1 Time evolution in quantum mechanics

It seems appropriate to begin these lectures by recalling and illustrating with simple examples in this chapter three ways of representing time evolution of quantum systems. This material is essentially standard (it can be found in standard quantum mechanics textbooks like the Schiff's one or many others) but it constitutes a good starting point for making a smooth transition from the ordinary quantum mechanics of a single particle to nonrelativistic and relativistic quantum theories of many particles and to quantum field theory: it is the time evolution of systems of particles (or fields) that is investigated in typical particle physics scattering experiments.

In addition, the interaction picture time evolution operator introduced in Section 1.1 will serve (in Section 1.2) to construct the lowest energy eigenvector (proportional to the normalized to unity ground-state vector) of the full Hamiltonian out of the normalized ground-state vector of the (appropriately chosen) free Hamiltonian. This construction, based on the adiabatic principle (which will be discussed in more detail in Section 2.4), will be then used in formulating the Dyson expansion of Green's functions in the nonrelativistic many body theory and in the relativistic quantum field theory (Chapter 13). Analysis of a simple solvable model presented in Section 1.3 will provide a simple illustration of this construction. The same model will also allow to introduce the notions of the *in* and *out* states and of the S-matrix, which is the object of prime interest in the scattering theory, together with two its representations: one in terms of matrix elements of the S-operator connecting the *in* and *out* states and another one in terms of matrix elements of the S_0 operator.

1.1 Three pictures

There are three different standard ways (traditionally called "pictures") of representing the time evolution of quantum systems.

1. *The Schrödinger picture* is the basic and most natural way of representing the time evolution in ordinary nonrelativistic quantum mechanics. In this picture vectors[1] $|\Psi\rangle$ representing states of the physical system and belonging to some Hilbert space change in time according to the Schrödinger equation:

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle_S = H^S |\Psi(t)\rangle_S \,, \tag{1.1}$$

in which the Hamiltonian H^S may or may not depend on time t. The symbol S is used (in this section only) to distinguish operators defined in this picture and time evolution

[1] We denote state-vectors by the upper case Greek letters in order to stress that the considerations are of a general character and apply to any quantum system, not only to the familiar one-particle nonrelativistic quantum mechanics.

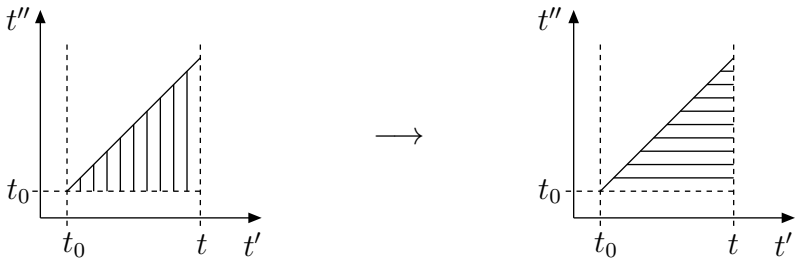

Figure 1.1: Changing the order of the integrations. Solid lines in the left (right) triangle mark the range of the integration over t'' (t') performed as the first one at fixed t' (t'').

of vectors in this picture. The formal solution of the equation (1.1) can be expressed in terms of the unitary evolution operator $U(t, t_0)$ such that

$$|\Psi(t)\rangle_S = U(t, t_0)|\Psi(t_0)\rangle_S \,. \tag{1.2}$$

The vector $|\Psi(t_0)\rangle_S$ specifying the state of the system at some arbitrary instant t_0 plays the role of the initial condition for the differential equation (1.1). The operator $U(t, t_0)$ satisfies the differential equation

$$i\hbar \frac{d}{dt} U(t, t_0) = H^S(t)\, U(t, t_0) \,, \tag{1.3}$$

with the boundary condition $U(t_0, t_0) = \hat{1}$ (the unit operator). The operator $U(t, t_0)$ is unitary,[2] $U(t, t_0)U^\dagger(t, t_0) = \hat{1}$, and has the following, physically obvious, properties:

$$U(t, t')\, U(t', t_0) = U(t, t_0) \,, \qquad U^{-1}(t, t_0) = U^\dagger(t, t_0) = U(t_0, t) \,. \tag{1.4}$$

If the Hamiltonian H^S is time-independent, the solution of (1.3) is well known and reads:

$$U(t, t_0) = \exp\left(-\frac{i}{\hbar} H^S (t - t_0) \right) . \tag{1.5}$$

If the Hamiltonian H^S depends on time t, one rewrites (1.3) in the form of the integral equation which automatically takes into account the initial condition $U(t_0, t_0) = \hat{1}$:

$$U(t, t_0) = \hat{1} - \frac{i}{\hbar} \int_{t_0}^{t} dt'\, H^S(t')\, U(t', t_0) \,. \tag{1.6}$$

[2]Indeed,

$$i\hbar \frac{d}{dt} \left(U(t, t_0) U^\dagger(t, t_0) \right) = \left(i\hbar \frac{d}{dt} U(t, t_0) \right) U^\dagger(t, t_0) + U(t, t_0) \left(i\hbar \frac{d}{dt} U^\dagger(t, t_0) \right) = 0 \,,$$

as follows from the equation (1.3) and its Hermitian conjugation. This, combined with the condition $U(t_0, t_0) = \hat{1}$, implies its unitarity.

