this peak scales as t^2, and its width scales as $1/t$. That is, for large t, only states $|n\rangle$ satisfying

$$t \sim \frac{2\pi}{|\omega|} = \frac{2\pi\hbar}{|E_n - E_i|} \tag{26}$$

have appreciable transition probability $|c_n^{(1)}|^2$ from the initial state $|i\rangle$. If we call the time t that the perturbation has been turned on Δt, then only those transitions have appreciable probability that satisfy

$$\Delta t \Delta E \sim \hbar. \tag{27}$$

This equation is not to be interpreted as of the same nature as the Heisenberg uncertainty principle. It indicates that for short time intervals Δt, the peak in Fig. 1 is broad, and therefore transitions to states with energy far detuned from the initial state have non-negligible probability. As time Δt this degree of energy nonconservation decreases, that is, only states with energy close to the initial state energy have appreciable transition probability from it.

Finally, note that for states $|n\rangle$ that are exactly degenerate with the initial state $|i\rangle$ in the spectrum of H_0, the transition probability depends quadratically on time

$$\left|c_n^{(1)}(t)\right|^2 = \frac{1}{\hbar^2}\left|V_{ni}\right|^2 t^2. \tag{28}$$

Note, however, that in practice, there is a continuum of states E_n around the energy E_i, as given by the density of states $\rho(E)$, where

$$\rho(E) dE \tag{29}$$

gives the number of states in the energy interval $[E, E + dE)$. The transition probability from the initial state $|i\rangle$ into those states with energy nearby E_i can therefore be expressed as

$$\begin{aligned} \sum_{n, E_n \approx E_i} \left|c_n^{(1)}\right|^2 &\to \int dE_n \rho\left(E_n\right) \left|c_n^{(1)}\right|^2 \\ &= 4 \int \sin^2\left[\frac{\left(E_n - E_i\right)t}{2\hbar}\right] \frac{\left|V_{ni}\right|^2}{\left|E_n - E_i\right|^2} \rho\left(E_n\right) dE_n, \end{aligned} \tag{30}$$

with the integral running over a neighborhood of E_i. Which neighborhood this is is not important in the limit $t \to \infty$, where we use

$$\frac{1}{\left|E_n - E_i\right|^2} \sin^2\left[\frac{\left(E_n - E_i\right)t}{2\hbar}\right] \sim \frac{\pi t}{2\hbar} \delta\left(E_n - E_i\right) \text{ as } t \to \infty. \tag{31}$$

We may then take the average of the matrix element squared over the states E_n with energy in the vicinity of E_i, $\overline{\left|V_{ni}\right|^2}$, outside of the integral sign, and perform the energy integral in Eq. (30) to get

$$\int dE_n \rho\left(E_n\right) \left|c_n^{(1)}(t)\right|^2 \sim \frac{2\pi}{\hbar} \overline{\left|V_{ni}\right|^2} \rho\left(E_n\right) t \bigg|_{E_n \approx E_i} \text{ as } t \to \infty. \tag{32}$$

Note that now the transition probability only scales linearly with the time t that the constant perturbation has been turned on, which is due to the fact that the total transition probability in the limit $t \to \infty$ should go like the area under the central peak of Fig. 1, that is $\sim t^2/t = t$. These facts all seem reasonable.

In practice, what we care about is the transition rate, that is the time-derivative of the transition probability $w_{i\to[n]} = \frac{d}{dt}\left(\sum_n \left|c_n^{(1)}\right|^2\right)$, where $[n]$ stands for the set of states with energy nearby E_i. Then

$$w_{i\to[n]} = \frac{2\pi}{\hbar}\overline{|V_{ni}|^2}\rho\left(E_n\right)_{E_n\simeq E_i}. \tag{33}$$

This is Fermi's Golden rule, a formula that we will be encountering again in this course. It gives a constant rate of transition, as a function of time, provided that first-order time-dependent perturbation theory is valid. This can be recast as

$$w_{i\to n} = \frac{2\pi}{\hbar}\left|V_{ni}\right|^2 \delta\left(E_n - E_i\right) \tag{34}$$

in the sense that it will be integrated over final state energies $\int dE_n \rho\left(E_n\right)$.

Second-order corrections. Virtual transitions

Going to next order in perturbation theory, we have

$$\begin{aligned} c_n^{(2)} &= \left(\frac{-i}{\hbar}\right)^2 \sum_m V_{nm}V_{mi}\int_0^t dt' e^{i\omega_{nm}t'}\int_0^{t'} dt'' e^{i\omega_{mi}t''} \\ &= \frac{i}{\hbar}\sum_m \frac{V_{nm}V_{mi}}{E_m - E_i}\int_0^t \left(e^{i\omega_{ni}t'} - e^{i\omega_{nm}t'}\right)dt'. \end{aligned} \tag{35}$$

The first term in the integrand has the same time dependence as the one in the first-order contribution. If this were the only term present, we would conclude that the only significant contribution as $t \to \infty$ occurs when the final state is near the initial state, i.e. $E_n \approx E_i$.

