2 Approximate solving time evolution

Physical problems which can be solved exactly are very rare. In some cases a physical insight allows to simplify the original problem, so that the exact solution of the resulting mathematical model can be found. In general, however, as it is generic for applications of many body quantum mechanics to solid state or condensed matter physics, even the simplified model problems are still too complicated to be solved (cf. the paradigmatic Hubbard models!). Such are also all relativistic quantum field theory models of interactions of elementary particles. Therefore approximate methods of solving quantum mechanical problems are necessary. Such methods fall into two broad classes. To the first one belong various Ansätze and clever guesses which allow to capture main features of the considered system and to obtain reasonable estimates of the quantities of interest, but are usually not easy to be further improved (by calculating corrections to the obtained approximate results). To the second class belong systematic methods which allow to obtain (at least in principle) the solution of the given problem in the form of a power series expansion in some (small) parameter.

One such systematic method is the well known stationary Rayleigh - Schrödinger perturbative expansion which allows to compute eigenvalues and eigenvectors of the time independent Hamiltonian $H = H_0 + \lambda V_{\rm int}$ in the form of a power series[1] in λ in terms of the (known) eigenvalues and eigenvectors of H_0. Another systematic method is known as the time-dependent perturbative expansion. This one is devised to perturbatively solve the Schrödinger equation (1.1) with the Hamiltonian $H = H_0 + \lambda\, V_{\rm int}(t)$ in which the (Schrödinger picture) interaction operator $V_{\rm int}$ is allowed to depend on time, that is to find the expansion of the state-vector $|\Psi(t)\rangle$ in a power series in λ in terms of the state-vector $|\Psi(t_0)\rangle$ specified at some initial instant t_0 using the basis of the H_0 eigenvectors and eigenvalues. In other words, this is a method of expanding the (interaction picture) evolution operator of the considered system. Here we recall first the usual formulation of this method and show that it is equivalent to the iterative construction of the interaction picture evolution operator $U_I(t, t_0)$ defined in (1.21), comment on its usage in the case when the spectrum of H_0 is continuous and then apply it to some illustrative model examples. Finally, we consider perturbations $V_{\rm int}(t)$ with harmonic time dependence, introduce the concept of transition probability per unit time and discuss how such probabilities should be interpreted and used.

2.1 Perturbative expansion of the evolution operator

The first step in formulating the standard perturbative expansion of the (interaction picture) evolution operator $U_I(t, t_0)$, called usually the time-dependent perturbative expansion, is the observation that without loss of generality the solution $|\Psi(t)\rangle_S \equiv |\Psi(t)\rangle$

[1] λ will be treated here as a formal expansion parameter and will be set to 1 at the end.

of the Schrödinger equation (1.1) can be at any instant t written as a superposition of the H_0 (time dependent) eigenvectors[2] $|n(t)\rangle = |n\rangle \exp(-iE_n t/\hbar)$ with time dependent coefficients $a_n(t)$:

$$|\Psi(t)\rangle = \sum_n |n(t)\rangle\, a_n(t) = \sum_n |n\rangle\, e^{-iE_n t/\hbar}\, a_n(t)\,. \tag{2.1}$$

The symbol $\sum_n$ denotes here summation over the discrete and integration over the continuous parts of the H_0 spectrum. Inserting (2.1) in the Schrödinger equation (1.1) gives

$$i\hbar \sum_n |n\rangle\, e^{-iE_n t/\hbar}\, \dot{a}_n(t) = \sum_n \lambda V_{\rm int}(t)|n\rangle\, e^{-iE_n t/\hbar}\, a_n(t)\,.$$

Taking the scalar product with the H_0 eigenvector $|k\rangle$ one obtains

$$\dot{a}_k(t) = \frac{1}{i\hbar} \sum_n e^{i\omega_{kn} t}\, \langle k|\lambda V_{\rm int}(t)|n\rangle\, a_n(t)\,, \tag{2.2}$$

where $\omega_{kn} = (E_k - E_n)/\hbar$. The infinite system of coupled equations (2.2) is, of course, fully equivalent to the original Schrödinger equation (1.1).

In fact, although no reference to the interaction picture has been made, (2.2) is precisely (the projection onto the state $\langle k|$ of) the interaction picture version (1.19) of the Schrödinger equation. To see this, it is sufficient to take the scalar product of both sides of the equation (1.19) with the time independent H_0 eigenvectors $|k\rangle$ and to notice (cf. (1.16)) that

$$\langle k|\Psi(t)\rangle_I = \langle k|e^{iH_0 t/\hbar}|\Psi(t)\rangle_S = \sum_n \langle k|e^{iH_0 t/\hbar}|n\rangle\langle n|\Psi(t)\rangle_S = a_k(t)\,,$$

because $\langle n|\Psi(t)\rangle_S = a_n(t)\exp(-iE_n t/\hbar)$, and that ($V^S_{\rm int}(t) \equiv V_{\rm int}(t)$)

$$\langle k|V^I_{\rm int}(t)|n\rangle = \langle k|e^{iH_0 t/\hbar}\, V^S_{\rm int}(t)\, e^{-iH_0 t/\hbar}|n\rangle = e^{i\omega_{kn} t}\, \langle k|V^S_{\rm int}(t)|n\rangle\,. \tag{2.3}$$

Therefore, (2.2) is simply the equation (1.19) written in the basis of the H_0 eigenstates.

In order to obtain the expansion in powers of λ of the solution of the system of equations (2.2), one seeks it in the form of the power series $a_k = a_k^{(0)} + \lambda\, a_k^{(1)} + \lambda^2 a_k^{(2)} + \ldots$ Equating then the coefficients of the same powers of λ on both sides of (2.2) yields the hierarchy of equations ($s = 0, 1, \ldots$)

$$\begin{aligned} &\dot{a}_k^{(0)}(t) = 0\,, \\ &\dot{a}_k^{(s+1)}(t) = \frac{1}{i\hbar} \sum_n e^{i\omega_{kn} t}\, \langle k|V_{\rm int}(t)|n\rangle\, a_n^{(s)}(t)\,. \end{aligned} \tag{2.4}$$

[2]The set of (time independent) vectors $|n\rangle$ is assumed to be complete, that is to form a basis of the Hilbert space. It may also include generalized (nonnormalizable) eigenvectors of the Hamiltonian H_0 which is assumed to be time independent.

Integrating them successively it is convenient to fix the constant coefficients $a_k^{(0)}$ so that[3]

$$|\Psi(t_0)\rangle = \sum_k |k\rangle\, e^{-iE_k t_0/\hbar}\, a_k^{(0)}\,, \tag{2.5}$$

and to impose on the remaining time dependent coefficients $a_k^{(s)}(t)$ with $s = 1, 2, \ldots$ the condition $a_k^{(s)}(t_0) = 0$. In this way $a_k(t_0) = a_k^{(0)}$ and the coefficients $a_k^{(s)}(t)$ (which implicitly depend also on t_0) are explicitly given by

$$\begin{aligned} a_k^{(1)}(t) &= \frac{1}{i\hbar}\int_{t_0}^{t} d\tau_1\, e^{i\omega_{kn_1}\tau_1}\, \langle k|V_{\rm int}(\tau_1)|n_1\rangle\, a_{n_1}^{(0)}\,, \qquad (2.6)\\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\ a_k^{(s)}(t) &= \left(\frac{1}{i\hbar}\right)^s \int_{t_0}^{t} d\tau_s \int_{t_0}^{\tau_s} d\tau_{s-1} \ldots \int_{t_0}^{\tau_2} d\tau_1\, e^{i\omega_{kn_s}\tau_s}\, e^{i\omega_{n_s n_{s-1}}\tau_{s-1}} \ldots e^{i\omega_{n_2 n_1}\tau_1} \\ &\qquad \times \sum_{n_s \ldots n_1} \langle k|V_{\rm int}(\tau_s)|n_s\rangle \ldots \langle n_2|V_{\rm int}(\tau_1)|n_1\rangle\, a_{n_1}^{(0)}\,, \end{aligned}$$

As in (2.1) the sums over n_i denote summations over the discrete and integration over the continuous parts of the H_0 spectrum. In view of (2.3), it is clear that, omitting the constant factor $a_{n_1}^{(0)}$ and the sum over n_1, the expression on the right is precisely the s-th terms of the iterative formula (1.22) for $U_I(t, t_0)$ sandwiched between the H_0 eigenvectors $\langle k|$ and $|n_1\rangle$. It makes, therefore, sense to write

$$a_k(t) = \sum_n \left[\delta_{kn} + \mathcal{A}_{kn}^{(1)}(t, t_0) + \mathcal{A}_{kn}^{(2)}(t, t_0) + \ldots\right] a_n^{(0)} \equiv \sum_n \mathcal{A}_{kn}(t, t_0)\, a_n(t_0)\,,$$

so that $a_k^{(s)}(t) = \sum_n \mathcal{A}_{kn}^{(s)}(t, t_0)\, a_n^{(0)}$ and

$$\mathcal{A}_{kn}(t, t_0) = \langle k|U_I(t, t_0)|n\rangle\,. \tag{2.7}$$

Having the solution $|\Psi(t)\rangle$ (usually only an approximation to it, consisting of only a few terms of the above expansion) one can in principle ask (independently of whether the interaction $V_{\rm int}$ is constant or time-dependent) what is the probability of finding the system at an instant t in a particular normalizable state $|\Phi\rangle$ (probabilities of transitions to nonnormalizable states, or, more precisely, to a group of nonnormalizable states, e.g. belonging to the continuous part of the spectrum of H_0, will be considered in Section 2.5), if at t_0 it was prepared[4] in a state $|\Psi_0\rangle \equiv |\Psi(t_0)\rangle$ of the general form (2.5). This probability $P(\Psi_0 \to \Phi;\, t, t_0)$ is given by:

$$P(\Psi_0 \to \Phi;\, t, t_0) = |\langle\Phi|\Psi(t)\rangle|^2\,. \tag{2.8}$$

[3] In other words $|\Psi(t_0)\rangle_I = \sum_n |n\rangle\, a_n^{(0)}$.

[4] It is a standard wisdom that systems can really be prepared only in normalizble states. Nevertheless, one can consider also nonnormalizable initial states $|\Psi_0\rangle$ (this may require introducing in expressions some extra factors ensuring convergence of integrals) as an idealization of well collimated (normalizable) states.

In general it strongly depends on t (and on t_0).

Even if the interaction depends explicitly on time and stationary eigenvectors of the Hamiltonian $H = H_0 + V_{\rm int}(t)$ do not exist in the strict sense, one may formally still ask about the probability of finding the system at an instant t in a normalized eigenstate $|k\rangle$ of H_0 (if H_0 has some proper eigenvectors) if at t_0 the system was prepared in the state $|\Psi_0\rangle$. Because one projects in this case $|\Psi(t)\rangle$ onto the exact H_0 eigenvector $|k\rangle$ and takes the modulus, the oscillatory factor $\exp(-iE_kt/\hbar)$ drops out and resulting transition probability is then simply equal $|a_k(t)|^2$ (it may still depend on time if $V_{\rm int}(t)$ is still nonzero at the instant t which is always true if $V_{\rm int}$ is time independent). The same probablity is, of course given by $|\mathcal{A}_{kn}(t,t_0)\, a_n(t_0)|^2$, that is, by the modulus squared of the amplitude

$$\langle k|e^{iH_0t/\hbar}|\Psi(t)\rangle = \langle k|\Psi(t)\rangle_I \equiv \langle k|U_I(t,t_0)|\Psi(t_0)\rangle_I\,. \tag{2.9}$$

Although the general principles allow to ask about such a probability of finding the system in a normalizable eigenstate of H_0, because of the still significant dependence of (2.9) on t and t_0 it is physically interesting mostly in some special situations, in particular when at the instant t the interaction $V_{\rm int}$ is already absent and the time evolution of the system is governed by H_0. It is only in such cases that t may also be taken to correspond to the infinite future ($t \to \infty$). Similarly, taking t_0 to correspond to the inifinite past (i.e. $t_0 \to -\infty$) is possible, strictly speaking, only if $V_{\rm int}$ switches off there. If the interaction is active at any time (e.g. because $V_{\rm int}$ is just a constant operator), using probabilities of transisions to H_0 eigenstates requires some care as will be seen below - such probabilities are well defined only in the lowest order of the perturbative expansion.

In many situations of interest the perturbation $V_{\rm int}(t)$ acts indeed only during a finite period, i.e. it vanishes when $t \to \mp\infty$, the system is prepared in the far past, (practically at $t_0 = -\infty$) in a H_0 eigenstate $|n\rangle$ (so that one particular $a_n^{(0)} = 1$ and $a_k^{(0)} = 0$ for $k \neq n$), and one is interested in the probability of finding it in a normalizable H_0 eigenstate $|k\rangle$ in the far future, after the interaction has already switched off. The corresponding transition amplitude which has well defined $t \to \infty$ and $t_0 \to -\infty$ limits is then $\mathcal{A}_{kn}(t,t_0)$. It should also be clear that this double limit, $\mathcal{A}_{kn}(\infty,-\infty)$, of the transition amplitude is just the element S_{kn} of the S-matrix introduced in the second example considered in Section 1.3. The transition probability $P(n \to k)$ of interest is in this situation equal $|\mathcal{A}_{kn}(\infty,-\infty)|^2 = |S_{kn}|^2$. In the lowest nontrivial approximation, if $k \neq n$, $P(n \to k) \approx |\mathcal{A}^{(1)}_{kn}(\infty,-\infty)|^2$ with

$$\mathcal{A}^{(1)}_{kn}(t,t_0) = \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, \langle k|V_{\rm int}(t')|n\rangle\, e^{i\omega_{kn}t'}\,. \tag{2.10}$$

In Section 2.2 this method of computing $P(n \to k)$ will be applied to the second example treated in Section 1.3. This will allow to discuss how unitarity of the S-matrix is realized in the perturbative expansion.

Another class of physically interesting situations is when $V_{\rm int}(t)$ does not vanish for $t \to \pm\infty$ but instead tends to well defined limits $V_{\rm int}^{(\pm)}$, where $V_{\rm int}^{(\pm)}$ are some time independent Hermitian operators. It is then most convenient to include $V_{\rm int}^{(-)}$ in H_0 and the most relevant question is one about transitions from a normalizable H_0 eigenstate prepared in the far past ($t_0 = -\infty$) to a normalizable eigenstate of $H(\infty) = H_0 + V_{\rm int}^{(+)}$ in the far future. Here the expansion of $U_I(t, t_0)$ in the basis of the H_0 eigenvectors becomes less useful,[5] but, as will be shown in section 2.3, in the first order in $V_{\rm int}$ the relevant probabilities can, nevertheless, be extracted from it.

The two types of changes of the Hamiltonian discussed above can occur at different rates. It will be seen below that in the two extreme cases - of a very fast change (occuring in a very short time interval) and of a very slow one - in the limit, occuring infinitely slowly - one can give useful special approximations which go beyond the perturbative expansion of the evolution operator $U_I(t, t_0)$. In the first case it is called the *instant* (or *impulse*) approximation. In the second case the special approximation is called *adiabatic*. It is based on the adiabatic theorem which was already exploited in Section 1.2 in the Gell-Mann - Low construction of the (normalizable) ground state vector of H out of the (normalized) ground-state vector of H_0. The theorem will be discussed in Section 2.4. An interesting aspect of the adiabatic approximation in the situation when the Hamiltonian returns after a long time to its initial form is the emergence of a phase, called after its discoverer the Berry's phase, of an essentially topological origin.