This can be solved iteratively (i.e. using the Banach's fixed point principle):

$$
\begin{aligned}
U^{(0)}(t,t_0) &= \hat{1}\,, \\
U^{(1)}(t,t_0) &= \hat{1} + \frac{1}{i\hbar}\int_{t_0}^{t} dt' H^S(t')\,, \\
U^{(2)}(t,t_0) &= \hat{1} + \frac{1}{i\hbar}\int_{t_0}^{t} dt' H^S(t') + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H^S(t') H^S(t'')\,,
\end{aligned}
\tag{1.7}
$$

and so on. The successive iterations yield the perturbative expansion of $U(t,t_0)$. The complete solution can be cast in a compact form by introducing the operation of chronological ordering. This is done as follows. Consider the last term in the expression for $U^{(2)}(t,t_0)$. Upon changing the order of the integrations $\int dt' \int dt'' \to \int dt'' \int dt'$ (see Figure 1.1) it becomes

$$
\int_{t_0}^{t} dt'' \int_{t''}^{t} dt'\, H^S(t')\, H^S(t'') \equiv \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\, H^S(t'')\, H^S(t')\,.
$$

Therefore, the integral in the last term in the expression for $U^{(2)}(t,t_0)$ can be rewritten in the form of the sum of two terms

$$
\begin{aligned}
\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, H^S(t')\, H^S(t'') &= \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, H^S(t')\, H^S(t'') \\
&+ \frac{1}{2}\int_{t_0}^{t} dt' \int_{t'}^{t} dt''\, H^S(t'')\, H^S(t') \equiv \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, \mathrm{T}\big[H^S(t')\, H^S(t'')\big]\,.
\end{aligned}
$$

We have introduced the time-ordered product (denoted T) of time dependent ("bosonic") operators[3] (here the Hamiltonians):

$$
\begin{aligned}
&\mathrm{T}[A(t')B(t'')] \equiv \theta(t'-t'')A(t')B(t'') + \theta(t''-t')B(t'')A(t')\,, \\
&\mathrm{T}[A(t')B(t'')B(t''')] \equiv \theta(t'-t'')\theta(t''-t''')A(t')B(t'')B(t''') + \ldots
\end{aligned}
\tag{1.8}
$$

The reasoning can be extended to higher order terms of the iterative solution (1.7) of the operator equation (1.3) defining $U(t,t_0)$. As a result one obtains the formal expression

$$
U(t,t_0) = \mathrm{T}\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, H^S(t')\right). \tag{1.9}
$$

The symbol T in front of the exponential means that in each term of its power series expansion the Hamiltonians under the multiple integrals have to be ordered from the left to the right in decreasing order of their time arguments. Obviously, if the Hamiltonian H^S does not depend on time, the formula (1.9) reduces to the more familiar form (1.5).

[3]Hamiltonians are always "bosonic" operators. Time-ordering of products of "fermionic" operators (which under rotations of the reference frame transform as half-integer spin representations of the rotation group - see Chapter 4) must be defined with the minus signs in front of the terms in which the ordering of operators differs by an odd permutation from their ordering under the sign of T in the left hand side.

Computing the time derivative of a matrix element of an operator O^S (which may or may not depend on time) between the vectors $|\Psi(t)\rangle_S$ and $|\Phi(t)\rangle_S$ satisfying the equation (1.1) one gets (with the help of the formulae (1.2), (1.3) and their Hermitian conjugations)

$$\frac{d}{dt}\,{}_S\langle\Phi(t)|O^S|\Psi(t)\rangle_S = {}_S\langle\Phi(t)|\,\frac{i}{\hbar}\big[H^S(t),\,O^S\big]|\Psi(t)\rangle_S + {}_S\langle\Phi(t)|\,\frac{\partial O^S}{\partial t}|\Psi(t)\rangle_S\,. \quad (1.10)$$

The last term is present only if the Schrödinger picture operator O^S depends explicitly on time. It follows that matrix elements of a time independent operator which commutes with the Hamiltonian (at every moment of time) are constant. The observable represented by O^S (if it is a Hermitian operator) is then a constant of motion - its matrix elements do not change with time. The result (1.10) shows, however, that there can also exist constants of motion represented by operators not commuting with the Hamiltonian: the two terms on the right hand side may cancel each other.

2. *The Heisenberg picture.* Physical predictions of the quantum theory are contained in matrix elements of operators, and not in state-vectors or operators separately. Therefore the Schrödinger picture discussed above is equivalent to another view, called the Heisenberg picture, on the time variation of the matrix elements. In this picture, specification of which requires singling out a particular instant t_0, Hilbert space vectors representing states of the system do not change with time; instead, the entire time dependence of matrix elements is attributed to operators. The time independent Heisenberg picture state-vectors $|\Psi\rangle_H$ are defined by

$$|\Psi\rangle_H \equiv U^\dagger(t,t_0)|\Psi(t)\rangle_S\,. \quad (1.11)$$

Therefore (cf. the formula (1.2)) $|\Psi\rangle_H = |\Psi(t_0)\rangle_S$. The choice of t_0 is arbitrary; usually one sets $t_0 = 0$. Correspondingly, the Heisenberg picture time-dependent counterpart $O^H(t)$ of a Schrödinger picture operator $O^S(t)$ (which, as indicated, may by itself depend on time) is defined as

$$O^H(t) = U^\dagger(t,t_0)\,O^S(t)\,U(t,t_0)\,, \quad (1.12)$$

so that the matrix elements like the one considered in (1.10) stay unchanged:

$${}_S\langle\Phi(t)|O^S|\Psi(t)\rangle_S = {}_H\langle\Phi|U^\dagger(t,t_0)\,O^S U(t,t_0)|\Psi\rangle_H = {}_H\langle\Phi|O^H(t)|\Psi\rangle_H\,.$$