Putting the two together gives rise to (*exercise:* prove this)

$$w_{i\to[n]} = \frac{2\pi}{\hbar}\left|V_{ni} + \sum_m \frac{V_{nm}V_{mi}}{E_i - E_m}\right|^2 \rho\left(E_n\right)\Bigg|_{E_n\simeq E_i}. \tag{36}$$

The first term corresponds to nearly energy conserving *real* transitions. In the second term, the system first has an energy-nonconserving transition $i \to m$, then an energy non-conserving transition $m \to n$, while maintaining overall energy conservation, i.e. the final state energy $E_n \approx E_i$. The two intermediate transitions are said to be *virtual transitions.*

B. Harmonic perturbation

In this section, we consider the same problem but for a time-periodic perturbation

$$V(t) = \mathscr{V} e^{i\omega t} + \mathscr{V}^\dagger e^{-i\omega t} \tag{37}$$

where $\mathscr{V}$ is a linear operator acting on the Hilbert space of H_0, not necessarily Hermitian.

As before, using Eq. (21), we arrive at the lowest order correction

$$\begin{aligned} c_n^{(1)} &= \frac{-i}{\hbar} \int_0^t \left(\mathscr{V}_{ni} e^{i\omega t'} + \mathscr{V}_{ni}^\dagger e^{-i\omega t'} \right) e^{i\omega_{ni} t'} dt' \\ &= \frac{1}{\hbar} \left[\frac{1 - e^{i(\omega + \omega_{ni})t}}{\omega + \omega_{ni}} \mathscr{V}_{ni} + \frac{1 - e^{i(\omega_{ni} - \omega)t}}{-\omega + \omega_{ni}} \mathscr{V}_{ni}^\dagger \right] \end{aligned} \tag{38}$$

We can readily see that this result is analogous to the one obtained previously for a constant perturbation turned on at $t = 0$, but with the following change

$$\omega_{ni} = \frac{E_n - E_i}{\hbar} \to \omega_{ni} \pm \omega. \tag{39}$$

Thus, $c_n^{(1)}$ will only be sizeable if the drive frequency ω matches the frequency associated with the transition $i \to n$, or $n \to i$, in the spectrum of H_0, that is

$$\begin{aligned} \omega_{ni} + \omega \simeq 0 \quad &\text{or} \quad E_n \simeq E_i - \hbar\omega, \\ \omega_{ni} - \omega \simeq 0 \quad &\text{or} \quad E_n \simeq E_i + \hbar\omega. \end{aligned} \tag{40}$$

In other words, the drive term $V(t)$ can either deexcite the system, by inducing a transition that lowers its energy $E_i - E_n \approx \omega$, or excite the system $E_n - E_i \approx \omega$ (see Fig. 2).

Following an analogous calculation as for the constant perturbation, we arrive at the emission and absorption rates, respectively,

$$\begin{aligned} w_{i \to [n]} &= \frac{2\pi}{\hbar} \overline{|\mathscr{V}_{ni}|^2} \rho(E_n) \Big|_{E_n \cong E_i - \hbar\omega}, \\ w_{i \to [n]} &= \frac{2\pi}{\hbar} \overline{\left|\mathscr{V}_{ni}^\dagger\right|^2} \rho(E_n) \Big|_{E_n \cong E_i + \hbar\omega}. \end{aligned} \tag{41}$$

This can be written more compactly as

$$w_{i \to n} = \frac{2\pi}{\hbar} \left\{ \begin{array}{c} |\mathscr{V}_{ni}|^2 \\ \left|\mathscr{V}_{ni}^\dagger\right|^2 \end{array} \right\} \delta(E_n - E_i \pm \hbar\omega). \tag{42}$$

Noting that,

$$|\mathscr{V}_{ni}|^2 = \left|\mathscr{V}_{in}^\dagger\right|^2 \tag{43}$$

FIG. 2. A drive 'photon' of frequency ω can be either i) emitted by the system, thereby deexciting the system (stimulated emission), or ii) absorbed, thereby exciting it. Reproduced from J. J. Sakurai, *Modern Quantum Mechanics*, Addison-Wesley 1994, page 335.

and swapping $i \leftrightarrow n$ in the second Eq. (41) to express the absorption rate from the state n into the states nearby i, we arrive at the following relation between rates, called *detailed balance*

$$\frac{\text{emission rate for } i \to [n]}{\text{density of final states for } [n]} = \frac{\text{absorption rate for } n \to [i]}{\text{density of final states for } [i]}. \tag{44}$$

C. Slow turning on of perturbation. Wigner-Weisskopf theory.

Assume that the perturbation is slowly turned on

$$V(t) = e^{\eta t} V. \tag{45}$$

We will in the end be interested in taking $\eta \to 0$ to consider the case of a perturbation that is turned on infinitely slowly.

