10.2.2.1 The Heisenberg Equation of Motion

Let us now derive the equation of motion that regulates the time evolution of operators within the Heisenberg picture. Assuming that $\hat{A}$ does not depend explicitly on time (i.e., $\partial\hat{A}/\partial t = 0$), and since $\hat{U}(t)$ is unitary we have

$$\begin{aligned} \frac{d\hat{A}_H(t)}{dt} &= \frac{\partial\hat{U}^\dagger(t)}{dt}\hat{A}\hat{U}_{(t)} + \hat{U}^\dagger(t)\hat{A}\frac{\partial\hat{U}(t)}{\partial t} = -\frac{1}{i\hbar}\hat{U}^\dagger\hat{H}\hat{U}\hat{U}^\dagger\hat{A}\hat{U} + \frac{1}{i\hbar}\hat{U}^\dagger\hat{A}\hat{U}\hat{U}^\dagger\hat{H}\hat{U} \\ &= \frac{1}{i\hbar}\left[\hat{A}_H, \hat{U}^\dagger\hat{H}\hat{U}\right], \end{aligned} \tag{10.12}$$

where we have used (10.3) to write $\partial\hat{U}(t)/\partial t = \hat{H}\hat{U}/i\hbar$ and $\partial\hat{U}^\dagger(t)/\partial t = -\hat{U}^\dagger\hat{H}/i\hbar$. Since $\hat{U}(t)$ and $\hat{H}$ commute, we have $\hat{U}^\dagger(t)\hat{H}\hat{U}(t) = H$, hence we can rewrite (10.12) as

$$\boxed{\frac{d\hat{A}_H}{dt} = \frac{1}{i\hbar}\left[\hat{A}_H, \hat{H}\right].} \tag{10.13}$$

This is the *Heisenberg equation of motion*. It plays the role of the Schrödinger equation within the Heisenberg picture. Since the Schrödinger and Heisenberg pictures are equivalent, we can use either picture to describe the quantum system under consideration. The Heisenberg equation (10.13), however, is in general difficult to solve.

Note that the structure of the Heisenberg equation (10.13) is similar to the classical equation of motion of a variable A that does not depend explicitly on time $dA/dt = \{A, H\}$ where $\{A, H\}$ is the Poisson bracket between A and H (see Chapter 3).

10.2.3 The Interaction Picture

The interaction picture, also called the *Dirac picture*, is useful to describe quantum phenomena with Hamiltonians that depend explicitly on time. In this picture *both state vectors and operators evolve in time*. We need, therefore, to find the equation of motion for the state vectors and for the operators.

10.2.3.1 Equation of Motion for the State Vectors

State vectors in the interaction picture are defined in terms of the Schrödinger states $\mid \psi(t)\rangle$by

$$\boxed{\mid \psi(t)\rangle_I = e^{i\hat{H}_0 t/\hbar} \mid \psi(t)\rangle.} \tag{10.14}$$

If $t = 0$ we have $\mid \psi(0)\rangle_I = \mid \psi(0)\rangle$. The time evolution of $\mid \psi(t)\rangle$ is governed by the Schrödinger equation (10.1) with $\hat{H} = \hat{H}_0 + \hat{V}$ where $\hat{H}_0$ is time independent, but $\hat{V}$ may depend on time.

To find the time evolution of $\mid \psi(t)\rangle_I$, we need the time derivative of (10.14):

$$\begin{aligned} i\hbar\frac{d \mid \psi(t)\rangle_I}{dt} &= -\hat{H}_0 e^{i\hat{H}_0 t/\hbar} \mid \psi(t)\rangle + e^{i\hat{H}_0 t/\hbar}\left(i\hbar\frac{d \mid \psi(t)\rangle}{dt}\right) \\ &= -\hat{H}_0 \mid \psi(t)\rangle_I + e^{i\hat{H}_0 t/\hbar}\hat{H} \mid \psi(t)\rangle, \end{aligned} \tag{10.15}$$

where we have used (10.1). Since $\hat{H} = \hat{H}_0 + \hat{V}$, and

$$e^{iH_0t/\hbar}\hat{V} = \left(e^{i\hat{H}_0t/\hbar}\hat{V}e^{-i\hat{H}_0t/\hbar}\right)e^{i\hat{H}_0t/\hbar} = \hat{V}_I(t)e^{i\hat{H}_0t/\hbar}, \tag{10.16}$$

with

$$\hat{V}_I(t) = e^{i\hat{H}_0t/\hbar}\hat{V}e^{-i\hat{H}_0t/\hbar}, \tag{10.17}$$

we can rewrite (10.15) as

$$i\hbar\frac{d \mid \psi(t)\rangle_I}{dt} = -\hat{H}_0 \mid \psi(t)\rangle_I + \hat{H}_0 e^{i\hat{H}_0t/\hbar} \mid \psi(t)\rangle + \hat{V}_I(t)e^{i\hat{H}_0t/\hbar} \mid \psi(t)\rangle, \tag{10.18}$$

or

$$\boxed{i\hbar\frac{d \mid \psi(t)\rangle_I}{dt} = \hat{V}_I(t) \mid \psi(t)\rangle_I.} \tag{10.19}$$

This is the Schrödinger equation in the interaction picture. It shows that the time evolution of the state vector is governed by the interaction $\hat{V}_I(t)$.