The derivative (1.10) with respect to time of the matrix element can be now represented in the form

$$\begin{aligned}\frac{d}{dt}\,{}_S\langle\Phi(t)|O^S|\Psi(t)\rangle_S &= \frac{d}{dt}\,{}_H\langle\Phi|O^H(t)|\Psi\rangle_H = {}_H\langle\Phi|\frac{d}{dt}\,O^H(t)|\Psi\rangle_H \\ &= {}_H\langle\Phi|\,\frac{i}{\hbar}\big[H^H(t),\,O^H(t)\big]\,|\Psi\rangle_H + {}_H\langle\Phi|\left(\frac{\partial O}{\partial t}\right)_H|\Psi\rangle_H\,. \quad (1.13)\end{aligned}$$

Here

$$H^H(t) \equiv U^\dagger(t,t_0)H^S(t)U(t,t_0)\,, \quad (1.14)$$

is the Hamiltonian in the Heisenberg picture and $(\partial O/\partial t)_H$ is the abbreviation for

$$U^\dagger(t,t_0)\,\frac{\partial O^S}{\partial t}\,U(t,t_0)\,,$$

(it is just the transformation to the Heisenberg picture of the Schrödinger picture operator $\partial O^S/\partial t$). Note that $H^H(t)$ equals H^S only if the latter is time independent (the operator $U(t,t_0)$ is then given by the formula (1.5) and commutes with H^S). Since the state-vectors $|\Psi\rangle_H$ and $|\Phi\rangle_H$ in (1.13) are arbitrary, one concludes that in the Heisenberg picture operators change with time according to the equation

$$\frac{d}{dt}\,O^H(t) = \frac{i}{\hbar}\,\big[H^H(t),\,O^H(t)\big] + \left(\frac{\partial O}{\partial t}\right)_H(t)\,, \tag{1.15}$$

called the Heisenberg equation of motion of the operator $O^H(t)$. The last term of this equation is present only if the Schrödinger picture operator O^S depends explicitly on time. The most prominent examples of such operators are the operators $\mathbf{K}$ which generate boosts of state-vectors i.e. changes of these related either to boosting the original system so that it acquires (in the original reference frame) an additional velocity or to making the transition to another reference frame moving with respect to the original one, both in nonrelativistic versions of quantum mechanics (see the formula (4.67)) and in relativistic quantum field theories.

Going over to the Heisenberg picture is a natural step in quantizing relativistic fields (see Chapter 11) because field operators depend then on both space and time variables $\mathbf{x}$ and t; this facilitates keeping the Poincaré covariance of the theory's formalism as much manifest as it is possible. The Heisenberg picture is also useful in problems with time dependent Hamiltonians $H^S(t)$ when, due to the uncertainty relation between time and energy (see Section 2.6), the instantaneous eigenvectors of $H^S(t)$ have no direct physical significance and one is rather interested in predicting transition rates (to be introduced in Section 1.3 and in Chapter 2) between appropriately defined states. In such situations it is sometimes easier (as in the example considered in Section 1.3) to solve the Heisenberg equation (1.15) for basic operators (out of which all observables can be built, i.e. for the ones forming the basis of the operator algebra of the given quantum theory) and to consider their matrix elements between constant in time state-vectors representing the entire time evolution of the system prepared in some state at some initial instant. Finally, it will be seen (Chapter 13) that in relativistic quantum field theories, similarly as in nonrelativistic quantum mechanics of many particles, the most important quantities are expectation values in the ground-state of the full Hamiltonian of chronologically ordered products of various Heisenberg picture operators: such expectation values encode essentially all physical information about the considered systems.

3. *The interaction (Dirac) picture.* Yet another view on the time evolution of matrix elements of operators is offered by the so-called interaction picture. Suppose the Hamiltonian H^S of the considered system can be divided into a time-independent part H_0^S, which will

be referred to as the free Hamiltonian because usually - though not necessarily - it is the Hamiltonian of the system in the absence of any interactions, and the perturbation $V^S_{\rm int}$ which may or may not depend on time. The splitting of the Hamiltonian allows to define the interaction picture time dependent state-vectors $|\Psi(t)\rangle_I$ by

$$|\Psi(t)\rangle_I \equiv e^{iH_0^S t/\hbar}|\Psi(t)\rangle_S = e^{iH_0^S t/\hbar}U(t,0)|\Psi(0)\rangle_S\,, \tag{1.16}$$

where we have chosen $t_0 = 0$ as the moment at which the corresponding state-vectors in the two pictures coincide. With this definition the free Hamiltonian part of the state-vector variation with time is removed. Correspondingly, operators in the interaction picture are given by

$$O^I(t) \equiv e^{iH_0^S t/\hbar}\, O^S(t)\, e^{-iH_0^S t/\hbar}\,. \tag{1.17}$$