We can ask the same question as in the previous sections, and find that for any state $n \neq i$,

$$\begin{aligned} c_n^{(0)}(t) &= 0 \\ c_n^{(1)}(t) &= \frac{-i}{\hbar} V_{ni} \lim_{t_0 \to -\infty} \int_{t_0}^{t} e^{\eta t'} e^{i\omega_{ni} t'} dt' \\ &= \frac{-i}{\hbar} V_{ni} \frac{e^{\eta t + i\omega_{ni} t}}{\eta + i\omega_{ni}}. \end{aligned} \tag{46}$$

Note that we have taken the limit $t_0 \to -\infty$ which signifies that the perturbation is null in the infinite past, and it is slowly turned on such that it takes value V at $t = 0$. The above leads to

$$\begin{aligned} |c_n(t)|^2 &\simeq \frac{|V_{ni}|^2}{\hbar^2}\frac{e^{2\eta t}}{\eta^2+\omega_{ni}^2}, \\ \frac{d}{dt}|c_n(t)|^2 &\simeq \frac{2|V_{ni}|^2}{\hbar^2}\left(\frac{\eta e^{2\eta t}}{\eta^2+\omega_{ni}^2}\right). \end{aligned} \tag{47}$$

Noting that in the limit of an infinitely slow turn on the Lorentzian gives the Dirac $\delta-$function,

$$\lim_{\eta\to 0}\frac{\eta}{\eta^2+\omega_{ni}^2} = \pi\delta\left(\omega_{ni}\right) = \pi\hbar\delta\left(E_n - E_i\right), \tag{48}$$

we recover the Fermi Golden Rule result of the previous subsections

$$w_{i\to n} \simeq \left(\frac{2\pi}{\hbar}\right)|V_{ni}|^2\,\delta\left(E_n - E_i\right). \tag{49}$$

This indicates, at least on an intuitive level, that the value of the transition rate is insensitive to the qualitative aspects of the turn on of the perturbation, which can be sudden at $t = 0$, or slow.

Following Sakurai, we may calculate higher-order corrections in order to understand the Fermi Golden Rule rate in yet another way, as the lowest-order correction to the *imaginary* energy shift of the eigenenergies, i.e. a linewidth. To do so, we evaluate $c_n^{(i)}$ up to second-order corrections in V

$$\begin{aligned} c_i^{(0)} &= 1 \\ c_i^{(1)} &= \frac{-i}{\hbar}V_{ii}\lim_{t_0\to-\infty}\int_{t_0}^{t} e^{\eta t'}dt' = \frac{-i}{\hbar\eta}V_{ii}e^{\eta t} \\ c_i^{(2)} &= \left(\frac{-i}{\hbar}\right)^2\sum_m |V_{mi}|^2\lim_{t_0\to-\infty}\int_{t_0}^{t} dt' e^{i\omega_{im}t'+\eta t'}\frac{e^{i\omega_{mi}t'+\eta t'}}{i\left(\omega_{mi}-i\eta\right)} \\ &= \left(\frac{-i}{\hbar}\right)^2|V_{ii}|^2\frac{e^{2\eta t}}{2\eta^2} + \left(\frac{-i}{\hbar}\right)\sum_{m\neq i}\frac{|V_{mi}|^2 e^{2\eta t}}{2\eta\left(E_i - E_m + i\hbar\eta\right)}, \end{aligned} \tag{50}$$

Note how the introduction of the inverse timescale η fixes the problem of the vanishing denominator of $c_i^{(1)}$. The above leads to the following expression depending explicitly on η

$$c_i(t) \simeq 1 - \frac{i}{\hbar\eta}V_{ii}e^{\eta t} + \left(\frac{-i}{\hbar}\right)^2|V_{ii}|^2\frac{e^{2\eta t}}{2\eta^2} + \left(\frac{-i}{\hbar}\right)\sum_{m\neq i}\frac{|V_{mi}|^2 e^{2\eta t}}{2\eta\left(E_i - E_m + i\hbar\eta\right)} \tag{51}$$