10.2.3.2 Equation of Motion for the Operators

The interaction representation of an operator $\hat{A}_I(t)$ is given, as shown in (10.17), in terms of its Schrödinger representation by

$$\boxed{\hat{A}_I(t) = e^{i\hat{H}_0t/\hbar}\hat{A}e^{-i\hat{H}_0t/\hbar}.} \tag{10.20}$$

Calculating the time derivative of $\hat{A}_I(t)$ and since $\partial\hat{A}/\partial t = 0$, we can show the time evolution of $\hat{A}_I(t)$ is governed by $\hat{H}_0$:

$$\boxed{\frac{d\hat{A}_I(t)}{dt} = \frac{1}{i\hbar}\left[\hat{A}_I(t),\ \hat{H}_0\right].} \tag{10.21}$$

This equation is similar to the Heisenberg equation of motion (10.13), save that $\hat{H}$ is replaced by $\hat{H}_0$. The basic difference between the Heisenberg and interaction pictures can be inferred from a comparison of (10.9) with (10.14), and (10.11) with (10.20): in the Heisenberg picture it is $\hat{H}$ that appears in the exponents, whereas in the interaction picture it is $\hat{H}_0$ that appears.

In conclusion we have seen that, within the Schrödinger picture, the states depend on time but not the operators; in the Heisenberg picture, only operators depend explicitly on time, state vectors are frozen in time. The interaction picture, however, is intermediate between the Schrödinger and the Heisenberg pictures, since both state vectors and operators evolve with time.

10.3 Time-Dependent Perturbation Theory

We consider here only those phenomena that are described by Hamiltonians which can be split into two parts, a time-independent part $\hat{H}_0$ and a time-dependent part $\hat{V}(t)$ that is small compared to $\hat{H}_0$:

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t), \tag{10.22}$$

where $\hat{H}_0$, which describes the system when unperturbed, is assumed to have exact solutions that are known. Such splitting of the Hamiltonian is encountered in the following typical problem. Consider a system which, when unperturbed, is described by a time-independent Hamilonian $\hat{H}_0$ whose solutions—the eigenvalues E_n and eigenstates, $\mid \psi_n\rangle$—are known,

$$\hat{H}_0 \mid \psi_n\rangle = E_n \mid \psi_n\rangle, \tag{10.23}$$

and whose most general state vectors are given by stationary states

$$\mid \Psi_n(t)\rangle = e^{-i\hat{H}_0 t/\hbar} \mid \psi_n\rangle = e^{-iE_n t/\hbar} \mid \psi_n\rangle. \tag{10.24}$$

In the time interval $0 \le t \le \tau$ we subject the system to an external time-dependent perturbation, $\hat{V}(t)$, that is small compared to $\hat{H}_0$:

$$\hat{V}(t) = \begin{cases} \hat{V}(t) & 0 \le t \le \tau \\ 0 & t < 0, \quad t > \tau. \end{cases} \tag{10.25}$$

During the time interval $0 \le t \le \tau$, the Hamiltonian of the system is $\hat{H} = \hat{H}_0 + \hat{V}(t)$, and the corresponding Schrödinger equation is

$$i\hbar \frac{d \mid \Psi(t)\rangle}{dt} = (\hat{H}_0 + \hat{V}(t)) \mid \Psi(t)\rangle. \tag{10.26}$$

where $\hat{V}(t)$ characterizes the interaction of the system with the external source of perturbation.

How does $\hat{V}(t)$ affect the system? When the system interacts with $\hat{V}(t)$, it either absorbs or emits energy. This process inevitably causes the system to undergo transitions from one unperturbed eigenstate to another. The main task of time-dependent perturbation theory consists of answering this question: If the system is initially in an (unperturbed) eigenstate $\mid \psi_i\rangle$ of $\hat{H}_0$, what is the probability that the system will be found at a later time in another unperturbed eigenstate $\mid \psi_f\rangle$?