In particular, $H_0^I = H_0^S$ but $H^I(t) \neq H^S$, because $V^I_{\rm int}(t) \neq V^S_{\rm int}$. They satisfy the equation

$$\frac{d}{dt}\,O^I(t) = \frac{i}{\hbar}\left[H_0^S,\, O^I(t)\right] + \left(\frac{\partial O}{\partial t}\right)_I(t)\,, \tag{1.18}$$

where $\left(\partial O/\partial t\right)_I(t)$ is the abbreviation for

$$e^{iH_0^S t/\hbar}\,\frac{\partial O^S}{\partial t}\,e^{-iH_0^S t/\hbar}\,.$$

Obviously, if $V^S_{\rm int} \equiv 0$, the interaction picture coincides with the Heisenberg one.

The interaction picture state-vectors evolve in time according to the equation

$$i\hbar\,\frac{d}{dt}|\Psi(t)\rangle_I = V^I_{\rm int}(t)|\Psi(t)\rangle_I\,, \tag{1.19}$$

which follows immediately by differentiating the definition (1.16) with respect to time and using the fact that

$$-H_0^S + e^{iH_0^S t/\hbar}\,H^S e^{-iH_0^S t/\hbar} = e^{iH_0^S t/\hbar}\,V^S_{\rm int}\,e^{-iH_0^S t/\hbar} \equiv V^I_{\rm int}(t)\,. \tag{1.20}$$

Since from the mathematical point of view the equation (1.19) has the same structure as (1.1) with the (possibly time-dependent) Hamiltonian H^S replaced by $V^I_{\rm int}(t)$, its solution must be given by

$$|\Psi(t)\rangle_I = U_I(t,t_0)|\Psi(t_0)\rangle_I\,, \tag{1.21}$$

with the interaction picture operator $U_I(t,t_0)$ satisfying the composition rules analogous to (1.4) and the differential equation analogous to (1.3) with the operator $V^I_{\rm int}(t)$ replacing $H^S(t)$ and with the initial condition $U_I(t_0,t_0) = \hat{1}$. The iterative solution of this equation is given by the series

$$U_I(t_2,t_1) = \hat{1} + \frac{1}{i\hbar}\int_{t_1}^{t_2} dt'\,V^I_{\rm int}(t') + \left(\frac{1}{i\hbar}\right)^2\int_{t_1}^{t_2}dt'\int_{t_1}^{t'}dt''\,V^I_{\rm int}(t')V^I_{\rm int}(t'') + \ldots \tag{1.22}$$

and can also be cast in the form

$$U_I(t_2,t_1) = \mathrm{T}\exp\left(-\frac{i}{\hbar}\int_{t_1}^{t_2} dt'\, V_{\mathrm{int}}^I(t')\right). \tag{1.23}$$

The iterative form (1.22) of $U_I(t_2,t_1)$, written down in the basis of H_0 eigenvectors, turns out to be simply equivalent to the standard time dependent perturbative expansion (recalled in Chapter 2). The form (1.23), instead, will lead to the Dyson expansion and Feynman diagrams. Applied to relativistic theories it will allow, unlike the expansion (1.22), to formulate the perturbative expansion in such a way that relativistic covariance of computed amplitudes is kept at every step as manifest as possible.

Finally it is not difficult to see that the two evolution operators: $U(t_2,t_1)$ given by (1.9) and $U_I(t_2,t_1)$ introduced here, are related by

$$U_I(t_2,t_1) = e^{iH_0^S t_2/\hbar}\, U(t_2,t_1)\, e^{-iH_0^S t_1/\hbar}. \tag{1.24}$$

Generalizing the definition (1.17) to operators depending on two time variables, one can view $U_I(t_2,t_1)$ as the evolution operator (1.9) transformed to the interaction picture.

1.2 The Gell-Mann - Low theorem

In many cases the ground-state vector $|\Omega_0\rangle$, i.e. the normalized lowest energy eigenvector of the free Hamiltonian H_0 is known[4] and one wants to have an explicit (even if formal) expression for the lowest energy eigenvector (proportional to the normalized ground-state vector $|\Omega\rangle$) of the time-independent Hamiltonian[5] $H = H_0 + V_{\mathrm{int}}$. Such an expression can be obtained by using the construction given by M. Gell-Mann and F. Low. Its essential technical element is the formula for the commutator of the free Hamiltonian H_0 with the interaction picture evolution operator $U_I^\varepsilon(0,-\infty)$ (or the $U_I^\varepsilon(0,+\infty)$ operator) corresponding to the modification of the original problem by giving the (Schrödinger picture) interaction operator V_{int} the explicit time dependence:

$$V_{\mathrm{int}} \longrightarrow V_{\mathrm{int}}(t) = e^{\varepsilon t}\, V_{\mathrm{int}}\,, \tag{1.25}$$

with $\varepsilon > 0$ ($\varepsilon < 0$). In the limit $\varepsilon \to 0^+$ ($\varepsilon \to 0^-$) the interaction is then switched on (off) "adiabatically", that is infinitely slowly. While the original interaction is certainly recovered in the limit $\varepsilon \to 0^+$ (0^-), it is to be noted that even with $\varepsilon \neq 0$ the time dependent Hamiltonian $H(t) = H_0 + V_{\mathrm{int}}(t)$ is at $t = 0$ just the original H. Correspondingly to this property of $H(t)$ one takes $t_0 = 0$ as the instant at which state-vectors of the (fictitious) system with the Hamiltonian $H(t) = H_0 + V_{\mathrm{int}}(t)$ in the three pictures