If the (Schrödinger picture) interaction operator $V_{\rm int}$ does not depend on time, the equations (2.4) can be straightforwardly integrated yielding in principle the explicit form of the perturbative expansion of the interaction picture evolution operator $U_I(t, t_0)$ (1.22) written in the basis of H_0 einenvectors. The expansion turns out however to be highly singular, a fact which has already been observed on the simplest example of the evolution operator of the harmonic oscillator (see the formula (1.51)) the spectrum of which is purely discrete. One way of regularizing the expansion, particularily convenient if one is interested in the limit $t_0 \to -\infty$, is to replace $V_{\rm int}$, as in Section 1.2, by $e^{\varepsilon t} V_{\rm int}$ and to take the limit $\varepsilon \to 0^+$ at the end. The explicit example considered in Section (1.3) shows (ifsoved exactly) that these singularities, if regularized in this way, should factorize into a singular phase factor at least in situations in which the interaction switches off asymptotically (and using the basis of H_0 einegvectors makes sense physically). Setting $t_0 = -\infty$ one then gets (recall, $\omega_{n_3 n_2} + \omega_{n_2 n_1} = \omega_{n_3 n_1}$ and $\omega_{n_j n_1} = -\omega_{n_1 n_j}$)

$$\mathcal{A}^{(s)}_{kn_1}(t, -\infty) = \sum_{n_s \ldots n_2} \frac{e^{(i\omega_{kn_1} + s\varepsilon)t}\, V_{kn_s} V_{n_s n_{s-1}} \ldots V_{n_2 n_1}}{\hbar^s (\omega_{n_1 k} + is\varepsilon) \ldots (\omega_{n_1 n_3} + i2\varepsilon)(\omega_{n_1 n_2} + i\varepsilon)}\,, \tag{2.11}$$

where $V_{n_i n_j} \equiv \langle n_i | V_{\rm int} | n_j \rangle$. In the limit $\varepsilon \to 0^+$ the factors $i\varepsilon$ in the denominator specify the way of going around the possible singularities. In this form the formula (and the

[5] One would rather preferred to find directly matrix elements of $U_I(t, t_0)$ between the eigenvectors H_0 and the eigenvectors $H_0 + V_{\rm int}^{(+)}$, i.e. matrix elements of the operator $U_I(t, t_0)$ between vectors of two different bases "on its two sides".

one below) remain valid even if the labels $n_1, \ldots, n_s$ run over a continuous (or partly discrete and partly continuos) set of values and the summations over them are replaced by appropriate integrals (or sums and integrals). In this limit one obtains

$$|\Psi(t)\rangle = \sum_{k,n_1} |k\rangle \left(\delta_{kn_1} + \frac{e^{\varepsilon t} V_{kn_1}}{E_{n_1} - E_k + i0} + \sum_{n_2} \frac{e^{2\varepsilon t} V_{kn_2} V_{n_2 n_1}}{(E_{n_1} - E_k + 2i0)(E_{n_1} - E_{n_2} + i0)} + \ldots \right) e^{-iE_{n_1} t/\hbar}\, a^{(0)}_{n_1} ,$$

where $a^{(0)}_{n_1}$ are the expansion coefficients of $\lim_{t_0 \to -\infty} e^{iH_0 t_0/\hbar} |\Psi(t_0)\rangle \equiv \lim_{t_0 \to -\infty} |\Psi(t_0)\rangle_I$ into the H_0 eigenvectors $|n_1\rangle$. However, in most cases of interest the basis of H_0 eigenvectors is not very physical (the true Hamiltonian of the closed system being $H_0 + V_{\rm int}$), particularily when H_0 has no normalizable eigenvectors, and beyond the first order the transition probabilities between the H_0 (generalized) eigenvectors become ill defined. Only if the interaction $V_{\rm int}$ is adjusted properly (essentially order by order), can these transition probabilities make sense. This will become clear in due course.

2.2 Finite time perturbation

Let us consider first a perturbation $V_{\rm int}(t)$ which vanishes in both limits, $t \to -\infty$ and $t \to +\infty$. One is then usually interested in probabilities of transitions from a H_0 eigenstate $|m\rangle$ at $t = -\infty$ to other H_0 eigenstates $|k\rangle$ at $t = +\infty$. To this class of problems belongs also the one-dimensional harmonic oscillator perturbed with a constant in space force $F(t)$ vanishing at $t = \mp\infty$, which was solved exactly in Section 1.3 using the Heisenberg picture and the formalism of the *in* and *out* states (and the corresponding *in* and *out* operators). In the approach based on the perturbative expansion discussed in Section 2.1, to obtain the amplitudes of the system's transitions from the H_0 eigenstate $|m\rangle$ in the far past to another H_0 eigenstate $|k\rangle$ in the far future, that is the element S_{km} of the S-matrix, one considers instead the time evolution of the system's interaction picture state-vector $|\Psi(t_0)\rangle_I$ which in the far past, i.e. in the limit $t_0 \to -\infty$, has the form

$$|\Psi(t_0)\rangle_I = |m\rangle ,$$

and projects $|\Psi(t)\rangle_I$ given by

$$\begin{aligned} |\Psi(t)\rangle_I &= \sum_k |k\rangle\, \mathcal{A}_{km}(t, -\infty) \\ &\approx |m\rangle + \sum_k |k\rangle \left(\mathcal{A}^{(1)}_{km}(t, -\infty) + \mathcal{A}^{(2)}_{km}(t, -\infty) + \ldots \right) , \end{aligned}$$

onto the H_0 eigenvector $|k\rangle$. Since the perturbation vanishes asymptotically, the amplitude $\mathcal{A}_{km}(t, -\infty)$ obtained in this way, as well as the amplitudes $\mathcal{A}^{(p)}_{km}(t, -\infty)$, tend to well

defined limits as $t \to \infty$. To the above expansion of $|\Psi(t)\rangle_I$ corresponds, of course, the expansion

$$S_{km} = \delta_{km} + S^{(1)}_{km} + S^{(2)}_{km} + \ldots , \tag{2.12}$$

of the S-matrix ($S^{(p)}_{km} = \mathcal{A}^{(p)}_{km}(\infty, -\infty)$). The probability that the system at $t = \infty$ will be found in the $|k\rangle$-th eigenstate of H_0 (probability of the transition to the state $|k\rangle$) is then given by

$$P(m \to k) = |S_{km}|^2 \approx \left| \delta_{km} + \frac{1}{i\hbar} \int_{-\infty}^{+\infty} dt\, e^{i\omega_{km} t} \, \langle k|V_{\rm int}(t)|m\rangle + \ldots \right|^2 . \tag{2.13}$$

The obvious criterion of applicability of the perturbative expansion (in powers of the interaction) of the coefficients $A_{km}(t)$ is the condition $|\mathcal{A}^{(s)}_{km}| \ll 1$, for $s \geq 1$. This imposes some restriction not only on the values of the relevant matrix elements of $V_{\rm int}(t)$ between the H_0 eigenstates, but also on the effective time duration Δt of the perturbation[6] (it is $\Delta t\, |\langle k|V_{\rm int}|m\rangle|/\hbar$ which is dimensionless).

As an illustrative example we will reconsider the one-dimensional harmonic oscillator of mass M and frequency ω, subject to the perturbation of the concrete form $V_{\rm int}(t) = -xF_0/(1+t^2/\tau^2)$ and will compute the probabilities $P(m \to k)$ of the transitions induced by

$$V_{\rm int}(t) = -\sqrt{\frac{\hbar}{2M\omega}}\, (a + a^\dagger)\, \frac{F_0}{1 + t^2/\tau^2} ,$$

using the time-dependent perturbative approach formulated in section 2.1. Computing the matrix elements of $V_{\rm int}$ is then straightforward:

$$\langle k|V_{\rm int}(t')|m\rangle = -\sqrt{\frac{\hbar}{2M\omega}} \left(\sqrt{m}\, \delta_{k,m-1} + \sqrt{m+1}\, \delta_{k,m+1} \right) \frac{F_0}{1 + t^2/\tau^2} . \tag{2.14}$$

It follows that to the first order in the perturbation possible are only the transitions $m \to m$ and $m \to m \pm 1$. (This means that other transitions, though possible, are suppressed, that is, their probabilities are proportional to higher powers of $\lambda \equiv F_0$). In this order the probability of the first one equals 1 because $S^{(0)}_{mm} = 1$, $S^{(1)}_{mm} = 0$ (we will return to the problem of the total transition probability shortly). Finding the probabilities of the other two transitions reduces to computing the integral

$$I = \int_{-\infty}^{+\infty} dt\, \frac{e^{i\omega_{km} t}}{1 + t^2/\tau^2} = \tau \int_{-\infty}^{+\infty} d\xi\, \frac{e^{i\omega_{km}\tau\xi}}{(\xi + i)(\xi - i)} .$$

[6] As will be seen on the example, the oscillatory factors present in (2.13) under the integral, can in some cases relax this criterion.

Using the method of residues and taking into account that for $k = m \pm 1$ $\omega_{km} = \pm\omega$, we find in both cases $I = \pi\tau \exp(-\omega\tau)$. Thus,

$$S^{(1)}_{m-1,m} = \frac{i}{\sqrt{2M\hbar\omega}}\, F_0 \pi\tau\, e^{-\omega\tau}\, \sqrt{m}\,, \tag{2.15}$$
$$S^{(1)}_{m+1,m} = \frac{i}{\sqrt{2M\hbar\omega}}\, F_0 \pi\tau\, e^{-\omega\tau}\, \sqrt{m+1}\,,$$

and, to the first order $P(m \to m) = 1$ and

$$P(m \to m-1) = \frac{F_0^2\pi^2\tau^2}{2M\hbar\omega}\; m\; e^{-2\omega\tau}\,,$$
$$P(m \to m+1) = \frac{F_0^2\pi^2\tau^2}{2M\hbar\omega}\,(m+1)\, e^{-2\omega\tau}\,. \tag{2.16}$$

Note that $P(m \to m+1) = P(m+1 \to m)$ as it should be (cf. (1.66)).

The probabilities (2.16) vanish in both limits: $\tau \to \infty$ and $\tau \to 0$. The first limit corresponds to the so-called "adiabatic" perturbation which affects the oscillator in a very gentle way.[7] The transition probabilities vanish then exponentially. This illustrates the adiabaticity principle. The other case corresponds to the force which displaces the equilibrium point of the oscillator for only a very short period $\Delta t \sim \tau$. The transition probabilities vanish in this case too, the heuristic explanation of this being that the quantum state-vector exhibits some "inertia" and cannot follow the abrupt change of the Hamiltonian immediately; since the Hamiltonian returns to its original form after a time $\sim \tau \to 0$, nothing happens (cf. the impulse approximation below).

In this simple example it is possible to easily go one step further in the perturbative expansion and consider the second order contributions to the transition probabilities. This will allow us to discuss unitarity of the S-matrix within the perturbative approach. Using the general formulae (2.10) and (2.4) with $t_0 = -\infty$ we get

$$\dot a^{(2)}_k(t) = \left(\frac{1}{i\hbar}\right)^2 \sum_n e^{i\omega_{kn}t}\, \langle k|V_{\rm int}(t)|n\rangle \int_{-\infty}^{t} dt'\, e^{i\omega_{nm}t'}\, \langle n|V_{\rm int}(t')|m\rangle\,.$$

Inserting here the matrix elements (2.14) we obtain

$$S^{(2)}_{km} = -\frac{F_0^2}{2M\hbar\omega}\int_{-\infty}^{+\infty} dt \int_{-\infty}^{t} dt' \sum_n \frac{e^{i\omega_{kn}t}\, e^{i\omega_{nm}t'}}{[1+t^2/\tau^2][1+t'^2/\tau^2]}$$
$$\times \left(\sqrt{n}\,\delta_{k,n-1} + \sqrt{n+1}\,\delta_{k,n+1}\right)\left(\sqrt{m}\,\delta_{n,m-1} + \sqrt{m+1}\,\delta_{n,m+1}\right).$$

From the structure of the matrix elements we see that in the second order of the perturbative expansion the following transitions are possible:

[7] Although the effective time duration $\Delta t \sim \tau$ tends in this case to infinity and $\tau|\langle k|V_{\rm int}(t)|m\rangle|/\hbar \to \infty$, and the simple criterion of applicability of the perturbative expansion formulated above seems to be violated, the oscilatory factors make the expansion, nevertheless, reliable.

i) to $|k\rangle = |m-2\rangle$, with $S^{(2)}_{km}$ proportional to $\sqrt{m(m-1)}$; in this case the double integral involves the factor $e^{-i\omega t}e^{-i\omega t'}$,
ii) to $|k\rangle = |m+2\rangle$, with $S^{(2)}_{km}$ proportional to $\sqrt{(m+2)(m+1)}$; here the double integral involves the factor $e^{+i\omega t}e^{+i\omega t'}$,
iii) to $|k\rangle = |m\rangle$; here two terms contribute to $S^{(2)}_{km}$: one proportional to m with the factor $e^{+i\omega t}e^{-i\omega t'}$ under the integral, and the second term proportional to $m+1$ with $e^{-i\omega t}e^{+i\omega t'}$ under the integral.

The integrals appearing in the elements $S^{(2)}_{km}$ with $k = m-2$ and $k = m+2$ are easy to compute: it suffices to notice that because the integrand $h(t,t') = f(t)f(t')$ is symmetric, $h(t,t') = h(t',t)$, one can write

$$\int_{-\infty}^{+\infty} dt \int_{-\infty}^{t} dt' f(t)f(t') = \int_{-\infty}^{+\infty} dt' \int_{t'}^{+\infty} dt f(t)f(t') = \int_{-\infty}^{+\infty} dt \int_{t}^{+\infty} dt' f(t')f(t)\,,$$

from which it follows that

$$\int_{-\infty}^{+\infty} dt \int_{-\infty}^{t} dt' f(t)f(t') = \frac{1}{2}\left[\int_{-\infty}^{+\infty} dt f(t)\right]^2 = \frac{1}{2}\, I^2.$$

Hence,

$$\begin{aligned} S^{(2)}_{m-2,m} &= -\frac{(F_0\pi\tau)^2}{4M\hbar\omega}\, e^{-2\omega\tau}\, \sqrt{m(m-1)}\,, \\ S^{(2)}_{m+2,m} &= -\frac{(F_0\pi\tau)^2}{4M\hbar\omega}\, e^{-2\omega\tau}\, \sqrt{(m+2)(m+1)}\,. \end{aligned} \tag{2.17}$$

and, therefore,

$$\begin{aligned} P(m \to m-2) &= \frac{1}{16M^2\hbar^2\omega^2}\, m(m-1)(F_0\pi\tau)^4 \exp(-4\omega\tau)\,, \\ P(m \to m+2) &= \frac{1}{16M^2\hbar^2\omega^2}\, (m+2)(m+1)(F_0\pi\tau)^4 \exp(-4\omega\tau)\,, \end{aligned}$$

that is, $P(m \to m+2) = P(m+2 \to m)$.

It is instructive to confront these results with the unitarity of the S-matrix. In terms of the expansion (2.12) the unitarity relation (1.57) takes the form

$$0 = \left(S^{(1)*}_{m,m'} + S^{(1)}_{m',m}\right) + \left(S^{(2)*}_{m,m'} + S^{(2)}_{m',m} + \sum_k S^{(1)*}_{k,m'} S^{(1)}_{k,m}\right) + \ldots \tag{2.18}$$

As the expressions in the successive brackets are proportional to different powers of the formal expansion parameter λ, they must vanish separately. In the considered example the first order equality $S^{(1)*}_{m,m'} + S^{(1)}_{m',m} = 0$ is clearly satisfied[8] by the elements (2.15). The

[8]The same follows also from the relation (1.66); being exact this formula also implies the general relation $S^{(1)*}_{m,m'} = (-1)^{m-m'} S^{(1)}_{m',m}$; in the case considered here $|m-m'| = 1$.

second order relation applied to $m' = m + 2$ and taking into account only the nonzero first order elements reads

$$S^{(2)*}_{m,m+2} + S^{(2)}_{m+2,m} + S^{(1)*}_{m+1,m+2} S^{(1)}_{m+1,m} = 0\,.$$

Using in it the results (2.15) confirms the correctness of the calculated second order S-matrix elements given by (2.17). The same second order unitarity relation applied to $m' = m$ gives

$$S^{(2)*}_{m,m} + S^{(2)}_{m,m} + S^{(1)*}_{m+1,m} S^{(1)}_{m+1,m} + S^{(1)*}_{m-1,m} S^{(1)}_{m-1,m} = 0\,. \tag{2.19}$$

Using the results (2.15) one finds

$$2\,\mathrm{Re}(S^{(2)}_{m,m}) = -\frac{(F_0\pi\tau)^2}{2M\hbar\omega}\,(2m+1)\,e^{-2\omega\tau}. \tag{2.20}$$