To prepare the ground for answering this question, we need to look for the solutions of the Schrödinger equation (10.26). The standard method to solve (10.26) is to expand $\mid \Psi(t)\rangle$ in terms of an expansion coefficient $c_n(t)$:

$$\mid \Psi(t)\rangle = \sum_n c_n(t) e^{-iE_n t} \mid \psi_n\rangle, \tag{10.27}$$

and then insert this into (10.26) to find $c_n(t)$ to various orders in the approximation. Instead of following this procedure, and since we are dealing with time-dependent potentials, it is more convenient to solve (10.26) in the interaction picture (10.19):

$$i\hbar \frac{d \mid \Psi(t)\rangle_I}{dt} = \hat{V}_I(t) \mid \Psi(t)\rangle_I, \tag{10.28}$$

where $\mid \Psi(t)\rangle_I = e^{iH_0 t/\hbar} \mid \Psi(t)\rangle$ and $\hat{V}_I(t) = e^{iH_0 t/\hbar}\hat{V}(t)e^{-iH_0 t/\hbar}$. The time evolution equation $\mid \Psi(t)\rangle = \hat{U}(t, t_i) \mid \Psi(t_i)\rangle$ may be written in the interaction picture as

$$\mid \Psi(t)\rangle_I = e^{i\hat{H}_0 t/\hbar} \mid \Psi(t)\rangle = e^{i\hat{H}_0 t/\hbar}\hat{U}(t, t_i) \mid \Psi(t_i)\rangle = e^{i\hat{H}_0 t/\hbar}\hat{U}(t, t_i)e^{-i\hat{H}_0 t_i/\hbar} \mid \Psi(t_i)\rangle_I, \tag{10.29}$$

or as

$$\mid \Psi(t)\rangle_I = \hat{U}_I(t, t_i) \mid \Psi(t_i)\rangle_I, \tag{10.30}$$

where the time evolution operator is given in the interaction picture by

$$\hat{U}_I(t, t_i) = e^{i\hat{H}_0 t/\hbar}\hat{U}(t, t_i)e^{-i\hat{H}_0 t_i/\hbar}. \tag{10.31}$$

Inserting (10.30) into (10.28) we end up with

$$i\hbar\frac{d\hat{U}_I(t, t_i)}{dt} = \hat{V}_I(t)\hat{U}_I(t, t_i). \tag{10.32}$$

The solutions of this equation, with the initial condition $\hat{U}_I(t_i, t_i) = \hat{I}$, are given by the *integral equation*

$$\hat{U}_I(t, t_i) = 1 - \frac{i}{\hbar}\int_{t_i}^{t}\hat{V}_I(t')\hat{U}_I(t', t_i)\,dt'. \tag{10.33}$$

Time-dependent perturbation theory provides *approximate* solutions to this integral equation. This consists in assuming that $\hat{V}_I(t)$ is *small then proceeding iteratively*. The first-order approximation is obtained by inserting $\hat{U}_I(t', t_i) = 1$ in the integral sign of (10.33), leading to $\hat{U}_I^{(1)}(t, t_i) = 1 - (i/\hbar)\int_{t_i}^{t}\hat{V}_I(t')\,dt'$. Substituting $\hat{U}_I(t', t_i) = \hat{U}_I^{(1)}(t', t_i)$ in the integral sign of (10.33) we get the second-order approximation:

$$\hat{U}_I^{(2)}(t, t_i) = 1 - \frac{i}{\hbar}\int_{t_i}^{t}\hat{V}_I(t')\,dt' + \left(-\frac{i}{\hbar}\right)^2\int_{t_i}^{t}\hat{V}_I(t_1)\,dt_1\int_{t_i}^{t_1}\hat{V}_I(t_2)\,dt_2. \tag{10.34}$$

The third-order approximation is obtained by substituting $\hat{U}_I^{(2)}(t, t_i)$ into (10.33), and so on. A repetition of this iterative process yields

$$\begin{aligned}\hat{U}_I(t, t_i) = 1 &- \frac{i}{\hbar}\int_{t_i}^{t}\hat{V}_I(t')dt' + \left(-\frac{i}{\hbar}\right)^2\int_{t_i}^{t}\hat{V}_I(t_1)dt_1\int_{t_i}^{t_1}\hat{V}_I(t_2)dt_2 + \cdots \\ &+ \left(-\frac{i}{\hbar}\right)^n\int_{t_i}^{t}\hat{V}_I(t_1)dt_1\int_{t_i}^{t_1}\hat{V}_I(t_2)dt_2\int_{t_i}^{t_2}\hat{V}_I(t_3)dt_3\cdots\int_{t_i}^{t_{n-1}}\hat{V}_I(t_n)dt_n + \cdots.\end{aligned} \tag{10.35}$$

This series, known as the *Dyson series*, allows for the calculation of the state vector up to the desired order in the perturbation.

We are now equipped to calculate the transition probability. It may be obtained by taking the matrix elements of (10.35) between the eigenstates of $\hat{H}_0$. Time-dependent perturbation theory, where one assumes knowledge of the solutions of the unperturbed eigenvalue problem (10.23), deals in essence with the calculation of the transition probabilities between the unperturbed eigenstates $|\,\psi_n\rangle$ of the system.