[4]Some Hamiltonians, like e.g. the one of quantum mechanics of a single free particle, $H = \hat{\mathbf{P}}^2/2M$, do not posses, however, normalizable eigenvectors.

[5]From now on we drop the superscript S from the Schrödinger picture operators.

introduced in Section 1.1 coincide. The interaction picture evolution operator $U_I^\varepsilon(t_2, t_1)$ corresponding to the modified interaction is given (cf. the formulae (1.23) and (1.20)) by

$$U_I^\varepsilon(t_2,\, t_1) = \mathrm{T}\exp\left(-\frac{i}{\hbar}\int_{t_1}^{t_2} d\tau\, e^{\varepsilon\tau}\, V_{\mathrm{int}}^I(\tau)\right), \tag{1.26}$$

with

$$V_{\mathrm{int}}^I(\tau) = e^{iH_0\tau/\hbar}\, V_{\mathrm{int}}\, e^{-iH_0\tau/\hbar}. \tag{1.27}$$

Although the commutator in question can be found without resorting to the perturbative expansion (see Appendix A), it will be computed here by using this technique because this will show how one can deal in practice with the chronological ordering of operators. In this approach the commutator $[H_0,\, U_I^\varepsilon(0, -\infty)]$ is given by (the commutator $[H_0,\, U_I^\varepsilon(0, +\infty)]$ with $\varepsilon < 0$ can be worked out analogously)

$$\sum_{n=1}^{\infty} \frac{(-i/\hbar)^n}{n!} \int_{-\infty}^{0} d\tau_1 \ldots \int_{-\infty}^{0} d\tau_n\, e^{\varepsilon(\tau_1+\ldots+\tau_n)} \left[H_0,\, \mathrm{T}\big(V_{\mathrm{int}}^I(\tau_1)\ldots V_{\mathrm{int}}^I(\tau_n)\big)\right].$$

The symbol T of the time ordering means that the domain of the integration should be split into $n!$ sub-domains in which the ordering of the time variables τ_i and, therefore, the ordering of the operators $V_{\mathrm{int}}^I(\tau_i)$ is fixed. Alternatively, $\mathrm{T}\big(V_{\mathrm{int}}^I(\tau_1)\ldots V_{\mathrm{int}}^I(\tau_n)\big)$ can be represented as the sum over $n!$ permutations P of terms of the form (cf. the formula (1.8))

$$\theta(\tau_{P(1)} - \tau_{P(2)})\, \theta(\tau_{P(2)} - \tau_{P(3)}) \ldots \theta(\tau_{P(n-1)} - \tau_{P(n)})\, V_{\mathrm{int}}^I(\tau_{P(1)}) \ldots V_{\mathrm{int}}^I(\tau_{P(n)}).$$

In each of these terms the commutator yields the sum of n terms

$$\begin{aligned}\left[H_0,\, V_{\mathrm{int}}^I(\tau_{P(1)})\ldots V_{\mathrm{int}}^I(\tau_{P(n)})\right] &= \left[H_0,\, V_{\mathrm{int}}^I(\tau_{P(1)})\right] V_{\mathrm{int}}^I(\tau_{P(2)})\ldots V_{\mathrm{int}}^I(\tau_{P(n)}) \\ &\quad + V_{\mathrm{int}}^I(\tau_{P(1)})\left[H_0,\, V_{\mathrm{int}}^I(\tau_{P(2)})\right]\ldots V_{\mathrm{int}}^I(\tau_{P(n)}) + \ldots\end{aligned}$$

Since the operator $V_{\mathrm{int}}^I(\tau)$ defined in (1.27) satisfies the equation

$$\frac{\hbar}{i}\frac{d}{d\tau} V_{\mathrm{int}}^I(\tau) = [H_0,\, V_{\mathrm{int}}^I(\tau)],$$

the commutator $[H_0,\, V_{\mathrm{int}}^I(\tau_{P(1)})\ldots V_{\mathrm{int}}^I(\tau_{P(n)})]$ can be written in the form

$$\frac{\hbar}{i}\left(\sum_{i=1}^{n}\frac{d}{d\tau_{P(i)}}\right) V_{\mathrm{int}}^I(\tau_{P(1)})\ldots V_{\mathrm{int}}^I(\tau_{P(n)}).$$

The crucial point is now that[6]

$$\left(\sum_{i=1}^{n}\frac{d}{d\tau_{P(i)}}\right)\theta(\tau_{P(1)} - \tau_{P(2)})\theta(\tau_{P(2)} - \tau_{P(3)})\ldots\theta(\tau_{P(n-1)} - \tau_{P(n)}) = 0.$$