This can be also computed directly. While the integral which is necessary for $S^{(2)}_{m,m}$ itself is not easy to compute because the integrand is not a symmetric function of t and t', the integral which gives $2\mathrm{Re}(S^{(2)}_{m,m})$ is simpler because the combined integrand of the sum of $S^{(2)}_{m,m}$ and $S^{(2)*}_{m,m}$ is effectively symmetric. Therefore

$$\begin{aligned}
2\,\mathrm{Re}\big(S^{(2)}_{m,m}\big) &= -\frac{F_0^2(2m+1)}{2M\hbar\omega}\int_{-\infty}^{+\infty} dt \int_{-\infty}^{t} dt'\,\frac{e^{-i\omega t}e^{+i\omega t'} + e^{i\omega t}e^{-i\omega t'}}{[1+t^2/\tau^2][1+t'^2/\tau^2]} \\
&= -\frac{F_0^2(2m+1)}{2M\hbar\omega}\frac{1}{2}\int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt'\,\frac{e^{-i\omega t}e^{+i\omega t'} + e^{i\omega t}e^{-i\omega t'}}{[1+t^2/\tau^2][1+t'^2/\tau^2]} \\
&= -\frac{F_0^2(2m+1)}{2M\hbar\omega}\int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt'\,\frac{e^{-i\omega t}e^{+i\omega t'}}{[1+t^2/\tau^2][1+t'^2/\tau^2]} \\
&= -\frac{F_0^2(2m+1)}{2M\hbar\omega}\left[\int_{-\infty}^{+\infty} dt\,\frac{e^{-i\omega t}}{1+t^2/\tau^2}\right]^2,
\end{aligned}$$

which is the result obtained from (2.19). In fact it is precisely $2\mathrm{Re}(S^{(2)}_{m,m})$, and not $S^{(2)}_{m,m}$ itself, which is needed to find the first nontrivial correction to the zero-th order result $P(m \to m) \approx 1$. Indeed,

$$P(m \to m) = \left|1 + S^{(2)}_{m,m} + S^{(4)}_{m,m} + \ldots\right|^2 = 1 + 2\mathrm{Re}\left(S^{(2)}_{m,m}\right) + \mathcal{O}(F_0^4)\,,$$

(from the structure of V_{int} it readily follows that $S^{(1)}_{m,m} = S^{(3)}_{m,m} = \ldots = 0$). The term $|S^{(2)}_{m,m}|^2$ contributes to the order F_0^4 term but the contribution $2\mathrm{Re}(S^{(4)}_{m,m})$ is also of the same (F_0^4) order. Thus, without computing $2\mathrm{Re}(S^{(4)}_{m,m})$ the probability $P(m \to m)$ can be found consistently only up to the F_0^2 order. Thus

$$P(m \to m) = 1 - \frac{(F_0\pi\tau)^2}{2M\hbar\omega}\,(2m+1)\,e^{-2\omega\tau} + \mathcal{O}(F_0^4)\,.$$

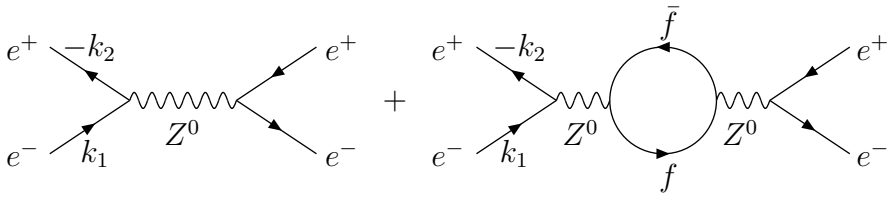

Figure 2.2: Example of the perturbative unitarization of quantum field theory transition amplitudes: because the Z^0 boson is an unstable particle, the amplitude of elastic electron-positron scattering should have a pole at a complex value of the Mandelstam variable $s \equiv (k_1 + k_2)^2 \approx M_Z^2 - iM_Z\Gamma_Z$ and not at the real value $s = M_Z^2$. To get the position of the pole shifted off the real axis one has however to compute the amplitude of the $e^-e^+ \to e^-e^+$ scattering up to the second order terms in the perturbative expansion.

Using this result as well as the probabilities $P(m \to m \pm 1)$ computed earlier (the probabilities $P(m \to m \pm 2)$ are of order F_0^4) it is straightforward to directly check (what anyway is secured by the relations (2.18)) that

$$\sum_k P(m \to k) = 1 + \mathcal{O}(F_0^3)\,.$$

This example shows that the unitarity is successively restored by including higher order contributions to $S_{k,m}$. Such a *perturbative unitarization* of transition amplitudes is a usual feature of calculations performed in the framework of quantum field theory (see Figure 2.2 for an illustration). The relation (2.18) which allows to obtain the p-th order $S^{(p)*}_{m,m'} + S^{(p)}_{m',m}$ from the S-matrix elements $S^{(s)}_{k,m}$ with $s < p$ is an example of the optical theorem which will be derived in Section 7.6.

The transition probabilities computed here can be compared with the ones following from the exact solution of the problem which was obtained in section 1.3. To this end, one has to set in the exact S-matrix given by (1.65)

$$c = \frac{i}{\sqrt{2M\hbar\omega}} \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, F(t) = \frac{i}{\sqrt{2M\hbar\omega}}\, F_0 \pi\tau\, e^{-\omega\tau}\,.$$

The expansion in powers of F_0 is then equivalent to the expansion in powers of $|c|$. Expanding for example the element $S_{m,m}$ of (1.65) we get

$$S_{m,m} = \left(1 - \frac{1}{2}|c|^2 + \ldots\right)\left(1 - m|c|^2 + \ldots\right) = 1 - \frac{1}{2}(2m+1)|c|^2 + \ldots\,,$$

(the lowest powers of $|c|$ arise from the terms with the largest values of k in the sum in (1.65)) and $2\mathrm{Re}(S_{mm})$ obtained in this way coincides with (2.20). (Incidentally, the comparison with the exact element S_{mm} shows that $\mathrm{Im}(S^{(2)}_{m,m}) = 0$). Other matrix elements can be checked similarly: $S_{m-1,m} = -c^*\sqrt{m} + \ldots$ and $S_{m+1,m} = c\,\sqrt{m+1} + \ldots$, etc.

2.3 Change of the Hamiltonian

Another interesting case to which the time dependent perturbative expansion can be applied is the situation in which the Hamiltonian of the system undergoes a finite change: $H(t) \to H_0$ as $t \to -\infty$ and $H(t) \to H_0 + V_{\rm int}^{(+)}$ in the limit $t \to +\infty$, that is $V_{\rm int}(-\infty) = 0$ but $V_{\rm int}(+\infty) = V_{\rm int}^{(+)}$. In this case one is naturally interested in probabilities of transitions from an eigenstate $|m\rangle$ of H_0 ($H_0|m\rangle = E_m|m\rangle$) prepared in the far past to a normalizable eigenstate $|\tilde{k}\rangle$ of $H_0 + V_{\rm int}^{(+)}$ at $t = +\infty$:

$$(H_0 + V_{\rm int}^{(+)})|\tilde{k}\rangle = (E_k + \Delta E_k)|\tilde{k}\rangle \equiv \tilde{E}_k|\tilde{k}\rangle \,.$$

Obviously, if $V_{\rm int}^{(+)}$ is a small perturbation in the usual sense, ΔE_k and the coefficients of the expansion of $|\tilde{k}\rangle$ in terms of the H_0 eigenvectors $|m\rangle$ can be computed perturbatively with the help of the ordinary Rayleigh-Schrödinger expansion. Furthermore, if the change of the Hamiltonian occurs (almost) instantaneously compared to a characteristic time of the system (determined by the inverse of the difference of its energy levels), the intuitive picture is that the system's state-vector does not change during the short period in which the Hamiltonian undergoes the change. However, even if before the perturbation has started to act the system was in an eigenstate of H_0, the corresponding initial state-vector is not an eigenvector of the ultimate Hamiltonian $H_0 + V_{\rm int}^{(+)}$ and will have, therefore, nonzero projections onto (in general all) its eigenvectors. In agreements with the general principles the transition probabilities (evaluated at any moment after the Hamiltonian has already assumed its final form $H_0 + V_{\rm int}^{(+)}$) should be, therefore, given by the squares of the absolute values of the scalar products of the initial system's state-vector with the eigenvectors of $H_0 + V_{\rm int}^{(+)}$.

This intuitively clear prescription for computing the probabilities of transitions induced by the sudden, ccuring in a short time interval $T = t_2 - t_1$, between the instants t_1 and t_2, change $\Delta H = V_{\rm int}^{(+)}$ of the Hamiltonian, can be justfied in a more formal way by replacing the time variable by a dimensionless parameter $\xi = (t - t_1)/T$ ($0 \le \xi \le 1$), and writing the system's (Schrödinger picture) evolution operator $U(t, t_1)$ corresponding to the time interval (t, t_1), where $t \le t_2$, as $U_T(\xi)$. The integral equation (1.6) can be then rewritten in the form

$$U_T(\xi) = \hat{1} - \frac{i}{\hbar}\, T \int_0^{\xi} d\xi'\, H(\xi')\, U_T(\xi') \,, \tag{2.21}$$

in which $H(\xi)$ is the Hamiltonian expressed through the parameter ξ. Under the adopted assumptions $H(0) = H_0$, $H(1) = H_0 + V_{\rm int}^{(+)}$ and it is clear that as $T \to 0$

$$U(t_2, t_1) = U_T(1) \to \hat{1} \,. \tag{2.22}$$

That is, if the system's state was at t_1 represented by a (normalized to unity) vector $|\Psi_1\rangle$, immediately after the instantaneous change of the Hamiltonian, at the moment t_2, it is

represented approximately by $U(t_2,t_1)|\Psi_1\rangle \approx |\Psi_1\rangle$. (Of course, the evolution operator corresponding to time intervals before t_1 has the form (1.5) with the Hamiltonian H_0 and after t_2, the same form but with the Hamiltonian $H_0 + V_{\rm int}^{(+)}$).

It is possible to obtain a simple estimate of the probability P of the system not being at t_2 in the state $|\Psi_1\rangle$. It is given by[9]

$$P = \langle\Psi_1|U^\dagger(t_2,t_1)\hat{P}_\perp U(t_2,t_1)|\Psi_1\rangle\,, \tag{2.23}$$

where $\hat{P}_\perp = \hat{1} - |\Psi_1\rangle\langle\Psi_1|$ is the projection operator onto the subspace (of the entire Hilbert space) orthogonal to $|\Psi_1\rangle$. Inserting in this formula the iterated solution to (2.21) and noticing that $\hat{P}_\perp|\Psi_1\rangle = 0$, one finds that

$$P = \frac{T^2}{\hbar^2}\langle\Psi_1|\overline{H}\hat{P}_\perp\overline{H}|\Psi_1\rangle + \mathcal{O}(T^3) \approx \frac{T^2}{\hbar^2}\left[\langle\Psi_1|\overline{H}^2|\Psi_1\rangle - (\langle\Psi_1|\overline{H}|\Psi_1\rangle)^2\right],$$

where

$$\overline{H} = \frac{1}{T}\int_{t_1}^{t_2} dt\, H(t) = \int_0^1 d\xi\, H(\xi)\,.$$

The probability P is (approximately) given by the squared dispersion $\Delta\overline{H}$ of the "mean" Hamiltonian $\overline{H}$ in the state $|\Psi_1\rangle$ and is small if $T \ll \hbar/\Delta\overline{H}$.

Let us now see how this intuitive picture can be recovered from the first order of the perturbative expansion of the evolution operator $U_I(t,t_0)$ despite the fact that it is formulated in the basis of the H_0 eigenvectors. For the sake of definiteness we will assume that $|\Psi(-\infty)\rangle_I = |m\rangle$ - in the far past the system was in the H_0 eigenstate $|m\rangle$. By integrating by parts its right hand side, the formula (2.10) for $\mathcal{A}^{(1)}_{km}(t,-\infty)$ can be rewritten as

$$-\frac{\langle k|V_{\rm int}(t')|m\rangle}{\hbar\omega_{km}}\,e^{i\omega_{km}t'}\Big|_{-\infty}^{t} + \int_{-\infty}^{t} dt'\,\frac{e^{i\omega_{km}t'}}{\hbar\omega_{km}}\,\frac{\partial}{\partial t'}\langle k|V_{\rm int}(t')|m\rangle\,, \tag{2.24}$$

for $k \neq m$, and as

$$+\frac{t'}{i\hbar}\,\langle m|V_{\rm int}(t')|m\rangle\Big|_{-\infty}^{t} - \frac{1}{i\hbar}\int_{-\infty}^{t} dt'\,t'\frac{\partial}{\partial t'}\langle m|V_{\rm int}(t')|m\rangle\,, \tag{2.25}$$

for $k = m$. It should be now noticed that the first terms of these two expressions

$$\begin{aligned} &\frac{\langle k|V_{\rm int}(t)|m\rangle}{E_m - E_k}\,e^{i(E_k-E_m)t/\hbar} \qquad &&\text{for} \quad k \neq m \\ &-\frac{i}{\hbar}\,t\,\langle m|V_{\rm int}(t)|m\rangle \qquad &&\text{for} \quad k = m, \end{aligned}$$

[9]Suppose $|\psi\rangle = \sum_n |n\rangle c_n$, where $|n\rangle$ is a basis of the Hilbert space. The probability $P_n = |c_n|^2$ of finding the system in the state $|n\rangle$ can be obtained as $\langle\psi|\hat{P}_n|\psi\rangle$ where $\hat{P}_n = |n\rangle\langle n|$. This readily generalizes to the joint probability of finding the system in any linear combination of a subset of basis states $|n\rangle$, i.e. in any state belonging to a subspace of the Hilbert space spanned by this subset of the basis state-vectors $|n\rangle$.

(in which the condition $V_{\rm int}(-\infty)=0$ has been used), give the changes of the eigenvectors and eigenvalues of the Hamiltonian: for $t\to\infty$ (when $V_{\rm int}(t)=V_{\rm int}^{(+)}$) the expression for $|\Psi(t)\rangle$

$$|\Psi(t)\rangle = |m\rangle\, e^{-iE_m t/\hbar} + \sum_k |k\rangle\, e^{-iE_k t/\hbar}\, \mathcal{A}^{(1)}_{km}(t,-\infty) + \ldots ,$$

which is obtained from the perturbative expansion can be rearranged to give

$$\begin{aligned}
|\Psi(t)\rangle &= |m\rangle\, e^{-iE_m t/\hbar} - \frac{i}{\hbar}\, t\, |m\rangle\, e^{-iE_m t/\hbar} \langle m|V_{\rm int}(t)|m\rangle \\
&\quad + \sum_{k\neq m} |k\rangle\, e^{-iE_k t/\hbar}\, \frac{\langle k|V_{\rm int}(t')|m\rangle}{E_m - E_k}\, e^{i(E_k-E_m)t/\hbar} + \ldots \\
&\approx e^{-i(E_m+\Delta E_m)t/\hbar} \left(|m\rangle + \sum_{k\neq m} |k\rangle \frac{\langle k|V^{(+)}_{\rm int}|m\rangle}{E_m - E_k} \right) + \ldots \\
&\approx e^{-i\tilde{E}_m t/\hbar}\, |\tilde{m}\rangle + \ldots ,
\end{aligned} \tag{2.26}$$

that is, up to higher order corrections these terms reproduce the energy $\tilde{E}_m$ and the eigenvector $|\tilde{m}\rangle$ of $H_0+V^{(+)}_{\rm int}$ (compare the formulae of the ordinary Rayleigh - Schrödinger perturbative expansion). Since the probabilities of transitions to the eigenstates of $H_0 + V^{(+)}_{\rm int}$ should be calculated by taking the scalar products of $|\Psi(t)\rangle$ with the eigenvectors $|\tilde{k}\rangle$ of $H_0 + V^{(+)}_{\rm int}$, the terms displayed in (2.26) should be treated as producing (together with the higher order terms) $\delta_{\tilde{k}\tilde{m}}$. Calculating the transition probabilities in the first order in the perturbation $V^{(+)}_{\rm int}$ one can treat in the remaining terms $|k\rangle$ as $|\tilde{k}\rangle$ and E_k as $\tilde{E}_k$ (the differences between $|k\rangle$ and $|\tilde{k}\rangle$ and between E_k and $\tilde{E}_k$ affects $P(m\to\tilde{k})$ only in higher orders). Thus

$$\begin{aligned}
P(m\to\tilde{k}) &= \frac{1}{\hbar^2\omega_{km}^2} \left| \int_{-\infty}^{+\infty} dt\, e^{i\omega_{km}t}\, \frac{\partial}{\partial t} \langle k|V_{\rm int}(t)|m\rangle + \ldots \right|^2 , \qquad k\neq m\,, \\
P(m\to\tilde{m}) &= \left| 1 - \frac{1}{i\hbar} \int_{-\infty}^{+\infty} dt\, t\, \frac{\partial}{\partial t} \langle m|V_{\rm int}(t)|m\rangle + \ldots \right|^2 .
\end{aligned} \tag{2.27}$$

Similar rearrangement of the perturbative series giving $|\Psi(t)\rangle$ should be also possible in higher orders, but would be, of course, considerably more complicated technically. The need for such a rearrangement is clearly due to the fact that obviously the expansion in terms of the eigenvectors of the free Hamiltonian H_0 is not appropriate when one is interested in transitions to eigenstates of $H_0 + V^{(+)}_{\rm int}$. As it will be seen in due course, it is analogous to the procedure (which is referred to as "correcting for wave functions renormalization") which must in general be applied (on their both "ends") to perturbatively calculated amplitudes (Green's functions) in relativistic field theories to extract proper transition amplitudes (S-matrix elements) because in general what one is interested in are transition probabilities between appropriately defined *in* and *out* eigenstates of the

full (time independent) Hamiltonian $H = H_0 + V_{\rm int}$ which differ from and correspond to different energies than eigenstates of the free Hamiltonian H_0 in terms of which the standard expansion is formulated.