10.3.1 Transition Probability

The transition probability corresponding to a transition from an initial unperturbed state $|\,\psi_i\rangle$ to another unperturbed state $|\,\psi_f\rangle$ is obtained from (10.35):

$$\begin{aligned}P_{if}(t) = \left|\langle\psi_f\,|\,\hat{U}_I(t, t_i)\,|\,\psi_i\rangle\right|^2 = \Bigg|\langle\psi_f\,|\,\psi_i\rangle &- \frac{i}{\hbar}\int_0^t e^{i\omega_{fi}t'}\langle\psi_f\,|\,\hat{V}(t')\,|\,\psi_i\rangle\,dt' \\ + \left(-\frac{i}{\hbar}\right)^2\sum_n\int_0^t e^{i\omega_{fn}t_1}\langle\psi_f\,|\,\hat{V}(t_1)\,|\,\psi_n\rangle\,dt_1&\int_0^{t_1}e^{i\omega_{ni}t_2}\langle\psi_n\,|\,\hat{V}(t_2)\,|\,\psi_i\rangle\,dt_2 + \cdots\Bigg|^2,\end{aligned} \tag{10.36}$$

where we have used the fact that

$$\langle \psi_f \mid \hat{V}_I(t') \mid \psi_i \rangle = \langle \psi_f \mid e^{iH_0t'/\hbar} \hat{V}(t') e^{-iH_0t'/\hbar} \mid \psi_i \rangle = \langle \psi_f \mid V(t') \mid \psi_i \rangle \exp\left(i\omega_{fi}t'\right), \tag{10.37}$$

where ω_{fi} is the transition frequency between the initial and final levels i and f

$$\omega_{fi} = \frac{E_f - E_i}{\hbar} = \frac{1}{\hbar}\Big(\langle \psi_f \mid \hat{H}_0 \mid \psi_f \rangle - \langle \psi_i \mid \hat{H}_0 \mid \psi_i \rangle\Big). \tag{10.38}$$

The transition probability (10.36) can be written in terms of the expansion coefficients $c_n(t)$ introduced in (10.27) as

$$P_{if}(t) = \left| c_f^{(0)} + c_f^{(1)}(t) + c_f^{(2)}(t) + \cdots \right|^2, \tag{10.39}$$

where

$$c_f^{(0)} = \langle \psi_f \mid \psi_i \rangle = \delta_{f,i}, \qquad c_f^{(1)}(t) = -\frac{i}{\hbar}\int_0^t \langle \psi_f \mid \hat{V}(t') \mid \psi_i \rangle e^{i\omega_{fi}t'} dt', \ldots. \tag{10.40}$$

The first-order transition probability for $\mid \psi_i\rangle \rightarrow \mid \psi_f \rangle$ with $i \neq f$ (and hence $\langle \psi_f \mid \psi_i \rangle = 0$) is obtained by terminating (10.36) at the first order in $V_I(t)$:

$$\boxed{P_{if}(t) = \left| -\frac{i}{\hbar}\int_0^t \langle \psi_f \mid \hat{V}(t') \mid \psi_i \rangle e^{i\omega_{fi}t'} dt' \right|^2.} \tag{10.41}$$

In principle we can use (10.36) to calculate the transition probability to any order in $\hat{V}_I(t)$. However, terms higher than the first order become rapidly intractable. For most problems of atomic and nuclear physics, the first order (10.41) is usually sufficient. In what follows, we are going to apply (10.41) to calculate the transition probability for two cases, which will have later usefulness when we deal with the interaction of atoms with radiation: a *constant* perturbation and a *harmonic* perturbation.

10.3.2 Transition Probability for a Constant Perturbation

In the case where $\hat{V}$ does not depend on time, (10.41) leads to

$$P_{if}(t) = \frac{1}{\hbar^2}\left| \langle \psi_f \mid \hat{V} \mid \psi_i \rangle \int_0^t e^{i\omega_{fi}t'} dt' \right|^2 = \frac{1}{\hbar^2}\left| \langle \psi_f \mid \hat{V} \mid \psi_i \rangle \right|^2 \left| \frac{e^{i\omega_{fi}t} - 1}{\omega_{fi}} \right|^2, \tag{10.42}$$

which, using $|e^{i\theta} - 1|^2 = 4\sin^2(\theta/2)$, reduces to

$$\boxed{P_{if}(t) = \frac{4|\langle \psi_f \mid \hat{V} \mid \psi_i \rangle|^2}{\hbar^2 \omega_{fi}^2} \sin^2\left(\frac{\omega_{fi}t}{2}\right).} \tag{10.43}$$

As a function of time, this transition probability is an oscillating sinusoidal function with a period of $2\pi/\omega_{fi}$. As a function of ω_{fi}, however, the transition probability, as shown in Figure 10.1, has an interference pattern: it is appreciable only near $\omega_{fi} \simeq 0$ and decays rapidly as ω_{fi} moves away from zero (here, for a fixed t, we have assumed that ω_{fi} is a continuous