In order to get at corrections to eigenenergies, we may try to recast the time-dependence of $c_i(t)$ into an exponential. To make this obvious, we look at the ratio

$$\begin{aligned}\frac{\dot{c}_i}{c_i} &\simeq \frac{\frac{-i}{\hbar}V_{ii} + \left(\frac{-i}{\hbar}\right)^2 \frac{|V_{ii}|^2}{\eta} + \left(\frac{-i}{\hbar}\right)\sum_{m\neq i}\frac{|V_{mi}|^2}{(E_i - E_m + i\hbar\eta)}}{1 - \frac{i}{\hbar}\frac{V_{ii}}{\eta}} \\ &\simeq \frac{-i}{\hbar}V_{ii} + \left(\frac{-i}{\hbar}\right)\sum_{m\neq i}\frac{|V_{mi}|^2}{E_i - E_m + i\hbar\eta}.\end{aligned} \tag{52}$$

The rhs of this differential equation is time-independent. This leads us to try the exponential Ansatz

$$c_i(t) = e^{-i\Delta_i t/\hbar}, \quad \frac{\dot{c}_i(t)}{c_i(t)} = \frac{-i}{\hbar}\Delta_i, \tag{53}$$

where, as usual in perturbation theory, we may expand the energy difference in the exponent in powers of the perturbation

$$\Delta_i = \Delta_i^{(1)} + \Delta_i^{(2)} + \cdots, \tag{54}$$

We find that the first order correction is real, and corresponds to the result expected from Rayleigh-Schrödinger perturbation theory

$$\Delta_i^{(1)} = V_{ii}. \tag{55}$$

Moreover, using the Sokhotski-Plemelj theorem

$$\lim_{\varepsilon\to 0}\frac{1}{x + i\varepsilon} = \mathrm{P}\,\frac{1}{x} - i\pi\delta(x) \tag{56}$$

we have for the real and imaginary parts of the second-order corrections to the eigenenergies

$$\begin{aligned}\mathrm{Re}\left(\Delta_i^{(2)}\right) &= \mathrm{P}\sum_{m\neq i}\frac{|V_{mi}|^2}{E_i - E_m}, \\ \mathrm{Im}\left(\Delta_i^{(2)}\right) &= -\pi\sum_{m\neq i}|V_{mi}|^2\,\delta\left(E_i - E_m\right).\end{aligned} \tag{57}$$

The real part is just the second-order Rayleigh-Schrödinger perturbation theory result for the energy correction. Moreover, inspecting our result from Fermi's Golden rule, we can readily identify the relaxation rate of state i as twice the imaginary part of the second-order energy correction

$$\sum_{m\neq i} w_{i\to m} = \frac{2\pi}{\hbar}\sum_{m\neq i}|V_{mi}|^2\,\delta\left(E_i - E_m\right) = -\frac{2}{\hbar}\,\mathrm{Im}\left[\Delta_i^{(2)}\right] \tag{58}$$

Let's go back to the weight of the state i as a function of time, which writes as

$$c_i(t) = e^{-(i/\hbar)[\mathrm{Re}(\Delta_i)t]+(1/\hbar)[\mathrm{Im}(\Delta_i)t]} \tag{59}$$

Denoting

$$\frac{\Gamma_i}{\hbar} \equiv -\frac{2}{\hbar}\,\mathrm{Im}\,(\Delta_i) \tag{60}$$

we have the following time-dependence for the population of the state i

$$|c_i|^2 = e^{2\,\mathrm{Im}(\Delta_i)t/\hbar} = e^{-\Gamma_i t/\hbar}. \tag{61}$$

To this order in perturbation theory, we can also readily check that the populations of all levels sum up to 1, i.e. there is conservation of the norm

$$|c_i|^2 + \sum_{m\neq i} |c_m|^2 = (1 - \Gamma_i t/\hbar) + \sum_{m\neq i} w_{i\to m} t = 1. \tag{62}$$

We can define the lifetime of the state i as

$$\frac{\hbar}{\Gamma_i} = \tau_i \tag{63}$$

which gives the characteristic decay time of the population of the state i into any other state

$$|c_i|^2 = e^{-t/\tau_i} \tag{64}$$

Defining the Fourier transform of the wavefunction coefficient as $f(E)$

$$\int f(E) e^{-iEt/\hbar} dE = e^{-i[E_i+\mathrm{Re}(\Delta_i)]t/\hbar - \Gamma_t t/2\hbar} \tag{65}$$

we find

$$|f(E)|^2 \propto \frac{1}{\{E - [E_i + \mathrm{Re}\,(\Delta_i)]\}^2 + \Gamma_i^2/4}, \tag{66}$$

i.e. Γ_i can be interpreted as the full width at half-maximum (FWHM) of the resonance at E_i.

The energy-time uncertainty relation

$$\Delta t \Delta E \sim \hbar \tag{67}$$

can be recovered once the FWHM is identified as the uncertainty in energy, and $\tau_i = \Delta t$ as the uncertainty in time.