If the change of the Hamiltonian occurs almost instantaneously at the instant $t_{\rm int}$, that is, if the derivative of $V_{\rm int}(t)$ in the matrix elements in (2.27) can be approximated by the derivative of $\langle k|V_{\rm int}^{(+)}\,\theta(t-t_{\rm int})|m\rangle$, one obtains[10] $P(m\to\tilde m)\approx 1$ and

$$P(m\to\tilde k)\approx\frac{\Big|\langle k|V_{\rm int}^{(+)}|m\rangle\Big|^2}{\hbar^2\omega_{km}^2}\,,\qquad \tilde k\neq m. \tag{2.28}$$

How this is related to the intuitive picture of the state-vector which "does not succeed" to change quickly enough? In this picture the same transition probability is simply given by

$$P(m\to\tilde k)=\Big|\langle\tilde k|m\rangle\Big|^2\,, \tag{2.29}$$

where $|m\rangle$ is the eigenvector of H_0 and $|\tilde k\rangle$ the eigenvectors of $H_0+V_{\rm int}^{(+)}$. Using in (2.29) the standard first order expression for $|\tilde k\rangle$

$$|\tilde k\rangle=|k\rangle+\sum_{n\neq k}|n\rangle\frac{\langle n|V_{\rm int}^{(+)}|k\rangle}{E_k-E_n}+\ldots,$$

given by Rayleigh - Schrödinger perturbative expansion reduces it to (2.28), if $k\neq m$, and gives $P(m\to\tilde m)=1$. From the general result (2.22) it should be, however, clear that if the time interval T, during which the change of the Hamiltonian effectively occurs, tends to zero, the prescription (2.29) goes beyond the perturbative method (the formula (2.29) becomes exact in the strict limit $T=0$).

As a first example of the application of the formula (2.29) we consider the one-dimensional harmonic oscillator of mass M and frequency ω whose center of equilibrium suddenly shifts (the change occurs during $\Delta t\ll 1/\omega$). The Hamiltonian perturbation is therefore $V_{\rm int}(t)=-xF(t)$ with $F(t)$ close in shape to $F_0\theta(t-t_{\rm int})$, that is $V_{\rm int}^{(+)}=-xF_0$. We will compute the probability of the transition from the ground state to the state $|\tilde n\rangle$ of the shifted oscillator.

Recall that the ground state wave function of the unshifted oscillator ($V_{\rm int}=0$) has the form

$$\psi_0(x)=(\alpha/\sqrt{\pi}\,)^{1/2}\,e^{-\frac{1}{2}\alpha^2x^2},$$

[10]Since $\langle m|V_{\rm int}^{(+)}|m\rangle$ is real, the first order correction to $P(m\to\tilde m)$ vanishes. Recall that in the approximation adopted here terms of order $\mathcal{O}((V_{\rm int}^{(+)})^2)$ in $P(m\to\tilde m)$ cannot be computed consistently.

in which $\alpha^2 = M\omega/\hbar$. The Hamiltonian of the shifted oscillator is

$$H_0 + V_{\rm int}^{(+)} = \frac{\hat{p}^2}{2M} + \frac{1}{2}M\omega^2(x - x_0)^2 + \text{const}\,,$$

where $x_0 = F_0/M\omega^2$. Therefore, the eigenfunctions $\tilde{\psi}_n(x)$ of the shifted oscillator read

$$\tilde{\psi}_n(x) = N_n\, H_n(\alpha(x - x_0))\, e^{-\frac{1}{2}\alpha^2(x-x_0)^2},$$

where $|N_n|^2 = \alpha/2^n n!\sqrt{\pi}$ and $H_n(z)$ are the Hermite polynomials ($H_0(z) = 1$, etc.). The transition probabilities are therefore given by

$$\begin{aligned} P(0 \to \tilde{n}) = |\langle\tilde{n}|0\rangle|^2 &= \left|\int_{-\infty}^{+\infty} dx\, \tilde{\psi}_n^*(x)\psi_0(x)\right|^2 \\ &= \frac{\alpha^2}{2^n n!\,\pi}\left|\int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}\alpha^2(x-x_0)^2} H_n(\alpha(x - x_0))\, e^{-\frac{1}{2}\alpha^2 x^2}\right|^2 \\ &= \frac{1}{2^n n!\,\pi}\, e^{-\xi_0^2}\left|\int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} e^{-\xi\xi_0} H_n(\xi)\right|^2, \end{aligned}$$

where $\xi = \alpha(x - x_0)$ and $\xi_0 = \alpha x_0$. Recalling now that $H_n(\xi) = (-1)^n\, e^{\xi^2}\frac{d^n}{d\xi^n}\, e^{-\xi^2}$ we can write

$$P(0 \to \tilde{n}) = \frac{1}{2^n n!\,\pi}\, e^{-\xi_0^2}\left|\int_{-\infty}^{+\infty} d\xi\, (-1)^n\, e^{-\xi\xi_0}\frac{d^n}{d\xi^n}\, e^{-\xi^2}\right|^2.$$

Integrating n times by parts (the boundary terms give always zero) we arrive at

$$\begin{aligned} P(0 \to \tilde{n}) &= \frac{1}{2^n n!\,\pi}\, e^{-\xi_0^2}\left|\int_{-\infty}^{+\infty} d\xi\, (-\xi_0)^n\, e^{-\xi\xi_0}\, e^{-\xi^2}\right|^2 \\ &= \frac{1}{2^n n!\,\pi}\,\xi_0^{2n}\, e^{-\xi_0^2/2}\left|\int_{-\infty}^{+\infty} d\xi\, e^{-(\xi+\xi_0/2)^2}\right|^2 = \frac{1}{2^n n!}\,\xi_0^{2n}\, e^{-\xi_0^2/2}\,. \end{aligned}$$

One recognizes easily in this expression the Poisson distribution with the mean excitement $\bar{n} = \sum_n nP(0 \to n)$ of the oscillator given by

$$\bar{n} = e^{-\xi_0^2/2}\sum_{n=0}^{\infty}\frac{n}{n!}\left(\frac{\xi_0^2}{2}\right)^n = e^{-\xi_0^2/2}\,\frac{\xi_0^2}{2}\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(\frac{\xi_0^2}{2}\right)^{n-1} = \frac{\xi_0^2}{2}\,,$$

that is, $\bar{n} = \xi_0^2/2 \equiv F_0^2/2M\hbar\omega^3$. Therefore

$$P(0 \to \tilde{n}) = \frac{(\bar{n})^n}{n!}\, e^{-\bar{n}}\,. \tag{2.30}$$

As the problem of the harmonic oscillator perturbed by an arbitrary external force $F(t)$ has been explicitly solved in Section 1.3, it is interesting to see, how the exact solution

reduces to (2.29) and (2.30) when $F(t) \to \theta(t)F_0$. Since at $t \gg 0$ the time evolution of the oscillator is governed by $H_0 + V_{\rm int}^{(+)}$ rather than by H_0, the transition amplitude $\mathcal{A}_{\tilde{k},m}(t,t_0)$ which will have well defined limits $t \to \infty$ and $t_0 \to -\infty$ should be defined (compare the expression (2.9)) as

$$\mathcal{A}_{\tilde{k},m}(t,t_0) = \langle \tilde{k}|e^{i(H_0+V_{\rm int}^{(+)})t/\hbar}|\Psi(t)\rangle = \langle \tilde{k}|e^{i(H_0+V_{\rm int}^{(+)})t/\hbar}e^{-iH_0t/\hbar}|\Psi(t)\rangle_I \,. \tag{2.31}$$

Thus, in the case at hands

$$\mathcal{A}_{\tilde{k},m}(t,t_0) = \langle \tilde{k}|e^{i(H_0+V_{\rm int}^{(+)})t/\hbar}e^{-iH_0t/\hbar}U_I(t,t_0)|m\rangle \,.$$

From the results of Section 1.3 it follows that[11]

$$H_0 + V_{\rm int}^{(+)} \equiv \Delta_\omega + \hbar\omega a^\dagger a + f_0\, a^\dagger + f_0^* a = S^\dagger(H_0 - \Delta_+)S \,, \tag{2.32}$$

where $f_0 = -\hbar F_0/\sqrt{2M\hbar\omega}$, $\Delta_+ = |f_0|^2/\hbar\omega$, $S = \exp(ba^\dagger - b^*a)$ and $b = f_0/\hbar\omega$. This also means that

$$e^{i(H_0+V_{\rm int}^{(+)})t/\hbar} = S^\dagger e^{i(H_0-\Delta_+)t/\hbar}S = e^{-i\Delta_+ t/\hbar}\, S^\dagger e^{iH_0t/\hbar}S \,.$$

Therefore, using the fact that $|\tilde{n}\rangle = S^\dagger|n\rangle$, which implies that $\langle\tilde{n}|S^\dagger = \langle n|$, one can write

$$\begin{aligned}\mathcal{A}_{\tilde{k},m}(t,t_0) &= e^{-i\Delta_+ t/\hbar}\langle k|e^{iH_0t/\hbar}Se^{-iH_0t/\hbar}U_I(t,t_0)|m\rangle \\ &= e^{-i\Delta_+ t/\hbar}\langle k|e^{b\,e^{i\omega t}a^\dagger - b^*e^{-i\omega t}a}U_I(t,t_0)|m\rangle \,.\end{aligned}$$

The operator $U_I(t,t_0)$ is given by (1.71). In the case of the force $F(t)$ considered here, the function $c(t,t_0)$ entering this operator, and defined in (1.53), does not have the limit $t \to \infty$ (the limit $t_0 \to -\infty$ still exists, owing to vanishing of $F(t)$ in the far past) but after integration by parts can be represented in the form

$$c(t,-\infty) = \frac{1}{\sqrt{2M\hbar\omega^3}}\left[F_0\, e^{i\omega t} - \int_{-\infty}^{t} d\tau\, e^{i\omega\tau}\,\frac{d}{d\tau}\,F(\tau)\right] \equiv -b\, e^{i\omega t} + \tilde{c}(t) \,, \tag{2.33}$$

where the function $\tilde{c}(t)$ already has the $t \to \infty$ limit $\tilde{c}_\infty$. With the help of the Baker-Hausdorff formula (1.49) the evolution operator $U_I(t,-\infty)$ can be brought into the form

$$U_I(t,-\infty) = e^{-b\,e^{i\omega t}a^\dagger + b^*e^{-i\omega t}a}e^{\tilde{c}(t)a^\dagger - \tilde{c}^*(t)a}e^{-i\tilde{\gamma}_t} \,, \tag{2.34}$$

with some irrelevant, time dependent phase factor $\tilde{\gamma}_t$. Therefore the exact transition amplitude takes the final form[12]

$$\mathcal{A}_{\tilde{k},m}(\infty,-\infty) = e^{-i\tilde{\gamma}_t - i\Delta_+ t/\hbar}\langle k|e^{\tilde{c}_\infty a^\dagger - \tilde{c}_\infty^* a}|m\rangle \,. \tag{2.35}$$

[11] The operator S introduced here should not be confused with the S operator discussed in Section 1.3.

[12] Although we have not computed the phase factors, the definition (2.31) of the amplitude should secure the existence of the $t \to \infty$ limit of the overall phase.

Since for $F(t) = \theta(t)F_0$ the factor $\tilde{c}_\infty$ goes over into $-b$, the operator between $\langle k|$ and $|m\rangle$ reduces to S, and on account of the relation $\langle k|S = \langle \tilde{k}|$ one recovers the formula (2.29). It is also easy to see that if $F(t)$ changes from 0 to F_0 smoothly, the transition probability

$$P(0 \to \tilde{n}) = e^{-|\tilde{c}_\infty|^2} \left| \langle n| e^{\tilde{c}_\infty a^\dagger} |0\rangle \right|^2 ,$$

has still the form (2.30) with $\bar{n} = |\tilde{c}_\infty|^2$ (which reduces to $F_0^2/2M\hbar\omega^3$ in the limit of the instantaneous change).

As the second example (which in Section 2.5 will also serve us to illustrate another important point) we consider the tritium β decay $^3\mathrm{H} \to ^3\mathrm{He} + e^- + \bar{\nu}_e$ and will calculate (neglecting complications related to spin and the antisimmetrization of all electron states) the probability that as a result of the decay the electron (not the one displayed here!) which is initially in the Hydrogen atom ground state $|(Z = 1)\, n = 0, l = 0, m = 0\rangle$ will make a transition to the Helium atom excited state $|(Z = 2)\, n', l', m'\rangle$.

The energy spectrum of the electrons emitted in a β decay is continuous.[13] In this particular reaction the maximal (kinetic) energy of the electron emitted from the nucleus is about 18 keV. Our first task is to check whether the approximation of the instant change of the Hamiltonian ($Z = 1 \to Z = 2$ in $H_0 = \hat{p}^2/2M_e - Ze^2/r$) can be justified. The characteristic atomic time is $\hbar/E$ where E is the typical difference of energies of the atomic levels. Taking 13.6 eV as a representative number we get[14]

$$\frac{\hbar}{E} = \frac{\hbar c}{E\, c} = \frac{197 \times 10^{-15}\ \mathrm{MeV \cdot m}}{13.6\ \mathrm{eV} \cdot 3 \times 10^8\ \mathrm{m/sec}} \approx 0.5 \times 10^{-16}\ \mathrm{sec}\,.$$

The time period Δt during which the change of the electrostatic field of the nucleus occurs ($Z = 1 \to Z = 2$), can be estimated as the time in which the electron emitted from the nucleus leaves the atom the spatial size of which is given by the Bohr radius $a_\mathrm{B} \approx 0.5 \times 10^{-10}$ m. The time $\Delta t \sim a_\mathrm{B}/v$ where v is the velocity of the electron produced in the β decay, that is, the velocity corresponding to electron kinetic energy $E_\mathrm{kin} \sim 18\,\mathrm{keV}$. Since $E_\mathrm{kin} = M_e v^2/2$, we get $v^2/c^2 = 2E_\mathrm{kin}/M_e c^2 \approx 0.07$. Thus,

$$\Delta t \sim \frac{\hbar}{M_e c^2 \alpha_\mathrm{EM}} \frac{1}{\sqrt{0.07}} \approx \frac{6.582 \times 10^{-22}\ \mathrm{MeV \cdot sec}}{0.511\ \mathrm{MeV}}\ \frac{137}{0.26} \approx 6.7 \times 10^{-19}\ \mathrm{sec}\,,$$

and we see that the change of the Hamiltonian is indeed fast compared to the characteristic atomic time,[15] and the use of the impulse approximation is justified. Therefore one can approximate

$$P(1S \to nlm_l(Z = 2)) = |\langle nlm_l(Z = 2)|1S(Z = 1)\rangle|^2 .$$

[13] The existence of the neutrino was postulated by W. Pauli in 1931 to explain this fact without resorting to nonconservation of the energy (which was desperately hypothesized by N. Bohr).

[14] Recall that $\hbar c \approx 197\ \mathrm{MeV} \times 10^{-15}\mathrm{m}$, $M_e c^2 \approx 0.511$ MeV and in the Gauss system of units used here the fine structure constant $\alpha_\mathrm{EM} = e^2/\hbar c \approx 1/137$ and $a_\mathrm{B} \equiv \hbar^2/M_e e^2 = \hbar c/M_e c^2 \alpha_\mathrm{EM}$.

[15] At least in the prevailing fraction of such decays, when the emitted electron energy is not too close to the lower end of the energy spectrum.