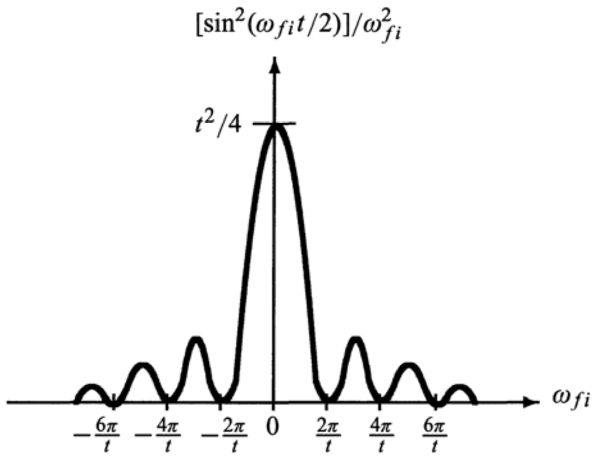

Figure 10.1 Plot of $[\sin^2(\omega_{fi}t/2)]/\omega_{fi}^2$ versus ω_{fi} for a fixed value of t; $\omega_{fi} = (E_f - E_i)/2$.

variable; that is, we have considered a continuum of final states; we will deal with this in more details in a moment). This means that the transition probability of finding the system in a state $\mid \psi_f\rangle$ of energy E_f is greatest only when $E_i \simeq E_f$ or when $\omega_{fi} \simeq 0$. The height and the width of the main peak, centered around $\omega_{fi} = 0$, are proportional to t^2 and $1/t$, respectively, so the area under the curve is proportional to t; since most of the area is under the central peak, the transition probability is proportional to t. The transition probability therefore grows linearly with time. The central peak becomes narrower and higher as time increases; this is exactly the property of a delta function. Thus, in the limit $t \to \infty$ the transition probability takes the shape of a delta function as we are going to see.

As $t \to \infty$ we can use the asymptotic relation (Appendix A)

$$\lim_{t\to\infty} \frac{\sin^2(yt)}{\pi y^2 t} = \delta(y) \tag{10.44}$$

to write the following expression:

$$\frac{1}{(\frac{1}{2}\omega_{fi})^2} \sin^2\left(\frac{\omega_{fi}t}{2}\right) = 2\pi t\hbar\delta(\hbar\omega_{fi}), \tag{10.45}$$

because $\delta(\omega_{fi}/2) = 2\hbar\delta(\hbar\omega_{fi})$. Now since $\hbar\omega_{fi} = E_f - E_i$, hence $\delta(\hbar\omega_{fi}) = \delta(E_f - E_i)$, we can reduce (10.43) in the limit of long times to

$$\boxed{P_{if}(t) = \frac{2\pi t}{\hbar} \left| \langle\psi_f \mid \hat{V} \mid \psi_i\rangle\right|^2 \delta(E_f - E_i).} \tag{10.46}$$

The *transition rate*, which is defined as a transition probability per unit time, is thus given by

$$\boxed{\Gamma_{if} = \frac{P_{if}(t)}{t} = \frac{2\pi}{\hbar} \left| \langle\psi_f \mid \hat{V} \mid \psi_i\rangle\right|^2 \delta(E_f - E_i).} \tag{10.47}$$

The delta term $\delta(E_f - E_i)$ guarantees the conservation of energy: in the limit $t \to \infty$, the transition rate is nonvanishing only between states of equal energy. Hence a constant (time independent) perturbation neither removes energy from the system nor supplies energy to it. It simply causes energy-conserving transitions.

Transition into a continuum of final states

Let us now calculate the total transition rate associated with a transition from an initial state $\mid \psi_i\rangle$ into a continuum[1] of final states $\mid \psi_f\rangle$. If $\rho(E_f)$ is the density of final states—the number of states per unit energy interval—the number of final states within the energy interval E_f and $E_f + dE_f$ is equal to $\rho(E_f)\,dE_f$. The total transition rate W_{if} can then be obtained from (10.47):

$$W_{if} = \int \frac{P_{if}(t)}{t}\rho(E_f)\,dE_f = \frac{2\pi}{\hbar}\mid\langle\psi_f \mid \hat{V} \mid \psi_i\rangle\mid^2 \int \rho(E_f)\delta(E_f - E_i)\,dE_f, \tag{10.48}$$

or

$$\boxed{W_{if} = \frac{2\pi}{\hbar}\left|\langle\psi_f \mid \hat{V} \mid \psi_i\rangle\right|^2 \rho(E_i).} \tag{10.49}$$

This relation is called the *Fermi golden rule*. It implies that, in the case of a constant perturbation, if we wait long enough, the total transition rate becomes constant (time independent).

10.3.3 Transition Probability for a Harmonic Perturbation

Consider now a perturbation which depends harmonically on time (i.e., the time between the moments of turning the perturbation on and off):

$$\hat{V}(t) = \hat{v}e^{i\omega t} + \hat{v}^\dagger e^{-i\omega t}, \tag{10.50}$$

where $\hat{v}$ is a time-independent operator. Such a perturbation is encountered, for instance, when charged particles (e.g., electrons) interact with an electromagnetic field. This perturbation provokes transitions of the system from a stationary state to another.