[6]Recall that $d\theta(t-t')/dt = \delta(t-t')$ and that $\delta(t-t') = \delta(t'-t)$. Of course

$$\sum_{i=1}^{n}\frac{d}{d\tau_{P(i)}} = \sum_{i=1}^{n}\frac{d}{d\tau_i}.$$

Therefore, the sum of time derivatives can be placed in front of the symbol T of the chronological ordering. Next, because the resulting expression

$$\sum_{n=1}^{\infty} \frac{(-i/\hbar)^n}{n!} \frac{\hbar}{i} \int_{-\infty}^{0} d\tau_1 \ldots \int_{-\infty}^{0} d\tau_n \, e^{\varepsilon(\tau_1+\ldots+\tau_n)} \left(\sum_{i=1}^{n} \frac{d}{d\tau_i} \right) \mathrm{T}\big(V_{\mathrm{int}}^I(\tau_1) \ldots V_{\mathrm{int}}^I(\tau_n)\big) \,,$$

is completely symmetric in its n time variables τ_i (the operators $V_{\mathrm{int}}^I(\tau_i)$ under the chronological product commute), the sum of n time derivatives can be replaced by $n\, d/d\tau_n$. The integral over $d\tau_n$ can be then taken by parts. This gives

$$\begin{aligned} &-\sum_{n=1}^{\infty} \frac{(-i/\hbar)^{n-1}}{(n-1)!} \int_{-\infty}^{0} d\tau_1 \ldots \int_{-\infty}^{0} d\tau_{n-1} \, e^{\varepsilon(\tau_1+\ldots+\tau_{n-1})} \big[e^{\varepsilon\tau_n} \mathrm{T}\big(V_{\mathrm{int}}^I(\tau_1) \ldots V_{\mathrm{int}}^I(\tau_n)\big) \big]_{-\infty}^{0} \\ &\quad + \varepsilon \sum_{n=1}^{\infty} \frac{(-i/\hbar)^{n-1}}{(n-1)!} \int_{-\infty}^{0} d\tau_1 \ldots \int_{-\infty}^{0} d\tau_n \, e^{\varepsilon(\tau_1+\ldots+\tau_n)} \, \mathrm{T}\big(V_{\mathrm{int}}^I(\tau_1) \ldots V_{\mathrm{int}}^I(\tau_n)\big) \,. \end{aligned}$$

In the first term, owing to the factor $e^{\varepsilon\tau_n}$, the lower limit $\tau_n = -\infty$ gives zero, while in the upper limit, $\tau_n = 0$, because $0 \geq \max(\tau_1, \ldots, \tau_{n-1})$, the operator $V_{\mathrm{int}}^I(0) \equiv V_{\mathrm{int}}$ can be taken out of the chronological ordering and placed in front of the remaining multiple integral. In the second term one can use the trick (we assume that the interaction operator V_{int} is proportional to some real coupling constant λ which at the end can be set equal 1)

$$\frac{(-i/\hbar)^{n-1}}{(n-1)!} \lambda^n = i\hbar\, \lambda \frac{\partial}{\partial\lambda} \frac{(-i/\hbar)^n}{n!} \lambda^n \,.$$

In this way one arrives at the final result[7]

$$[H_0,\, U_I^{\varepsilon}(0,-\infty)] = -V_{\mathrm{int}}\, U_I^{\varepsilon}(0,-\infty) + i\hbar\,\varepsilon\,\lambda \frac{\partial}{\partial\lambda} U_I^{\varepsilon}(0,-\infty) \,, \tag{1.28}$$

which equivalently can be written in the form

$$H U_I^{\varepsilon}(0,-\infty) = U_I^{\varepsilon}(0,-\infty) H_0 + i\hbar\,\varepsilon\,\lambda \frac{\partial}{\partial\lambda} U_I^{\varepsilon}(0,-\infty) \,, \tag{1.29}$$

with the original Hamiltonian $H = H_0 + V_{\mathrm{int}}$ on the left hand side.

This formal result can be used in various ways. One possible application is the construction of the normalizable lowest energy (denoted E_Ω) eigenvector (proportional to the normalized to unity ground-state vector $|\Omega\rangle$) of the time independent Hamiltonian $H = H_0 + V_{\mathrm{int}}$ in terms of the (normalized) ground-state vector $|\Omega_0\rangle$ of H_0. To this end, following Gell-Mann and Low, one considers the time evolution generated by $U_I^{\varepsilon}(t_2, t_1)$ given by (1.26) of the particular interaction picture state-vector $|\Psi^{\varepsilon}(t)\rangle_I$ which in the

[7]The result in this form is also valid with $U_I^{\varepsilon}(0,+\infty)$ replacing $U_I^{\varepsilon}(0,-\infty)$ provided ε is assumed to be negative.

infinite past, i.e. at $t = -\infty$, is the normalized H_0 eigenvector $|\Omega_0\rangle$ corresponding to its lowest eigenvalue E_{Ω_0}:

$$|\Psi^\varepsilon(t)\rangle_I = U_I^\varepsilon(t,-\infty)|\Psi^\varepsilon(-\infty)\rangle_I = U_I^\varepsilon(t,-\infty)|\Omega_0\rangle\,. \tag{1.30}$$