For example, for $m = 1S$ or $2S$, using the explicit form of the wave functions:

$$\psi_{1S} = 2\left(\frac{Z}{a_{\rm B}}\right)^{3/2} \exp\!\left(-Z\frac{r}{a_{\rm B}}\right) Y_{00} = \sqrt{\frac{Z^3}{\pi a_{\rm B}^3}}\, \exp\left(-Z\frac{r}{a_{\rm B}}\right),$$

$$\psi_{2S} = \frac{1}{2\sqrt{2}}\left(\frac{Z}{a_{\rm B}}\right)^{3/2} \left(2 - Z\frac{r}{a_{\rm B}}\right) \exp\left(-Z\frac{r}{2a_{\rm B}}\right) Y_{00}\,,$$

we find

$$\begin{aligned} P(1S \to 1S) &= \left| \int d^3\mathbf{r}\, \psi^*_{1S}(Z=2)\, \psi^*_{1S}(Z=1) \right|^2 \\ &= \left| \frac{2^{7/2}}{a_{\rm B}^3} \int_0^\infty dr\, r^2\, e^{-3r/a_{\rm B}} \right|^2 = \left| \frac{2^{7/2}}{a_{\rm B}^3} \frac{\partial^2}{\partial\alpha^2} \int_0^\infty dr\, e^{-\alpha r} \right|^2_{\alpha=3/a_{\rm B}} \\ &= \left| \frac{2^{7/2}}{a_{\rm B}^3} \frac{\partial^2}{\partial\alpha^2} \frac{1}{\alpha} \right|^2_{\alpha=3/a_{\rm B}} = \left| \frac{2^{7/2}}{a_{\rm B}^3} \frac{2}{(3/a_{\rm B})^3} \right|^2 = \left(\frac{8}{9}\right)^3 = 0.702\,. \end{aligned}$$

Similarly, one finds that $P(1S \to 2S) \approx 0.25$. Transitions to the states other than the S-states have in this approximation vanishing probabilities (due to the orthogonality of the spherical harmonics).

2.4 Slow change of the Hamiltonian

Here we would like to give a proof of the adiabatic theorem which says that if the time-dependent Hamiltonian $H(t)$ of a system undergoes a finite change in a very long time period $T = t_2 - t_1$, the system which at the instant t_1 was in an instaneous eigenstate of the Hamiltonian $H(t_1)$ will, after the change is completed, with probability aproaching unity in the limit $T \to \infty$, be found in the instantaneous eigenstate of the Hamiltonian $H(t_2)$ connected by continuity with the initial state. We will use the already introduced notation $t = T\xi + t_1$ and assume that the spectrum of the Hamiltonian $H(t) = H(\xi)$ consists of discrete energy levels $E_n(\xi)$ which do not intersect, so the changes of the spectrum can be unambigously followed. To each of these levels corresponds the projection operator $P_n(\xi)$ ($P_n(\xi)P_n(\xi) = P_n(\xi)$, $P_n(\xi)P_{n'}(\xi) = \hat{0}$ if $n \neq n'$, $\sum_n P_n(\xi) = \hat{1}$) onto the subspace spanned by the instantaneous eigenvectors of $H(\xi)$ corresponding to the eigenvalue $E_n(\xi)$. The instantaneous Hamiltonian can be therefore written in the form (spectral decomposition)

$$H(\xi) = \sum_n P_n(\xi)\, E_n(\xi)\,. \tag{2.36}$$

The (Schrödinger picture) evolution operator $U(t, t_1)$ of the system corresponding to the time interval (t_1, t_2) will be written as $U(T, \xi)$. The operator form of the adiabatic theorem is

$$\lim_{T\to\infty} U(T,\xi)\, P_n(0) = P_n(\xi) \lim_{T\to\infty} U(T,\xi)\,. \tag{2.37}$$

It says that if the system starts at $t = t_1$ (i.e. $\xi = 0$) in a state belonging to the n-th energy level, it will remain, in the adiabatic limit in a state belonging to the same (evolved) energy level. The relation (2.37) remains obviously true in the special (somewhat artificial) case in which despite the changes of the Hamiltonian eigenvalues $E_n(\xi)$, the projectors $P_n(\xi)$ do not depend on time: $P_n(\xi) = P_n(0)$. The Hamiltonian splits then into a sum of ξ dependent operators $H_n(\xi) \equiv P_n(0)\, E_n(\xi)$ and the evolution operator takes the form (T_ξ denotes the ξ-time ordering operation)

$$\begin{aligned} U(T,\xi) &= \mathrm{T}_\xi \exp\left(-\frac{i}{\hbar}\, T \int_0^\xi d\xi'\, H(\xi') \right) \\ &= \sum_n P_n(0) \exp\left(-\frac{i}{\hbar}\, T \int_0^\xi d\xi'\, E_n(\xi') \right), \end{aligned} \tag{2.38}$$

because $[H(\xi),\, H(\xi')] = 0$. The proof of the adiabatic theorem relies on reducing the general situation to this particular case.

As the first step one introduces the unitary operator $A(\xi)$ which maps the $H(0)$ eigenvectors $|n(0)\rangle$ into the corresponding eigenvectors $|n(\xi)\rangle$ of $H(\xi)$:

$$A(\xi)|n(0)\rangle = |n(\xi)\rangle\,. \tag{2.39}$$

Since $P_n(\xi)$ is the sum of the operators $|n(\xi)\rangle\langle n(\xi)|$ with $n(\xi)$ corresponding to $E_n(\xi)$, it follows that

$$P_n(\xi) = A(\xi)\, P_n(0)\, A^\dagger(\xi)\,. \tag{2.40}$$

The operator $A(\xi)$ will be constructed by integrating the differential equation

$$i\hbar\, \frac{d}{d\xi}\, A(\xi) = K(\xi)\, A(\xi)\,, \tag{2.41}$$

with the initial condition $A(0) = \hat{1}$. Provided $K(\xi)$ is Hermitian, this way of constructing $A(\xi)$ yields a unitary operator. As can be checked differentiating the projectors $P_n(\xi)$ with respect to ξ, the operator $A(\xi)$ constructed in this way will have the properties (2.39) if

$$[K(\xi),\, P_n(\xi)] = i\hbar\, \frac{d}{d\xi}\, P_n(\xi)\,. \tag{2.42}$$

This does not fix the operator $K(\xi)$ uniquely - a sum $\sum_n P_n(\xi)\, O_n(\xi)\, P_n(\xi)$ with arbitrary operators $O_n(\xi)$ can always be added to it. (Such a sum always commutes with $P_n(\xi)$ because $P_n(\xi)P_m(\xi)$ equals either $P_n(\xi)$ or zero.) The ambiguity is fixed by imposing on $K(\xi)$ a set of subsidiary conditions

$$P_n(\xi)\, K(\xi)\, P_n(\xi) = 0\,, \qquad \text{all } n\,, \tag{2.43}$$

which will play an important role in the proof. The operator $K(\xi)$ satisfying the relations (2.42) and (2.43) has the form

$$K(\xi) = i\hbar \sum_m \frac{dP_m(\xi)}{d\xi}\, P_m(\xi) = -i\hbar \sum_m P_m(\xi)\, \frac{dP_m(\xi)}{d\xi}\,. \tag{2.44}$$

The equivalence of the two forms (which is crucial in checking the property (2.42) and the Hermiticity of $K(\xi)$) follows readily by differentiating with respect to ξ the second equality in the identities

$$\sum_n P_n(\xi) = \sum_n P_n(\xi)\, P_n(\xi) = \hat{1}\,.$$

Differentiating instead the relation $P_nP_n = P_n$ gives the identity which can be written as $P_n\dot{P}_n = \dot{P}_n(1 - P_n)$ and upon multiplication from the right by P_n yields the identity $P_n\dot{P}_nP_n = \hat{0}$ which is necessary to check that (2.44) satisfies also the subsidiary conditions (2.43).

With the help of the unitary operator $A(\xi)$ one can define the "A-picture" - the analog of the interaction picture introduced in Section 1.1 - in which the system's states are represented by vectors obtained from the corresponding Schrödinger picture vectors with help of the transformation

$$|\Psi(\xi)\rangle_A \equiv A^\dagger(\xi)|\Psi(\xi)\rangle_S\,. \tag{2.45}$$

The A-picture evolution operator $U_A(T,\xi)$ is related to the Schrödinger picture one by (cf. the formula (1.24))

$$U_A(T,\xi) = A^\dagger(\xi)\, U(T,\xi)\, A(0) = A^\dagger(\xi)\, U(T,\xi)\,,$$

and satisfies, therefore, together with the condition $U_A(T,0) = \hat{1}$, the equation

$$i\hbar\, \frac{d}{d\xi}\, U_A(T,\xi) = \big(T\, H^A(\xi) - K^A(\xi)\big)\, U_A(T,\xi)\,, \tag{2.46}$$

in which $K^A(\xi) = A^\dagger(\xi)\, K(\xi)\, A(\xi)$ and

$$H^A(\xi) = A^\dagger(\xi)\, H(\xi)\, A(\xi) = \sum_n P_n(0)\, E_n(\xi)\,. \tag{2.47}$$

If the term with the operator $K^A(\xi)$ on the right hand side of this equation is neglected in comparison with the one explicitly proportional to T, the resulting approximate evolution operator $\tilde{U}_A(T,\xi)$ (satisfying the initial condition $\tilde{U}_A(T,0) = \hat{1}$) is precisely, owing to the above form of $H^A(\xi)$, given by the right hand side of (2.38) and the corresponding approximate Schrödinger picture evolution operator $A(\xi)\,\tilde{U}_A(T,\xi)$ satisfies (owing to the relation (2.39)) the relation (2.37).

To show that in the limit $T \to \infty$ the evolution operator $U_A(T,\xi)$ can be approximated by $\tilde{U}_A(T,\xi)$ one can write $U_A(T,\xi) = \tilde{U}_A(T,\xi)\, W(\xi)$ and study the operator $W(\xi)$ which satisfies the equation

$$i\hbar \frac{d}{d\xi} W(\xi) = -\tilde{U}_A^\dagger(T,\xi)\, K_A(\xi)\, \tilde{U}_A(T,\xi)\, W(\xi) \equiv -\overline{K}(\xi)\, W(\xi)\,, \tag{2.48}$$

with the initial condition $W(0) = \hat{1}$, which can be converted into the integral equation

$$W(\xi) = \hat{1} + \frac{i}{\hbar}\int_0^\xi d\xi'\, \overline{K}(\xi')\, W(\xi')\,. \tag{2.49}$$

The point now is that the kernel $\overline{K}(\xi)$ is a sum of terms oscillating with frequencies which become infinite in the $T \to \infty$ limit. To see this one writes it in the form

$$\overline{K}(\xi) = \sum_{n,n'} P_n(0)\, \overline{K}(\xi)\, P_{n'}(0) \equiv \sum_{n,n'} \overline{K}_{n,n'}(\xi)\,, \tag{2.50}$$

in which, owing to the special form (2.38) of $\tilde{U}_A(T,\xi)$ and the relation (2.39)),

$$\overline{K}_{n,n'}(\xi) = A^\dagger(\xi)\, P_n(\xi)\, K(\xi)\, P_{n'}(\xi)\, A(\xi) \exp\left(iT \int_0^\xi d\xi'\, \omega_{nn'}(\xi') \right), \tag{2.51}$$

where $\omega_{nn'}(\xi') \equiv (E_n(\xi) - E_{n'}(\xi))/\hbar$. All off-diagonal terms (i.e. ones with $n \neq n'$ $\overline{K}_{n,n'}(\xi)$ involve phase factors oscillating with increasing, as $T \to \infty$, effective frequencies while owing to the subsidiary condition (2.43) $\overline{K}_{n,n}(\xi) = 0$. To see that these rapid oscillations kill the integral term in (2.49) one can, upon integrating by parts, cast it in the form,

$$W(\xi) = \hat{1} + \frac{i}{\hbar}\, F(\xi)\, W(\xi) - \frac{i}{\hbar}\int_0^\xi d\xi'\, F(\xi')\, \frac{d}{d\xi'}\, W(\xi')\,. \tag{2.52}$$

Of interest is the large T behaviour of the operators

$$F_{nn'}(\xi) \equiv \int_0^\xi d\xi'\, \overline{K}_{n,n'}(\xi')\,,$$

with $n \neq n'$ (as $F_{nn}(\xi) = 0$). As the operators $A^\dagger(\xi)\, P_n(\xi)\, K(\xi)\, P_{n'}(\xi)\, A(\xi)$ in (2.51) do not depend on T and are continuous functions of ξ, the operators $F_{nn'}(\xi)$ vanish in the limit $T \to \infty$, essentially like $1/T$. Since this means that $W(\xi) = \hat{1} + \mathcal{O}(1/T)$,

$$U(T,\xi) = A(\xi)\, \tilde{U}_A(T,\xi)\, [1 + \mathcal{O}(1/T)]\,,$$

which is what was to be shown.

An important aspect of the adiabatic theorem applied to slow *cyclic* changes of the Hamiltonian is the appearance of the "geometric" phase, called also Berry's phase, which

complements the usual "dynamical" phase. Suppose the Hamiltonian of the system depends on time through a set of parameters $\lambda^i(t)$, $i = 1, \ldots, r$, collectively denoted $\boldsymbol{\lambda}(t)$

$$\hat{H}(t) = \hat{H}(\boldsymbol{\lambda}(t))\,,$$

and that $|l(\boldsymbol{\lambda})\rangle$ are the eigenvectors of $\hat{H}(\boldsymbol{\lambda})$ with the eigenvalues $E_l(\boldsymbol{\lambda})$ (when $\boldsymbol{\lambda}$ depends on time they are the instantaneous eigenvectors and eigenvalues of $\hat{H}(\boldsymbol{\lambda}(t))$). Seeking the solution of the Schrödinger equation with $\hat{H}(\boldsymbol{\lambda}(t))$ in the form

$$|\psi(t)\rangle = \sum_l |l(\boldsymbol{\lambda}(t)\rangle\, a_l(t)\, \exp\!\left\{-\frac{i}{\hbar}\int_0^t dt' E_l(\boldsymbol{\lambda}(t'))\right\}, \tag{2.53}$$

with the initial condition $|\psi(0)\rangle = |n(\boldsymbol{\lambda}(0)\rangle$, i.e. $a_l(0) = \delta_{ln}$, one finds that the coefficients $a_l(t)$ satisfy the system of differential equations ($\omega_{ll'} = (E_l - E_{l'})/\hbar$)

$$\dot{a}_l(t) = -\sum_{l'} \langle l(\boldsymbol{\lambda}(t))|\, \frac{d}{dt}\, |l'(\boldsymbol{\lambda}(t))\rangle\, a_{l'}(t) \exp\!\left\{i\int_0^t dt'\, \omega_{ll'}(\boldsymbol{\lambda}(t'))\right\}. \tag{2.54}$$

The scalar product $\langle l(\boldsymbol{\lambda}(t)|\, d|l'(\boldsymbol{\lambda}(t)\rangle/dt$ can be worked out by differentiating with respect to time the relation $\hat{H}(t)|l'(t)\rangle = E_{l'}(t)|l'(t)\rangle$ and closing the resulting equality from the left with $\langle l(t)|$ with $l \neq l'$. This gives

$$\langle l(\boldsymbol{\lambda})|\, \frac{d}{dt}\, |l'(\boldsymbol{\lambda})\rangle = -\frac{1}{E_l(\boldsymbol{\lambda}) - E_{l'}(\boldsymbol{\lambda})}\, \langle l(\boldsymbol{\lambda})|\, \frac{d\hat{H}}{dt}\, |l'(\boldsymbol{\lambda})\rangle\,, \qquad l \neq l'\,.$$

For $l = l'$ instead one differentiates the equality $\langle l(\boldsymbol{\lambda})|l(\boldsymbol{\lambda})\rangle = 1$ which leads to the relation (written in the more appropriate notation)

$$(\dot{l}|l) + (l|\dot{l}) = (l|\dot{l})^* + (l|\dot{l}) = 0\,,$$

from which it follows that

$$(l|\dot{l}) \equiv \langle l(\boldsymbol{\lambda}(t)|\, \frac{d}{dt}\, |l(\boldsymbol{\lambda}(t)\rangle = i\gamma_l(t)\,, \tag{2.55}$$

where $\gamma_l(t)$ is real. The (exact) set of differential equations for the cefficients $a_l(t)$ takes therefore the form

$$\begin{aligned}\dot{a}_l(t) = &\sum_{l' \neq l} \frac{\langle l(\boldsymbol{\lambda})|\, d\hat{H}/dt\, |l'(\boldsymbol{\lambda})\rangle}{E_l(\boldsymbol{\lambda}) - E_{l'}(\boldsymbol{\lambda})}\, a_{l'}(t) \exp\!\left\{i\int_0^t dt'\, \omega_{ll'}(\boldsymbol{\lambda}(t'))\right\} \\ &-i\,\gamma_l(t)\, a_l(t)\,.\end{aligned} \tag{2.56}$$

According to the adiabatic theorem, when a fixed change of the Hamiltonian occurs very slowly, i.e. it takes a very long time, and the system at the instant $t = 0$ starts in the (instantaneous) eigenvector $|n(\boldsymbol{\lambda}(0))\rangle$ of $\hat{H}(\boldsymbol{\lambda}(0))$, the coefficients $a_l(t)$ with $l \neq n$ remain very small and can be in the first approximation set equal zero. The evolution of the only

significantly different from zero coefficient $a_n(t)$ is in this limit determined by the simple equation $\dot{a}_n(t) = -i\gamma_n(t)\, a_n(t)$ the solution of which is

$$a_n(t) = \exp\left(-i\int_0^t dt'\,\gamma_n(t')\right) \equiv \exp(-i\Gamma_n(t))\,,$$

that is, a_n remains a pure phase factor, $|a_n(t)| = 1$, and the evolution of the system's state vector is

$$|\psi(t)\rangle \approx |n(\boldsymbol{\lambda}(t))\rangle \exp\left\{-i\Gamma_n(t) - \frac{i}{\hbar}\int_0^t dt' E_n(\boldsymbol{\lambda}(t'))\right\}, \tag{2.57}$$

The system remains in the instantaneous eigenstate of $\hat{H}(\boldsymbol{\lambda})$ but the corresponding state-vector acquires a phase which consists of two parts: the dynamical one, depending on the integral of the instantaneous eigenvalues $E_n(\boldsymbol{\lambda})$ of the changing Hamiltonian - this generalizes the well-known phase factor $\exp(-iE_nt/\hbar)$ acquired by a vector representing the system which at $t = 0$ was in the eigenstate $|n\rangle$ of a time-independent Hamiltonian - and the phase $\Gamma_n(t)$.