The transition probability corresponding to this perturbation can be obtained from (10.41):

$$P_{if}(t) = \frac{1}{\hbar^2}\left|\langle\psi_f \mid \hat{v} \mid \psi_i\rangle \int_0^t e^{i(\omega_{fi}+\omega)t'}dt' + \langle\psi_f \mid \hat{v}^\dagger \mid \psi_i\rangle \int_0^t e^{i(\omega_{fi}-\omega)t'}dt'\right|^2. \tag{10.51}$$

Neglecting the cross terms, for they are negligible compared with the other two (because they induce no lasting transitions), we can rewrite this expression as

$$P_{if}(t) = \frac{1}{\hbar^2}\left|\langle\psi_f \mid \hat{v} \mid \psi_i\rangle\right|^2 \left|\frac{e^{i(\omega_{fi}+\omega)t} - 1}{\omega_{fi}+\omega}\right|^2 + \frac{1}{\hbar^2}\left|\langle\psi_f \mid \hat{v}^\dagger \mid \psi_i\rangle\right|^2 \left|\frac{e^{i(\omega_{fi}-\omega)t} - 1}{\omega_{fi}-\omega}\right|^2, \tag{10.52}$$

which, using $|e^{i\theta} - 1|^2 = 4\sin^2(\theta/2)$, reduces to

$$P_{if}(t) = \frac{4}{\hbar^2}\left[\left|\langle\psi_f \mid \hat{v} \mid \psi_i\rangle\right|^2 \frac{\sin^2((\omega_{fi}+\omega)t/2)}{(\omega_{fi}+\omega)^2} + \left|\langle\psi_f \mid \hat{v}^\dagger \mid \psi_i\rangle\right|^2 \frac{\sin^2((\omega_{fi}-\omega)t/2)}{(\omega_{fi}-\omega)^2}\right]. \tag{10.53}$$

As displayed in Figure 10.2, the transition probability peaks either at $\omega_{fi} = -\omega$, where its maximum value is $P_{if}(t) = (t^2/4\hbar^2)|\langle\psi_f \mid \hat{v} \mid \psi_i\rangle|^2$, or at $\omega_{fi} = \omega$, where its maximum

[1] F. Schwabl, *Quantum Mechanics*, 2nd ed., Springer–Verlag, Berlin, 1995, Section 16.3.3.

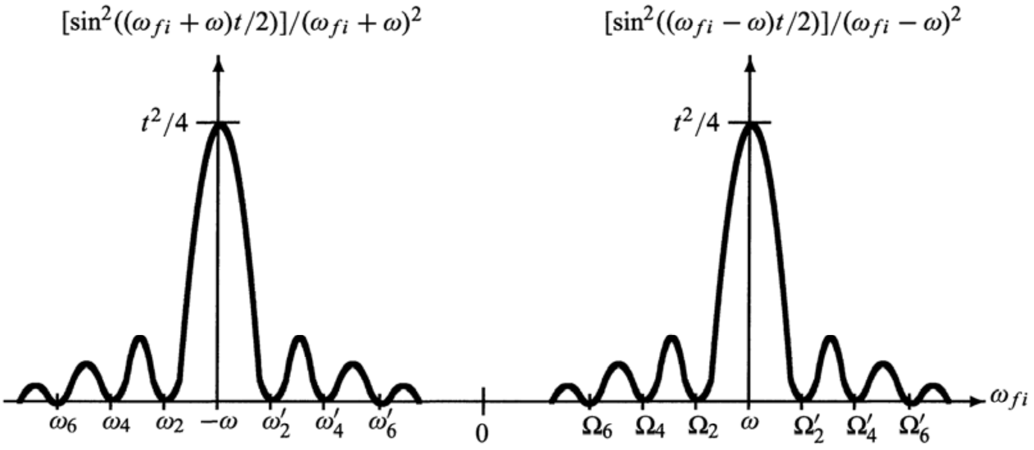

Figure 10.2 Plot of $[\sin^2((\omega_{fi} \pm \omega)t/2)]/(\omega_{fi} \pm \omega)^2$ versus ω_{fi} for a fixed value of t, where $\omega_n = -\omega - n\pi/t$, $\omega'_n = -\omega + n\pi/t$, $\Omega_n = \omega - n\pi/t$, and $\Omega'_n = \omega + n\pi/t$.

value is $P_{if}(t) = (t^2/4\hbar^2)|\langle \psi_f \mid \hat{v}^\dagger \mid \psi_i\rangle|^2$. These are conditions for resonance; this means that the probability of transition is greatest only when the frequency of the perturbing field is close to $\pm\omega_{fi}$. As ω moves away from $\pm\omega_{fi}$, P_{fi} decreases rapidly.