The Gell-Mann - Low theorem states that *if* the vector

$$\frac{|\Psi^\varepsilon(0)\rangle_I}{\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I} \equiv \frac{U_I^\varepsilon(0,-\infty)|\Omega_0\rangle}{\langle\Omega_0|U_I^\varepsilon(0,-\infty)|\Omega_0\rangle}\,, \tag{1.31}$$

is well defined in the limit $\varepsilon \to 0^+$, it is in this limit an eigenvector of the original (time-independent) Hamiltonian $H = H_0 + V_{\rm int}$. This can be understood in the following way. In general, the instantaneous spectrum of the modified Hamiltonian $H(t) = H_0 + e^{\varepsilon t}V_{\rm int}$ changes with time. If a discrete eigenvalue of $H(t)$, as the time flows from $-\infty$ to 0, does not become degenerate nor crosses with any of the other $H(t)$ energy levels (including the levels belonging to the continuous part of the $H(t)$ spectrum), the changes of the corresponding instantaneous normalizable eigenvector can be (in most cases - see the comments below) traced unambiguously and the discrete eigenvector of $H(-\infty) = H_0$ has its unique $t = 0$ counterpart which is the eigenvector of $H(0) = H$. Under these assumptions the adiabatic theorem (Section 2.4) ensures that if $|\Omega_0\rangle$ is the normalized ground-state[8] of $H(-\infty) = H_0$, the vector $|\Psi^\varepsilon(0)\rangle_I$ should be in the "adiabatic" limit[9] $\varepsilon \to 0^+$ proportional to the normalized ground-state vector $|\Omega\rangle$ of $H(0) = H$. If these requirements are fulfilled, applying the equality (1.29) to the vector $|\Omega_0\rangle$ one gets (the limit $\varepsilon \to 0^+$ is understood)

$$(H - E_{\Omega_0})|\Psi^\varepsilon(0)\rangle_I = i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}|\Psi^\varepsilon(0)\rangle_I\,. \tag{1.32}$$

Closing this relation from the left with $\langle\Omega_0|/\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I$, remembering that $|\Omega_0\rangle$, being an eigenvector of H_0, does not depend on λ, we get the relation

$$\frac{\langle\Omega_0|V_{\rm int}|\Psi^\varepsilon(0)\rangle_I}{\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I} = i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\ln\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I\,. \tag{1.33}$$

If the limit $\varepsilon \to 0^+$ of $|\Psi^\varepsilon(0)\rangle_I$ existed, the result (1.32) would imply that this limit is an eigenvector of H with the eigenvalue E_{Ω_0}, the same as the energy of the ground-state of

[8]It should be clear that if $|\phi_0\rangle$ is any discrete eigenvector of H_0 which has its counterpart $|\phi\rangle$ in the H spectrum, one could replace in the Gell-Mann - Low construction $|\Omega_0\rangle$ by $|\phi_0\rangle$ to construct a H eigenvector proportional to $|\phi\rangle$. The formula (1.34) would then give the difference $E_\phi - E_{\phi_0}$ of the respective energies of these discrete levels. The main reason for concentrating in the Gell-Mann - Low construction on the ground-state eigenvectors of H_0 and H is that in quantum field theory formulated in the continuum $|\Omega_0\rangle$ and $|\Omega\rangle$ are assumed to be the only (in the selected Fock space - this will become more clear in due course) normalizable eigenvectors of H_0 and of H, respectively.

[9]If $\varepsilon \neq 0$, the time evolution of $|\Omega_0\rangle$, that is application to $|\Omega_0\rangle$ of the evolution operator $U_I^\varepsilon(t,-\infty)$, takes this vector in general (as indicates the presence of the second term in the right hand side of the relation (1.29)) into a complicated superposition of instantaneous eigenvectors of $H_0 + e^{\varepsilon t}V_{\rm int}$.

H_0. Unless $V_{\rm int}$ is judiciously adjusted (as will be done in the formulation of quantum field theory based on the relativistic quantum mechanics of particles developed in Chapters 7, 8 and 9) this is impossible. Therefore, the limit $\varepsilon \to 0^+$ of $|\Psi^\varepsilon(0)\rangle_I$ must in general be singular (in Section 1.3 it will be shown on a simple example that the phase of the vector $|\Psi^\varepsilon(0)\rangle_I$ diverges as $1/\varepsilon$). However, it is easy to check that for $\varepsilon \neq 0$ the equality (1.32) is equivalent to

$$\left(H - E_{\Omega_0} - i\hbar\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\ln\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I\right)\frac{|\Psi^\varepsilon(0)\rangle_I}{\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I} = i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,\frac{|\Psi^\varepsilon(0)\rangle_I}{\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I}\,.$$

From this formula one concludes that if the vector $|\Psi^\varepsilon(0)\rangle_I/\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I$ does have the $\varepsilon \to 0^+$ limit (that is, the right-hand side of this formula vanishes when $\varepsilon \to 0^+$), this limit is the eigenvector of the full Hamiltonian $H = H_0 + V_{\rm int}$ and, moreover,

$$\lim_{\varepsilon\to 0}\left[i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\ln\langle\Omega_0|U_I^\varepsilon(0,-\infty)|\Omega_0\rangle\right] = E_\Omega - E_{\Omega_0}\,. \tag{1.34}$$