At first sight it may seem that the phase $\Gamma_n(t)$ is unphysical and can be eliminated. Indeed, in choosing the eigenvectors of the Hamiltonian $\hat{H}(\boldsymbol{\lambda})$ it is always possible to change their phases and take instead of the eigenvectors $|n(\boldsymbol{\lambda})\rangle$ (to which correspond the factors γ_n defined by the relation (2.55)), the eigenvectors $|n(\boldsymbol{\lambda})\rangle'$ which differ from $|n(\boldsymbol{\lambda})\rangle$ by phases:

$$|n(\boldsymbol{\lambda})\rangle' = |n(\boldsymbol{\lambda})\rangle \exp(i\chi_n(\boldsymbol{\lambda}))\,.$$

The corresponding phase γ_n' is then

$$i\gamma_n'(t) = {}'\langle n(\boldsymbol{\lambda}(t)|\,\frac{d}{dt}\,|n(\boldsymbol{\lambda}(t)\rangle' = i\gamma_n(t) + i\,\frac{d}{dt}\,\chi_n\,, \tag{2.58}$$

so taking

$$\chi_n(t) = -\int_0^t dt'\,\gamma_n(t')\,,$$

indeed seems to lead to $\Gamma_n'(t) \equiv 0$.

To show that elimination of the phase Γ_n is in fact not possible globally, when after a long (for adiabaticity) time T the parameters λ^i return to their initial values, $\lambda^i(T) = \lambda^i(0)$, it is convenient to write the factor $\gamma_n(t)$ in the form

$$\gamma_n(t) = \mathscr{A}_i^{(n)}\,\dot{\lambda}^i\,, \qquad \mathscr{A}_i^{(n)} = -i\,\langle n(\boldsymbol{\lambda})|\,\frac{\partial}{\partial\lambda^i}\,|n(\boldsymbol{\lambda})\rangle\,, \tag{2.59}$$

introducing thereby the "gauge fields" $\mathscr{A}_i^{(n)}$, which can be treated as the analogs of the vector potential known from classical electrodynamics. The phase Γ_n in (2.57) acquired

by the state vector representing the system (remaining in the instantaneous eigenstate of the changing Hamiltonian) after the parameters λ^i have returned to their initial values after (a long) time T can be then written in the form

$$\Gamma_n(T) = \int_0^T dt\, \gamma_n(t) = \int_0^T dt\, \mathscr{A}_i^{(n)}\, \dot{\lambda}^i(t) = \oint_C \mathscr{A}_i^{(n)}\, d\lambda^i\,.$$

It is therefore given by the integral of the one-form $\omega_{\mathscr{A}} = \mathscr{A}_i^{(n)}\, d\lambda^i$ over the closed path C traced in the abstract parameter space by the vector $\boldsymbol{\lambda}$. One can now use the Stokes theorem to write $\Gamma_n(T)$ as

$$\Gamma_n(T) = \oint_{C=\partial\Sigma} \mathscr{A}_i^{(n)}\, d\lambda^i = \int_\Sigma d\omega_{\mathscr{A}} = \int_\Sigma \frac{\partial \mathscr{A}_i^{(n)}}{\partial \lambda^j}\, d\lambda^j \wedge d\lambda^i\,,$$

that is as the integral of the two-form $d\omega_{\mathscr{A}}$ over a dwo-dimensional surface Σ (in the abstract parameter space) the boundary of which is the closed curve C. (If the parameter space is three-dimensional, one can directly use the analogy with the A-Ampsio rule of electrodynamics which states that the line integral of the vector potential $\mathbf{A}$ over a closed contour is equal to the flux of the magnetic induction $\mathbf{B}$ through a surface spanned on this contour.) Since the transformation $\gamma_n \longrightarrow \gamma_n'$ (2.58) is equivalent to a "gauge transformation"

$$\mathscr{A}_i^{(n)} \longrightarrow \mathscr{A}_i^{(n)\prime} = \mathscr{A}_i^{(n)} + \partial\chi_n/\partial\lambda^i\,,$$

it does not affect the two-form $d\omega_{\mathscr{A}}$ and, hence, cannot eliminate (nor change its value) the phase factor $\Gamma_n(T)$ similarly as in electrodynamics a gauge transformation of the vector potential cannot change the inducton $\mathbf{B}$ of the magnetic field (and therefore its flux).

To understand the origin of the name "geometric phase" one can consider the matrix Hamiltonian

$$\hat{H} = -\,\text{const.}\,\boldsymbol{\lambda}\cdot\boldsymbol{\sigma}\,,$$

($\boldsymbol{\sigma} = (\sigma^1, \sigma^2, \sigma^3)$ are the three Pauli matrices) which may be treated as the Hamiltonian of the magnetic moment of a spin $\frac{1}{2}$ particle in an external magnetic field directed along the vector $\boldsymbol{\lambda}$ (which changes with time). Introducing another parametrization by writing $\lambda^1 = r\sin\theta\cos\varphi$, $\lambda^2 = r\sin\theta\sin\varphi$, $\lambda^3 = r\cos\theta$ the eigenvector corresponding e.g. to the lower energy level can be written in the form

$$\begin{pmatrix} e^{-i\varphi/2}\cos(\theta/2) \\ e^{i\varphi/2}\sin(\theta/2) \end{pmatrix}.$$

Treating (r, θ, φ) as a new set of parameters one readily obtains from (2.59) $\mathscr{A}_r = \mathscr{A}_\theta = 0$, $\mathscr{A}_\varphi = -\frac{1}{2}\cos\theta$. Assuming that the Hamiltonian returned to its initial form after a long time T, one can compute the resulting phase Γ. This can be done by integrating $d\omega_{\mathscr{A}} = \frac{1}{2}\sin\theta\, d\theta \wedge d\varphi$ over the region in the (θ, φ) space which is the image of the surface surface

spanned on the closed contour traced out in the real space of the parameters $\boldsymbol{\lambda}$ by the vector $\boldsymbol{\lambda}(t)$ and parametrized by the coordinates (θ, φ). This gives $\Gamma = \frac{1}{2}\Omega$ where Ω is the solid angle cut out from the parameter space by the contour traced by $\boldsymbol{\lambda}$. The same result can be also obtained by writing $\varphi = \mathrm{arctg}(y/x)$ so that (to make the notation easier we use x for λ^x, etc.)

$$\omega_{\mathscr{A}} = -\frac{1}{2}\cos\theta\, d\varphi = \frac{1}{2}\,\frac{z}{(x^2+y^2)\sqrt{x^2+y^2+z^2}}\,(y\,dx - x\,dy)\,,$$

i.e. to $\mathscr{A}_x = yz/2r(x^2+y^2)$, $\mathscr{A}_y = -xz/2r(x^2+y^2)$ and $\mathscr{A}_z = 0$. The corresponding $\mathscr{B}$ field has then the form $\mathscr{B} = \boldsymbol{\nabla}\times\mathscr{A} = \mathbf{r}/2r^3$, i.e. it is of the same form as the magnetic field created by a pointlike magnetic monpole of the magnetic charge $q = 1/2$. By analogy with the Gauss law it is then clear that the flux of $\mathscr{B}$ throught any surface spanned on the closed contour traced in space is the same as computed above. The result can be generalized to spin s in which case $\Gamma = s\,\Omega$.

2.5 Transitions to nonnormalizable states

Up to this point only transitions (induced by a perturbation) from a prepared state to states normalized to unity have been considered. This covers naturally transitions to states corresponding to the discrete part of the H_0 spectrum or, as in section 2.3, of the $H_0 + V_{\mathrm{int}}^{(+)}$ spectrum, or to any other physically interesting and realizable states. Here we will consider transitions to nonormalizable states. Of course, strictly speaking, states represented by nonnormalizable (generalized) vectors[16] cannot be realized physically and it should be possible to formulate all questions concerning any physically realizable measurement in terms of probabilities of transitions to normalized states only. Nevertheless, in the scattering theory and other akin problems in which the measuring devices are able to detect particles with well defined momenta (physical states detected in such measurements are represented by normalizable but well collimated in the momentum space superpositions of momentum operator generalized eigenvectors) the use of nonnormalizable vectors in place of normalizable ones is very convenient, enormously simplifying practical calculations.

Sets of nonnormalizable vectors, e.g. generalized eigenvectors of H_0, corresponding to the continuous part of its spectrum, are always labeled by one or more continuous parameter(s) and, perhaps, some additional discrete labels, which all together will be here collectively denoted α. Vectors $|\alpha\rangle$ will be assumed to be normalized to a generalized delta function $\delta(\beta-\alpha)$:

$$\langle\beta|\alpha\rangle = \delta(\beta-\alpha) \equiv \delta_{\beta\alpha}\,, \tag{2.60}$$

[16]Generalized or nonnormalizable vectors, like e.g. plane waves in quantum mechanics of a single particle, do not belong to the proper Hilbert space; they are, roughly speaking, elements of the space of linear forms over the proper Hilbert space and as such are only convenient mathematical devices which should be used with some care.

which is a product of several Dirac and Kronecker deltas and some factors depending on the adopted convention. For example in quantum mechanics of a single particle moving in the continuum (i.e. not confined to a finite domain of the three-dimensional space) the generalized vectors $|\mathbf{k}\rangle$ will be (in the nonrelativistic case) normalized so that $\langle\mathbf{k}'|\mathbf{k}\rangle = (2\pi)^3\delta^{(3)}(\mathbf{k}'-\mathbf{k})$. If the particle has a nonzero spin s, the vectors $|\mathbf{k},\sigma\rangle$, where $\sigma = -s, -s+1, \ldots, +s$ is the particle's spin projection, will be normalized so that $\langle\mathbf{k}',\sigma'|\mathbf{k},\sigma\rangle = (2\pi)^3\delta^{(3)}(\mathbf{k}'-\mathbf{k})\delta_{\sigma'\sigma}$. The vectors $|\mathbf{k}\rangle$ or $|\mathbf{k},\sigma\rangle$ are in this case generalized eigenvectors of $H_0 = \mathbf{P}^2/2M$ and correspond to its eigenvalues $\hbar^2\mathbf{k}^2/2M$ forming the continuous spectrum; H_0 in this case has no normalizable eigenvectors at all. If the spectrum of H_0 (or H) consists of the discrete and continuous parts with the eigenvectors $|n\rangle$ (normalized to unity) and $|\alpha\rangle$ (generalized), the decomposition of the unit operator $\hat{1}$ will be (symbolically) written as

$$\hat{1} = \sum_n |n\rangle\langle n| + \int d\alpha\, |\alpha\rangle\langle\alpha|\,. \tag{2.61}$$

The measure $d\alpha$ in (2.61) corresponds to the generalized delta in (2.60). Because of the arbitrariness inherent in the normalization (2.60) of generalized vectors,[17] the amplitude

$${}_I\langle\alpha|\Psi(t)\rangle_I = \langle\alpha|U_I(t,t_0)|\Psi(t_0)\rangle_I\,,$$

(in which $|\Psi(t_0)\rangle_I$ can be a normalizable or a nonnormalizable vector) usually is not dimensionless and for this reason alone its modulus squared cannot be the probability of finding the system (at the instant t after its evolution from the state $|\Psi(t_0)\rangle$ at t_0) in the state $|\alpha\rangle$. Instead, in this case one is interested in the (differential) probability

$$dP = |{}_I\langle\alpha|\Psi(t)\rangle_I|^2\, d\alpha\,, \tag{2.62}$$

of finding the system in any state of the continuous set of (generalized) states $|\alpha\rangle$ with the label α in the range $(\alpha, \alpha+d\alpha)$. If $|\Psi(t_0)\rangle$ is normalized to unity,[18] the expression (2.62) is dimensionless (as follows from (2.61)) and does not depend on the arbitrariness of the normalization (2.60). If $|\alpha\rangle$ are generalized eigenvectors of H_0 which is has a simple form, the justification of the probabilistic interpretation of (2.62) can be also obtained by enclosing the system in a large box of volume $V = L^3$ so that all states become normalizable.

To illustrate this and another important and somewhat subtle point we consider once again the problem of Tritium β decay of Section 2.3 and ask about the probability that as a result of the decay of the nucleus the atom gets ionized and the electron (initially bound

[17] For instance, generalized eigenvectors $|\mathbf{k}\rangle$ of the operator $\mathbf{P}^2/2M$ in quantum mechanics of a single particle can be normalized as here to $(2\pi)^3\delta^{(3)}(\mathbf{k}'-\mathbf{k})$ (in which case $d\alpha$ stands for $d^3\mathbf{k}/(2\pi)^3$) or to $\delta^{(3)}(\mathbf{k}'-\mathbf{k})$ (with $d\alpha = d^3\mathbf{k}$) or, as in relativistic theories, to $(2\pi)^3 2E_{\mathbf{k}}\delta^{(3)}(\mathbf{k}'-\mathbf{k})$, with $E_{\mathbf{k}} = \sqrt{c^2\hbar^2\mathbf{k}^2 + M^2c^4}$ and $d\alpha = d^3\mathbf{k}/(2\pi)^3 2E_{\mathbf{k}}$.

[18] If it is not normalizable, measurable quantities involve additional factors related to the experimental meaning of the initial state. This will be discussed in Chapter 10.

in the Tritium atom in the $|1S\rangle$ state) is detected[19] (far away from the atom) with the momentum in the range between $\mathbf{k}$ and $\mathbf{k} + d\mathbf{k}$. Using the same approach as in Section 2.3 one can, simplifying the calculation, compute this probability approximately by using the plane waves in place of the true generalized eigenvectors of $H_{\rm fin} = H_0 + V_{\rm int}^{(+)} = P^2/2M - 2e^2/r$ (the final nucleus has $Z = 2$). Since the plane waves are simple, one can easily enclose the system in the box of volume $V = L^3$ imposing on the plane waves periodic boundary conditions. One then deals with the discrete set of the state-vectors $|\mathbf{k}\rangle$ such that

$$\langle \mathbf{r}|\mathbf{k}\rangle = \frac{1}{\sqrt{V}}\, e^{i\mathbf{k}\cdot\mathbf{r}}\,, \qquad \text{with} \quad \mathbf{k} = \frac{2\pi}{L}\,\mathbf{n}\,, \tag{2.63}$$

where the components of the vectors $\mathbf{n}$ are integers. In the momentum space the allowed vectors $\mathbf{k}$ form, therefore, a three-dimensional lattice of points. The number of such points contained in the volume $\Delta k_x \Delta k_y \Delta k_z$ equals

$$\text{number of points} = \frac{V}{(2\pi)^3}\Delta k_x \Delta k_y \Delta k_z\,.$$

Consequently, the factor $V/(2\pi)^3$ plays the role of the density of allowed points in the momentum space. The differential element of the phase space $d^3\mathbf{k} \equiv dk_x dk_y dk_z$ contains therefore $V d^3\mathbf{k}/(2\pi)^3$ states. In the adopted approximation, the (differential) probability of finding the final electron in the specified group of states therefore is

$$\begin{aligned} dP(1S \to \mathbf{k}) &= |\langle \mathbf{k}|1S(Z=1)\rangle|^2\, \frac{V}{(2\pi)^3}\, d^3\mathbf{k} \\ &= \left|\frac{1}{\sqrt{V}}\int d^3\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\, \psi_{1S}(\mathbf{r})\right|^2 \frac{V}{(2\pi)^3}\, d^3\mathbf{k} \equiv \left|\tilde{\psi}_{1S}(\mathbf{k})\right|^2 \frac{d^3\mathbf{k}}{(2\pi)^3}\,. \end{aligned}$$

It is clear that the arbitrary volume factors cancel out reflecting the independence of the probability dP of the arbitrariness in the normalization of nonnormalizable state-vectors. Notice also, that the implicit limit $V \to \infty$ allows one to work from the beginning with the wave function of the $|1S\rangle$ state normalized in the continuum.