Note that the expression (10.53) is similar to that derived for a constant perturbation as shown in (10.43). Using (10.45) we can reduce (10.53) in the limit $t \to \infty$ to

$$\boxed{\Gamma_{if} = \frac{2\pi}{\hbar}\left|\langle \psi_f \mid \hat{v} \mid \psi_i\rangle\right|^2 \delta(E_f - E_i + \hbar\omega) + \frac{2\pi}{\hbar}\left|\langle \psi_f \mid \hat{v}^\dagger \mid \psi_i\rangle\right|^2 \delta(E_f - E_i - \hbar\omega).} \tag{10.54}$$

This transition rate is nonzero only when either of the following two conditions is satisfied:

$$E_f = E_i - \hbar\omega, \tag{10.55}$$

$$E_f = E_i + \hbar\omega. \tag{10.56}$$

These two conditions cannot be satisfied simultaneously; their physical meaning can be understood as follows. The first condition $E_f = E_i - \hbar\omega$ implies that the system is initially excited, since its final energy is smaller than the initial energy; when acted upon by the perturbation, the system deexcites by giving up a photon of energy $\hbar\omega$ to the potential $\hat{V}(t)$ as shown in Figure 10.3. This process is called *stimulated emission*, since the system easily emits a photon of energy $\hbar\omega$. The second condition, $E_f = E_i + \hbar\omega$ shows that the final energy of the system is larger than its initial energy. The system then *absorbs* a photon of energy $\hbar\omega$ from $\hat{V}(t)$ and ends up in an excited state of (higher) energy E_f (Figure 10.3). We may thus view the terms $e^{i\omega t}$ and $e^{-i\omega t}$ in $\hat{V}(t)$ as responsible, respectively, for the emission and the absorption of a photon of energy $\hbar\omega$.

In conclusion the effect of a harmonic perturbation is to transfer to the system, or to receive from it, a photon of energy $\hbar\omega$. In sharp contrast, a constant (time-independent) perturbation neither transfers energy to the system nor removes energy from it.

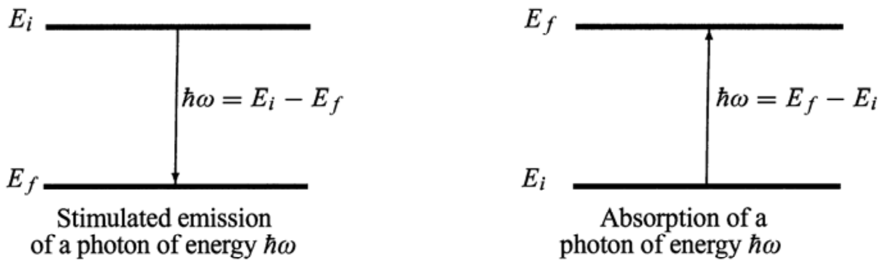

Figure 10.3 Stimulated emission and absorption of a photon of energy $\hbar\omega$.

Remark

For transitions into a continuum of final states, we can show, by analogy with the derivation of (10.49), that (10.54) leads to the absorption and emission transition rates:

$$W_{if}^{abs} = \frac{2\pi}{\hbar}\left|\langle\psi_f \mid \hat{V}^\dagger \mid \psi_i\rangle\right|^2 \left.\rho(E_f)\right|_{E_f=E_i+\hbar\omega}, \tag{10.57}$$

$$W_{if}^{emi} = \frac{2\pi}{\hbar}\left|\langle\psi_f \mid \hat{V} \mid \psi_i\rangle\right|^2 \left.\rho(E_f)\right|_{E_f=E_i-\hbar\omega}. \tag{10.58}$$

Since the perturbation (10.50) is Hermitian, $\langle\psi_f \mid \hat{v} \mid \psi_i\rangle = \langle\psi_i|\hat{v}^\dagger \mid \psi_f\rangle^*$, we have $|\langle\psi_f \mid \hat{v} \mid \psi_i\rangle|^2 = |\langle\psi_f \mid \hat{v}^\dagger \mid \psi_i\rangle|^2$, hence

$$\frac{W_{if}^{abs}}{\left.\rho(E_f)\right|_{E_f=E_i+\hbar\omega}} = \frac{W_{if}^{emi}}{\left.\rho(E_f)\right|_{E_f=E_i-\hbar\omega}}. \tag{10.59}$$

This relation is known as the condition of *detailed balancing*.

Example 10.1

A particle, which is initially ($t = 0$) in the ground state of an infinite, one-dimensional potential box with walls at $x = 0$ and $x = a$, is subjected for $0 \le t \le \infty$ to a perturbation $\hat{V}(t) = \hat{x}^2 e^{-t/\tau}$. Calculate to first order the probability of finding the particle in its first excited state for $t \ge 0$.

Solution

For a particle in a box potential, with $E_n = n^2\pi^2\hbar^2/(2ma^2)$ and $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$, the ground state corresponds to $n = 1$ and the first excited state to $n = 2$. We can use (10.41) to obtain

$$P_{12} = \frac{1}{\hbar^2}\left|\int_0^\infty \langle\psi_2|\hat{V}(t)|\psi_1\rangle e^{i\omega_{21}t}dt\right|^2 = \frac{1}{\hbar^2}\left|\langle\psi_2|\hat{x}^2|\psi_1\rangle\right|^2 \left|\int_0^\infty e^{-(1/\tau - i\omega_{21})t}dt\right|^2, \tag{10.60}$$

where

$$\langle\psi_2|\hat{x}^2|\psi_1\rangle = \int_0^a x^2\psi_2^*(x)\psi_1(x)\,dx = \frac{2}{a}\int_0^a x^2 \sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right)dx = -\frac{16a^2}{9\pi^2}, \tag{10.61}$$

$$\left| \int_0^t e^{-(1/\tau - i\omega_{21})t} dt \right|^2 = \left| \frac{e^{-(1/\tau - i\omega_{21})t} - 1}{1/\tau - i\omega_{21}} \right|^2 = \frac{1 + e^{-2t/\tau} - 2e^{-t/\tau}\cos(\omega_{21}t)}{\omega_{21}^2 + 1/\tau^2}, \tag{10.62}$$

which, in the limit $t \to \infty$, reduces to

$$\left| \int_0^\infty e^{-(1/\tau - i\omega_{21})t} dt \right|^2 = \left[\omega_{21}^2 + \frac{1}{\tau^2} \right]^{-1} = \left[\frac{9\pi^4\hbar^2}{4m^2a^4} + \frac{1}{\tau^2} \right]^{-1}, \tag{10.63}$$

since $\omega_{21} = (E_2 - E_1)/\hbar = 3\pi^2\hbar/(2ma^2)$. A substitution of (10.61) and (10.63) into (10.60) leads to

$$P_{12} = \left(\frac{16a^2}{9\pi^2\hbar} \right)^2 \left[\frac{9\pi^4\hbar^2}{4m^2a^4} + \frac{1}{\tau^2} \right]^{-1}. \tag{10.64}$$

10.4 Adiabatic and Sudden Approximations

In discussing the time-dependent perturbation theory, we have dealt with phenomena where the perturbation $\hat{V}(t)$ is small, but we have payed no attention to the rate of change of the perturbation. In this section we want to discuss approximation methods treating phenomena where $\hat{V}(t)$ is not only small but also switched on either *adiabatically* (slowly) or *suddenly* (rapidly). We assume here that $\hat{V}(t)$ is switched on at $t = 0$ and off at a later time t (the turning on and off may be smooth or abrupt).

Since $e^{i\omega_{fi}t} = (1/i\omega_{fi})\partial e^{i\omega_{fi}t}/\partial t$ an integration by parts yields

$$\begin{aligned} -\frac{i}{\hbar}\int_0^t \langle \psi_f \mid \hat{V}(t') \mid \psi_i \rangle e^{i\omega_{fi}t'} dt' &= -\frac{1}{\hbar\omega_{fi}} \int_0^t \langle \psi_f \mid \hat{V}(t') \mid \psi_i \rangle \left(\frac{\partial}{\partial t'} e^{i\omega_{fi}t'} \right) dt' \\ &= -\frac{1}{\hbar\omega_{fi}} \langle \psi_f \mid \hat{V}(t) \mid \psi_i \rangle e^{i\omega_{fi}t} \Big|_{t=0}^{t} + \frac{1}{\hbar\omega_{fi}} \int_0^t e^{i\omega_{fi}t'} \left(\frac{\partial}{\partial t'} \langle \psi_f \mid \hat{V}(t') \mid \psi_i \rangle \right) dt' \\ &= \frac{1}{\hbar\omega_{fi}} \int_0^t e^{i\omega_{fi}t'} \left(\frac{\partial}{\partial t'} \langle \psi_f \mid \hat{V}(t') \mid \psi_i \rangle \right) dt', \end{aligned} \tag{10.65}$$

where we have used the fact that $\hat{V}(t)$ vanishes at the limits (when it is switched on at $t = 0$ and off at time t). The calculation of the integral depends on the rate of change of $\hat{V}(t)$. In what follows we are going to consider the cases where the interaction is switched on slowly or rapidly.

10.4.1 Adiabatic Approximation

First, let us discuss briefly the adiabatic approximation without combining it with perturbation theory. This approximation applies to phenomena whose Hamiltonians evolve *slowly* with time; we should highlight the fact that the adiabatic approximation does not require the Hamiltonian to split into an unperturbed part $\hat{H}_0$ and a weak time-dependent perturbation $\hat{V}(t)$. Essentially, it consists in approximating the solutions of the Schrödinger equation at every time by the stationary states (energy E_n and wave functions ψ_n) of the instantaneous Hamiltonian such that