Yet the approximation which uses the plane waves (even if it may prove quite satisfactory numerically) is wrong from the fundamental point of view. To see this it is sufficient to sum up the probabilities of finding the electron in any possible final state (we have passed to the normalization in the continuum):

$$\sum_{nlm_l} P(1S \to nlm_l) + \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, |\langle \mathbf{k}|1S(Z=1)\rangle|^2 > 1\,,$$

[19] In this qualitative discussion we neglect the electron spin and, more importantly effects due to the identity of the two electrons - the one which was initial bound on the atom's orbit and the one which is created in the nuclear β decay.

because the Parseval's identity implies that

$$\int \frac{d^3\mathbf{k}}{(2\pi)^3}\,|\tilde{\psi}_{1S}(\mathbf{k})|^2 = \int d^3\mathbf{r}\,|\psi_{1S}(\mathbf{r})|^2 = 1\,.$$

Obviously this violation of the unitarity results from the fact that the vectors $|\mathbf{k}\rangle$ used to represent the electron final states form by themselves a complete set of (generalized) vectors. (Using $|\mathbf{k}\rangle$ as $|\alpha\rangle$ in (2.61) leaves no room for the first term in this formula - the vectors $|\mathbf{k}\rangle$ span the entire Hilbert space of the single particle). To avoid the problem with the unitarity one has to use the exact generalized eigenvectors of $H_{\rm fin}$. From the elementary potential scattering theory of a single particle it is known, however, that there are many possible choices of the set of generalized eigenvectors spanning the subspace of the Hilbert space corresponding to the continuous part of the spectrum of this Hamiltonian. One such set form the states, labeled by $\mathbf{k}$, the wave functions of which have the asymptotic (i.e. when $r \equiv |\mathbf{r}| \to \infty$) form[20]

$$\langle \mathbf{r}|\mathbf{k}_+\rangle \approx e^{i\mathbf{k}\cdot\mathbf{r}} + f(\hat{\mathbf{r}},\hat{\mathbf{k}})\,\frac{e^{ikr}}{r}\,,$$

(see Appendix E) and correspond to the eigenvalue $E_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2M_e$ of $H_{\rm fin}$. Another set form the vectors, also labeled by $\mathbf{k}$ and corresponding to the same $H_{\rm fin}$ eigenvalue, which in the same limit have the form

$$\langle \mathbf{r}|\mathbf{k}_-\rangle \approx e^{i\mathbf{k}\cdot\mathbf{r}} + f(-\hat{\mathbf{r}},\hat{\mathbf{k}})\,\frac{e^{-ikr}}{r}\,.$$

(One could also form superpositions of $|\mathbf{k}_+\rangle$ and $|\mathbf{k}_-\rangle$). The question then arises, which set of generalized eigenvectors should be used to compute the probabilities of finding the electron with the momentum $\mathbf{k}$. We touch here upon the problem which will be discussed more thoroughly in Chapter 7. The answer is that, because one detects the electron which behaves as free for $t \to \infty$, the time evolution generated by $H_{\rm fin}$ of the true *normalized* to unity electron state which is an appropriately formed (usually well collimated) superposition of the generalized $H_{\rm fin}$ eigenvectors, should match, as $t \to \infty$, the evolution generated by $\hat{\mathbf{P}}^2/2M_e$ of a similar superposition of the generalized eigenvectors $|\mathbf{k}\rangle$ of $\hat{\mathbf{P}}^2/2M_e$. It is the set of $|\mathbf{k}_-\rangle$ generalized eigenvectors of $H_{\rm fin}$ which satisfies this requirement (see Section 7.3):

$$e^{-iH_{\rm fin}t/\hbar}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\,|\mathbf{k}_-\rangle\,g(\mathbf{k}) \to e^{-i\hat{\mathbf{P}}^2t/2M_e\hbar}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\,|\mathbf{k}\rangle\,g(\mathbf{k})\,,$$

(the convergence is to be understood in the usual sense of convergence of sequences of vectors in Hilbert spaces). Thus, provided the the vectors $|\mathbf{k}_-\rangle$ are normalized to

[20] We disregard here the, unimportant for our point, fact that the Coulombic wave functions have in fact a more complicated form.

$(2\pi)^3\delta^{(3)}(\mathbf{k}' - \mathbf{k})$, the correct (within the approximation of the sudden change of the Hamiltonian) formula for the probability of interest is

$$dP(1S \to \mathbf{k}) = |\langle \mathbf{k}_-|1S(Z=1)\rangle|^2 \, \frac{d^3\mathbf{k}}{(2\pi)^3} \, . \tag{2.64}$$

As will be elucidated in Chapter 7, the generalized states $|\mathbf{k}_+\rangle$ and $|\mathbf{k}_-\rangle$ are, as far as their physical meaning is concerned, analogous to the (normalizable) *in* and *out* vectors introduced in the perturbed harmonic oscillator problem discussed in Section 1.3. It is also clear that finding the (normalizable) eigenvectors of H_{fin} in the finite volume V (which in the limit $V \to \infty$ would correspond to the continuous part of the spectrum) and counting the number of states, as it was possible with the plane waves, is prohibitively difficult. Fortunately the arguments based on the dimension and independence of the adopted concrete normalization prescription (to the Dirac delta functions) of the generalized vectors suffice to write down the formula (2.64).

2.6 Harmonic perturbations

We now consider the very important case of a perturbation which has harmonic time dependence of frequency ω of the general (Hermitian) form

$$V_{\text{int}}(t) = O\, e^{-i\omega t} + O^\dagger \, e^{+i\omega t} \, , \tag{2.65}$$

in which O is a time independent operator. Without loss of generality we can assume that $\omega \geq 0$.

Assuming that H_0 has some normalized eigenvectors corresponding to its discrete energy levels, we will first consider transitions between such H_0 eigenstates. In this case we can assume that at some instant t_0 for which, without loss of generality[21] we can take $t_0 = 0$, the system was in the discrete H_0 eigenstate $|n\rangle$ with energy E_n and ask about the probability of finding it at the instant t in another discrete H_0 eigenstate $|k\rangle$ with energy E_k. Inserting the form (2.65) of $V_{\text{int}}(t)$ into the formula (2.10) we get

$$\mathcal{A}^{(1)}_{kn}(t,0) = -\frac{1}{\hbar}\left[\frac{e^{i(\omega_{kn}-\omega)t}-1}{\omega_{kn}-\omega}\,\langle k|O|n\rangle + \frac{e^{i(\omega_{kn}+\omega)t}-1}{\omega_{kn}+\omega}\,\langle k|O^\dagger|n\rangle\right] . \tag{2.66}$$

This result means that the transition probability between two discrete states $|n\rangle$ and $|k\rangle$ (given in this approximation by $|\mathcal{A}^{(1)}_{kn}(t)|^2$) is, in general, a complicated function of time

[21] If $t_0 \neq 0$ in all the formulae of this section t should be replaced by $t - t_0$ and the matrix elements of the operator O (of the operator $O^\dagger$) multiplied by the phase factor $e^{i(\omega_{kn}-\omega)t_0}$ (the factor $e^{i(\omega_{kn}+\omega)t_0}$). This would only slightly change the precise form of the result of the two-state approximation discussed in the first part of this Section (but not the qualitative picture of the time evolution of the system) but would not affect the results discussed in the further part.

t. Moreover, from (2.66) it is seen that for a given state $|n\rangle$ the probability of the transition to the state $|k\rangle$ such that either $\omega_{kn} \approx \omega$, if $E_k > E_n$, or $\omega_{kn} \approx -\omega$, if $E_k < E_n$ (that is, if the frequency ω of the perturbation is tuned to be very close to the energy difference of the initial state $|n\rangle$ and another state $|k\rangle$), is particularly big. If ω is tuned to be precisely equal ω_{kn} or $-\omega_{kn}$ the coefficient $\mathcal{A}^{(1)}_{kn}(t)$ grows linearly with time and necessarily after some (short) time the condition $|\mathcal{A}^{(1)}_{kn}| \ll 1$ of applicability of the perturbative expansion becomes violated. This means that if ω is tuned to the energy difference between the initial state $|n\rangle$ and another discrete state $|k\rangle$, the time evolution of the system cannot be analyzed perturbatively.[22] One has then to go back to the original set of equations (2.2) and either solve them exactly or invent another approximation scheme.

One such a possible scheme is the two-state approximation which can be applied if the perturbation frequency ω is (almost exactly) tuned to the energy difference of only one pair of the discrete H_0 eigenstates: the initial state $|n\rangle$ and another state $|k\rangle$. This enables one to neglect all remaining discrete energy eigenstates and the states corresponding to the continuous part of the H_0 spectrum. Setting in (2.2) to zero all coefficients $a_m(t)$ except for $a_n(t)$ and $a_k(t)$ one obtains the system of two coupled equations ($\omega_{nk} = -\omega_{kn}$)

$$
\begin{aligned}
i\hbar\,\dot{a}_k &= \left(e^{i(\omega_{kn}-\omega)t}O_{kn} \;+\; e^{i(\omega_{kn}+\omega)t}O^*_{nk}\right) a_n + \left(e^{-i\omega t}O_{kk} + e^{i\omega t}O^*_{kk}\right) a_k\,,\\
i\hbar\,\dot{a}_n &= \left(e^{-i(\omega_{kn}+\omega)t}O_{nk} + e^{-i(\omega_{kn}-\omega)t}O^*_{kn}\right) a_k + \left(e^{-i\omega t}O_{nn} + e^{i\omega t}O^*_{nn}\right) a_n\,,
\end{aligned}
$$

in which O_{kn} stands for $\langle k|O|n\rangle$ and the relation $(O^\dagger)_{kn} = \langle k|O^\dagger|n\rangle = \langle n|O|k\rangle)^* = O^*_{nk}$ has been used. If $E_k > E_n$ ($\omega_{kn} > 0$) it is the two terms with $\omega_{kn} - \omega$ in the exponents which produce the linear growth with t of the coefficient $\mathcal{A}^{(1)}_{kn}$ observed for $\omega \approx \omega_{kn}$. Setting $\omega = \omega_{kn} - \varepsilon$, one can then discard all the remaining terms in the right hand sides of these equations obtaining the simple system of two equations

$$
i\hbar\,\dot{a}_k = O_{kn}\,e^{i\varepsilon t}\,a_n\,, \qquad\qquad i\hbar\,\dot{a}_n = O^*_{kn}\,e^{-i\varepsilon t}\,a_k\,.
$$

This system can be easily transformed into the linear second order equation

$$
\frac{d^2a_k}{dt^2} - i\varepsilon\,\frac{da_k}{dt} + \frac{|O_{kn}|^2}{\hbar^2}\,a_k = 0\,,
$$

the most general solution of which is

$$
a_k(t) = A_1\,e^{i\Omega_1 t} + A_2\,e^{i\Omega_2 t}\,, \qquad \Omega_{1,2} = \frac{\varepsilon}{2} \pm \sqrt{\frac{\varepsilon^2}{4} + \frac{|O_{kn}|^2}{\hbar^2}} \equiv \frac{\varepsilon}{2} \pm \Omega\,,
$$

The corresponding solution for $a_n(t)$ is then

$$
a_n(t) = -\frac{\hbar}{O_{kn}}\left(A_1\Omega_1\,e^{i\Omega_1 t} + A_2\Omega_2\,e^{i\Omega_2 t}\right)e^{-i\varepsilon t}\,.
$$

[22] Also, as will be seen on the example, the notion of the transition probability, which is appropriate for situations in which the probability of the system's return to the initial state is practically negligible, should be in this case replaced by just the probability of finding the system in this or another state at a given instant.

The initial conditions $a_n(0) = 1$, $a_k(0) = 0$ determine A_1 and A_2 and therefore also the state-vector $|\psi(t)\rangle$ of the system for any instant t:

$$|\psi(t)\rangle = e^{-i\varepsilon t/2}\left(\cos\Omega t + \frac{i\varepsilon}{2\Omega}\sin\Omega t\right)e^{-iE_n t/\hbar}|n\rangle - \frac{iO_{kn}}{\hbar\Omega}\,e^{i\varepsilon t/2}\sin\Omega t\,e^{-iE_k t/\hbar}|k\rangle\,.$$

Therefore, the probabilities of finding the system in the state $|k\rangle$ and in the state $|n\rangle$ change with the time as

$$P(n\to k) = \frac{|O_{kn}|^2}{\hbar^2\Omega^2}\sin^2\Omega t = \frac{|O_{kn}|^2}{2\hbar^2\Omega^2}\,(1-\cos 2\Omega t)\,,$$
$$P(n\to n) = \cos^2\Omega t + \frac{\varepsilon^2}{4\Omega^2}\,\sin^2\Omega t\,.$$

When $\varepsilon \neq 0$ the unitarity is not preserved by the two-states approximation because $P(n\to n) + P(n\to k) \neq 1$. It is restored only for $\varepsilon = 0$ (exact tuning of ω), when $|O_{kn}|^2/\hbar^2\Omega^2 = 1$. $\varepsilon = 0$, i.e. $\omega = \omega_{kn}$, corresponds to the exact resonance, at which the system jumps periodically between the two states and the probability of finding it in the state $|k\rangle$ changes between 0 and 1 with the period $2\pi\hbar/|O_{kn}|$.

The calculation done above does not apply to the harmonic oscillator which is special in that if $\omega = \omega_{kn} + \varepsilon$ for some n and k, there are infinitely many other pairs of states for which the same holds. For this reason one cannot restrict the equation (2.2) to two states only. Indeed, to see this, and to understand what can happen in this case, one can use as an illustrative example (taking corresponding to $O = a^\dagger$) the exact solution of the harmonic oscillator problem formulated in (1.38) setting there $f(t) = \lambda\exp(-i\omega_p t)$ (ω_p is the frequency of the perturbation). If the oscillator was prepared at $t = 0$ in the state $|n\rangle$, its interaction picture state-vector at time t is given by $|\psi(t)\rangle_I = U_I(t,0)|n\rangle$ with the operator $U_I(t,0)$ which, up to an irrelevant phase factor is the same as (1.47) with

$$h(t) = -\frac{i}{\hbar}\,\lambda\int_0^t d\tau\, e^{i(\omega-\omega_p)\tau} = -\frac{i}{\hbar}\,\lambda\, e^{i\Delta\omega t/2}\,\frac{\sin\Delta\omega t/2}{\Delta\omega/2}\,,$$

where $\Delta\omega = \omega - \omega_p$. The probability of finding the oscillator at the instant t in the H_0 eigenstate $|k\rangle$ can be then easily computed using the methods of Section 1.3 as $|\langle k|U_I(t,0)|n\rangle|^2$; in particular, it is easy to see, that if $\omega_p = \omega$, the probability $P(0\to k)$ of finding in the state $|k\rangle$ the oscillator which at $t = 0$ started in the ground state, is given by the Poisson distribution (2.30) with the mean excitement $\bar{k}$ growing quadratically with the time t.

The above considerations show that time evolution of systems, the unperturbed energy spectrum of which has, in addition to the continuous part, several discrete levels (or, as the harmonic oscillator, has solely the discrete spectrum), caused by an external harmonic perturbation of the form (2.65) with the frequency ω smaller than $(E^{\rm cont}_{\rm min} - E_i)/\hbar$, where $E^{\rm cont}_{\rm min}$ is the lowest limit of the continuous spectrum and E_i is the energy of the state in

which the system was prepared initially, is either very complicated and irregular or, if ω is tuned to the energy difference of two discrete levels, cannot be analyzed using the perturbative expansion described in this section. Also, the notion of transition probability looses to some extent its usual meaning in this case, because the system will jump forth and back between its discrete levels. However, as we shall now see, the situation changes qualitatively when the frequency ω of the perturbation is greater than $(E^{\rm cont}_{\rm min} - E_i)/\hbar$.

Suppose a system, the unperturbed spectrum of which determined by H_0 consists of a continuous part and a discrete part, is prepared at $t = 0$ in the normalized discrete eigenstate $|i\rangle$ of H_0, the frequency ω of the perturbation (2.65) is greater than $(E^{\rm cont}_{\rm min} - E_i)/\hbar$, and we consider the coefficient $\mathcal{A}_{\alpha i}(t) = \mathcal{A}^{(1)}_{\alpha i}(t) + \ldots$ which gives the projection of the system's state-vector $|\Psi(t)\rangle_I$ (in the interacting picture) at the instant t onto the generalized H_0 eigenvector $|\alpha\rangle$. From the formula (2.10) one gets

$$|\mathcal{A}^{(1)}_{\alpha i}(t)|^2 = |O_{\alpha i}|^2 \left[\frac{\sin(\omega^-_{\alpha i}t/2)}{\hbar\omega^-_{\alpha i}/2}\right]^2 + |O_{i\alpha}|^2 \left[\frac{\sin(\omega^+_{\alpha i}t/2)}{\hbar\omega^+_{\alpha i}/2}\right]^2 \qquad (2.67)$$
$$+ \left(O_{\alpha i}O_{i\alpha}\, e^{-i\omega t} + O^*_{\alpha i}O^*_{i\alpha}\, e^{i\omega t}\right) \left[\frac{\sin(\omega^-_{\alpha i}t/2)}{\hbar\omega^-_{\alpha i}/2}\right] \left[\frac{\sin(\omega^+_{\alpha i}t/2)}{\hbar\omega^+_{\alpha i}/2}\right],$$

where $\omega^{\mp}_{\alpha i} \equiv (\omega_\alpha - \omega_i) \mp \omega$. Because $\omega \geq 0$ by definition, and $\omega_{\alpha i} \equiv \omega_\alpha - \omega_i > 0$ (we assume the energy spectrum of the system is "normal"), $|\mathcal{A}^{(1)}_{\alpha i}(t)|^2$ treated as a function the energy of E_α exhibits a strong peak at $E_\alpha = E_i + \hbar\omega$ of height $h_{\rm princ} \propto |O_{\alpha i}|^2 t^2/\hbar^2$. Formally this principal peak is accompanied by secondary peaks which from the physical point of view, however, are completely negligible compared to the principal one. Indeed, the height $h_{\Delta E}$ of a secondary peak separated by ΔE from the principal one is suppressed by the factor

$$\frac{h_{\Delta E}}{h_{\rm princ}} \approx \left(\frac{2}{\Delta E}\right)^2 \frac{\hbar^2}{t^2} \approx \left[\frac{\rm eV}{\Delta E}\right]^2 \left[\frac{\rm sec}{t}\right]^2 \times 10^{-30}\,.$$

Thus, already after e.g. $t \sim 10^{-6}$ sec. from the moment at which the system was prepared in the state $|i\rangle$, the height of the secondary peak at $\Delta E \sim 10^{-6}$ eV is suppressed by the factor 10^6 relative to the height of the principal one. The contribution of the second term of (2.67) to the principal peak is clearly also negligible, while the contribution of the last term of (2.67) to it can be estimated as

$$\frac{2}{\hbar\omega^+_{\alpha i}}\frac{t}{\hbar} : \frac{t^2}{\hbar^2} \approx \left[\frac{\rm eV}{\hbar\omega_{\alpha i}}\right] \left[\frac{\rm meter}{c\,t}\right] \left[\frac{2\hbar c}{\rm eV \cdot meter}\right] \approx \left[\frac{\rm eV}{\hbar\omega_{\alpha i}}\right] \left[\frac{\rm meter}{c\,t}\right] \times 4 \times 10^{-7}\,,$$

that is, it is also negligible already for $t \sim 10^{-6}$ sec, provided the energy difference $\hbar\omega_{\alpha i} = E_\alpha - E_i$ is not too small. All this means that for times t relevant for real measurements the behaviour of $|\mathcal{A}^{(1)}_{\alpha i}(t)|^2$ can be safely approximated by

$$|\mathcal{A}^{(1)}_{\alpha i}(t)|^2 \approx \left[\frac{\sin(\omega^-_{\alpha i}t/2)}{\hbar\omega^-_{\alpha i}/2}\right]^2 |\langle\alpha|O|i\rangle|^2\,. \qquad (2.68)$$

Furthermore, the width of the principal peak (determined by the first zero of the sine function) decreases as $2\pi\hbar/t$. Thus, as the time t increases, the principal peak becomes higher and sharper. Still, the narrow range of energies around $E_\alpha = E_i + \hbar\omega$, within which $|\mathcal{A}^{(1)}_{\alpha i}(t)|^2$ is appreciably different from zero, covers, if t is not taken to infinity (as it will be discussed shortly, this cannot be done), a huge number of states belonging to the continuous part of the H_0 spectrum[23] and probabilities of transitions to all these states are therefore nonnegligible. This simply reflects the uncertainty principle $\Delta E \Delta t \gtrsim 2\pi\hbar$ which generally restricts the accuracy ΔE with which the conservation of energy can be assessed in any measurement taking a time shorter than Δt: at the time t after the preparation of the initial state $|i\rangle$ one cannot determine the energy of the final system's state with an accuracy better than $2\pi\hbar/t$.

The final factor which has to be taken into account is the experimental resolution $\Delta_{\rm ex}E$ which is always finite, so that after a time $t \sim 2\pi\hbar/\Delta_{\rm ex}E \approx [10^{-6}{\rm eV}/\Delta_{\rm ex}E] \times 10^{-9}$ sec. it becomes much larger than the width of the principal peak (thus making the uncertainty principle invoked above somewhat irrelevant in this case from the practical point of view). The quantity of interest, therefore, is the probability of finding the system at the instant t in any of the states $|\alpha\rangle$ having energies E_α which are within the experimental resolution around the center of the principal peak located at $E_\alpha = E_i + \hbar\omega$. Since, as illustrated above, the factor $|\mathcal{A}^{(1)}_{\alpha i}|^2$ (which, let us recall, is not dimensionless and, therefore, is not yet the probablility) is practically negligible outside the window of the width $2\pi\hbar/t$ around $E_i + \hbar\omega$, the quantity of physical interest is

$$\int_{E_\alpha \sim E_i + \hbar\omega \pm \frac{2\pi\hbar}{t}} d\alpha \, |\mathcal{A}^{(1)}_{\alpha i}(t)|^2 \, ,$$

where it is understood that the integration is only over the energy variable dE_α which is a part of $d\alpha$. This is already dimensionless (see section 2.5) and is usually written in the form

$$\int_{E_\alpha \sim E_i + \hbar\omega \pm \frac{2\pi\hbar}{t}} dE_\alpha \, \rho(E_\alpha) \, |\mathcal{A}^{(1)}_{\alpha i}(t)|^2 \, , \tag{2.69}$$

with the density of states $\rho(E_\alpha)$ which itself may still have a differential character (it gives the number of states per unit energy interval and contained within $d\alpha_{\rm rest}$ of the remaining continuous parameters involved in the label α). The integral (2.69) gives the probability that after the time t from preparing it in the state $|i\rangle$, the system will be found in any

[23] These can be counted by enclosing the system in a cubic box of volume $V = L^3$, so that the etire H_0 energy spectrum becomes discrete; the energy levels which in the limit $L \to \infty$ merge to form the continuous spectrum are separated by gaps $\delta E \propto 1/L^2$ (low lying states) and $\delta E \propto 1/L$ (higher states). For instance, in the box of $V = 1$ m^3 states of free electron are separated by (cf. section 2.5) $\delta E \sim 4\pi^2(\hbar^2c^2/Mc^2L^2)n \approx n\,[1\ {\rm meter}/L]^2 \times 10^{-18}$ eV; even the levels corresponding to the electron velocity $|\mathbf{v}| \equiv \hbar|\mathbf{k}|/M \sim c$ (i.e. $n \sim (Mc/\hbar)(L/2\pi)$) are separated by gaps $\delta E \sim 2\pi\hbar c/L \approx [1\ {\rm meter}/L] \times 10^{-6}$ eV. Of course the gaps δE can be made arbitrarily small by increasing L. Therefore the number of states in a given finite energy interval, however small, can be made arbitrarily large.

of the states $|\alpha\rangle$ of energy E_α within the range $2\pi\hbar/t$ around $E_i + \hbar\omega$, so also within the range $\Delta_{\rm ex}E$, and $d\alpha_{\rm rest}$.

Since the height of the peak at $E_\alpha = E_i + \hbar\omega$ grows as t^2 and its width decreases as $1/t$, the area under the plot of the function $f(E_\alpha) = |\mathcal{A}^{(1)}_{\alpha i}|^2$, within the range $2\pi\hbar/t$ (or, as has been explained, within $\Delta_{\rm ex}E$, from $E_i + \hbar\omega$), that is the value of the integral (2.69), grows only *linearly* with time t. This can be also made clear with the help of the following representation[24]

$$\delta(\kappa) = \lim_{t\to\infty} \frac{\sin^2 \kappa t}{\pi\kappa^2 t}\,, \tag{2.70}$$

of the Dirac delta-function which allows us to rewrite (2.69) with $|\mathcal{A}^{(1)}_{\alpha i}(t)|^2$ given by (2.68) in the formal limit $t \to \infty$ as

$$\begin{aligned}\int dE_\alpha\, \rho(E_\alpha)\, |\mathcal{A}^{(1)}_{\alpha i}|^2 &\approx \frac{\pi}{\hbar^2} \int dE_\alpha\, \rho(E_\alpha)\, |\langle\alpha|O|i\rangle|^2\, t\, \delta\!\left(\frac{\omega_{\alpha i} - \omega}{2}\right) \\ &= \frac{2\pi}{\hbar}\, |\langle\alpha|O|i\rangle|^2\, \rho(E_\alpha)\, t\,, \end{aligned} \tag{2.71}$$

where in the last line $E_\alpha \equiv E_i + \hbar\omega$ (the integral in (2.71) has been explicitly performed exploiting the property of the delta function: $\delta(ax) = \delta(x)/|a|$). Of course in this formal limit[25] the transition can only occur to the states having energies E_α equal exactly $E_i + \hbar\omega$, but the aim of the discussion preceding the formula (2.71) was to make clear that from the practical point of view (2.71) stays valid for times t which are not asymptotic and correspond in fact to measurements which can be made on real systems.

Of course, the linear with time t growth of the probability seen in (2.71) cannot continue indefinitely because otherwise after some finite time the probability of finding the system in the group of states specified above would exceed unity (no matter how small the matrix element squared $|\langle\alpha|O|i\rangle|^2$ were), that is would violate the unitarity constraint: as the evolution (generated by the operator $U_I(t, 0)$ defined in section 1.1) of the system's state vector is unitary,

$$\int d\alpha\, |\mathcal{A}_{\alpha i}(t)|^2 + \sum_k |\mathcal{A}_{ki}(t)|^2 = 1\,,$$

at any instant t. This means that higher order corrections to the coefficient $\mathcal{A}_{\alpha i}(t) = \mathcal{A}^{(1)}_{\alpha i}(t) + \ldots$ must necessarily cut the linear growth of the probability observed in (2.71).

[24] For $\kappa \neq 0$ the limit of (2.70) is obviously 0, whereas for $\kappa = 0$ it is infinite; moreover, $\int_{-\infty}^{+\infty} d\kappa\, \frac{\sin^2 \kappa t}{\pi\kappa^2 t} = \frac{1}{\pi}\int_{-\infty}^{+\infty} d\xi\, \frac{\sin^2 \xi}{\xi^2} = 1$.

[25] Alternatively, one can keep t finite and, relying on the presented arguments that $|\mathcal{A}^{(1)}_{\alpha i}(E)|^2$ is practically zero outside the window $E_i + \hbar\omega \pm 2\pi\hbar/t$, extend the integral over dE_α in the left hand side of (2.71) to the entire E_α axis (from $-\infty$ to $+\infty$) and take the density $\rho(E_\alpha) \approx \rho(E + \hbar\omega)$ outside the integral. This procedure leads to the same result.

The question then arises whether one can make any sense at all out of this result. Recall that in the case of the frequency ω of the perturbation tuned exactly to the energy difference of two discrete levels, discussed at the beginning of this Section, the transition probability obtained in the first order of the perturbative expansion grew quadratically with time leading to a very quick unitarity violation and it was necessary to employ a different approach to investigate the true evolution of the system. The answer to the posed question is, however, in the affirmative owing to the following two important circumstances which make the case of transitions from a discrete state to states belonging to the continuous part of the spectrum different. Firstly, the transition probability (2.71) depends not only on t, but also on the magnitude of the matrix element. Owing to the only linear (and not quadratic) growth with t, for small but still realistic values of $|\langle\alpha|O|i\rangle|^2$, the probability (2.71) can remain much smaller than unity for times t sufficiently long that the principal peak of (2.68) covers practically only states of energies E_α indistinguishable from $E_i + \hbar\omega$ within the experimental resolution. Secondly, the crucial role plays the fact that we consider transitions to the states belonging to the continuous part of the H_0 spectrum. Owing to this circumstance the constant *transition probability per unit time*, obtained from the formula[26]

$$w_{\alpha i} = \frac{2\pi}{\hbar} \, |\langle\alpha|O|i\rangle|^2 \, \rho(E_\alpha) \, , \tag{2.72}$$

(in which $E_\alpha = E_i + \hbar\omega$), called the Fermi's Golden Rule, can be applied to an ensemble of N systems prepared at $t = 0$ in the same state $|i\rangle$ to compute the fraction dN_i (proportional to dt and to the actual number $N_i(t)$ of systems in the state $|i\rangle$) of systems in the ensemble which in the infinitesimal time interval dt (with dt so long from the microscopic point of view that transitions occur only to the states covered by the principal peak) will make the transition to the specified group of states belonging to the continuous part of the H_0 spectrum. The resulting differential equation

$$dN_i = -dt \, N_i(t) \, w_{\alpha i} \, , \tag{2.73}$$

for $N_i(t)$ can be then solved giving the number $N_i(t)$ of systems in the ensemble which in the time interval $[0, t]$ have passed from the state $|i\rangle$ to the specified group of states. In the reasoning leading to the differential equation one neglects altogether the possibility that the systems which have already made the transition could at later times return to the initial state $|i\rangle$. The probability (per unit time) of such "returns" is negligibly small compared to the overwhelming probability that systems in the ensemble which once passed

[26] If the label α consists of more continuous parameters (in addition to energy E_α), the formula (2.72) for probability per unit time can be also written in the form (changing the symbol $w_{\alpha i}$ to the more appropriate $dw_{\alpha i}$)

$$dw_{\alpha i} = d\alpha \, |\langle\alpha|O|i\rangle|^2 \, \frac{2\pi}{\hbar} \, \delta(E_\alpha - E_i - \hbar\omega) \, .$$

Notice the difference with the formula (2.62) for the probability.

to the continuous part of the spectrum will further migrate in it almost forever.[27]

A variant of the above reasoning arises when one considers transitions between discrete states of H_0 induced by a perturbation which consists of an incoherent superposition of perturbations characterized by some frequency profiles in the frequency space. The prominent example are here atomic transitions induced by the presence of the radiation, considered in section 3.2. In this case one finds that probabilities of transitions $i \to f$ computed in the first order also grow linearly with time. The constant transition probabilities w_{fi} per unit time can then again be used to write down a system of differential equations for the numbers of systems in the ensemble making transitions $i \to f$ in any finite interval $[0, t]$. In this case, however, the probability of "returns" from other discrete states is not negligible (the "returns" from the states belonging to the continuous part of the spectrum can still be neglected) and have to be taken into account in the system

$$dN_i(t) = -dt\, N_i(t) \sum_f w_{fi} - dt\, N_i(t) \int d\alpha_{\text{cont part}}\, w_{\alpha i} + dt \sum_f w_{if} N_f(t)\,,$$

of coupled differential equations for the instantaneous numbers $N_i(t)$ of the ensemble systems in the state $|i\rangle$.

[27] Their behaviour is in this respect similar to the behaviour of the harmonic oscillator of frequency ω subject to a perturbation with ω_p tuned to ω. The mean excitement of such a system grows, as we have found, as t^2 (at the cost of energy absorbed from the external source and transmitted to it through the perturbation). This similarity owes to the simple fact that for a given state $|\alpha\rangle$ in the continuous part of the spectrum there are always other states $|\beta\rangle$ with $(E_\beta - E_\alpha)/\hbar$ matching the frequency of the applied perturbation.