It should be clear that the same construction of the lowest energy H eigenvector can be repeated taking in (1.25) $\varepsilon < 0$ and considering the time evolution of the (interaction picture) state-vector which becomes $|\Omega_0\rangle$ in the far future, that is at $t = +\infty$. One then gets that the $\varepsilon \to 0^-$ limit of

$$\frac{U_I^\varepsilon(0,+\infty)|\Omega_0\rangle}{\langle\Omega_0|U_I^\varepsilon(0,+\infty)|\Omega_0\rangle}\,, \tag{1.35}$$

if it exists, is the eigenvector of $H = H_0 + V_{\rm int}$. Since the scalar products of the vectors (1.31) and (1.35) with $|\Omega_0\rangle$ are both equal 1, they must be the same vector (including the phase).[10]

It is perhaps worth stressing that the construction given here is merely a mathematical trick and in no way entails unphysical switching on and off interactions of the considered physical system the true Hamiltonian of which is $H = H_0 + V_{\rm int}$ (and not $H(t) = H_0 + e^{\varepsilon t}V_{\rm int}$). Let us also remark that an eigenvector of H proportional to the normalized H ground-state vector $|\Omega\rangle$ could be also constructed by using the ordinary Rayleigh-Schrödinger stationary perturbative expansion. The resulting formula would, however, have a form less convenient from the point of view of formulating the Dyson expansion (formulated in Section 5.8).

The general result (1.29), which is a formal operator relation, can be also applied to generalized (non-normalizable) eigenvectors of H_0. For example, in the nonrelativistic scattering theory the free Hamiltonian H_0 has no normalizable eigenvectors and the operators $U_I^\varepsilon(0,\mp\infty)$ become in the limits $\varepsilon \to 0^\pm$ the so-called Møller operators $\Omega_\pm$ which will be introduced in Section 7.1. In this case matrix elements of the term proportional

[10]Notice that the vectors (1.31) and (1.35) are not normalized to unity.

to ε on the right-hand side of (1.29) between (normalizable) vectors of any arbitrarily chosen basis of the proper Hilbert space all vanish, which means that this term should be treated just as the zero operator. The left-hand side of (1.29) becomes then the operator intertwining relation $H\Omega_{\pm} = \Omega_{\pm}H_0$ playing an important role in the formal scattering theory (outlined in Chapter 7).

In the relativistic theory of interacting particles presented in Chapters 7, 8 and 9, which can be treated as a formulation (though not the most convenient one) of the relativistic quantum field theory, the term explicitly proportional to ε on the right-hand side of (1.29) vanishes owing to the already mentioned tuning of $V_{\rm int}$, which is necessary to fulfill the assumptions on which this formulation is based (see Chapter 7). In the limit $\varepsilon \to 0^{\pm}$ the operators $U_I^{\varepsilon}(0, \mp\infty)$ become then again the Møller operators satisfying the intertwining relation $H\Omega_{\pm} = \Omega_{\pm}H_0$. When applied to generalized (non-normalizable) eigenvectors of H_0 the Møller operators yield then the corresponding (in the sense which will be explained in Chapter 7) *in* and *out* generalized eigenvectors of H, whereas when applied to the single normalized eigenvector $|\Omega_0\rangle$ of H_0 (its normalized to unity ground-state) they yield a normalizable eigenvector of H proportional to the single (up to a phase factor), normalized to unity lowest energy eigenvector $|\Omega\rangle$ of H.

Finally, in the approach to nonrelativistic quantum mechanics of many particles based on Green's functions and in relativistic quantum field theory formulated (in the infinite space) as in Chapter 13 (without the restrictive assumptions of Chapter 7) it is usually assumed that the operators $U_I^{\varepsilon}(0, \mp\infty)$ acting on the single normalized to unity H_0 eigenvector $|\Omega_0\rangle$ produce a vector proportional to the single normalized to unity H eigenvector $|\Omega\rangle$ and the formulae (1.34), or (1.36) given below give the nonzero difference of the respective ground-state energies.[11] The Gell-Mann - Low theorem constitutes in this case the cornerstone of the Dyson perturbative expansion discussed in Section 5.8 of Green's functions which are, in some sense, the most important quantities of theoretical interest (see Section 5.7 and Chapter 13). The situation can however in these cases be more complicated. As mentioned, the presented construction of the H eigenvectors out of the H_0 eigenvectors requires that the relevant parts of the spectra (the ground-states) of these two Hamiltonians are continuously and uniquely related to one another. In particular this means that switching on the interaction (by a continuous change of a parameter of $V_{\rm int}$ such as $e^{\varepsilon t}$) must cause a continuous transition of the ground-state of H_0 into a unique ground-state of H. Direct application of the Gell-Mann - Low construction of the lowest energy eigenvector of H must therefore necessarily fail when the interaction term $V_{\rm int}$ induces the phenomenon of (dynamical) symmetry breaking resulting in the energy spectrum which typically has lower symmetry than it would follow[12] from the symmetry

[11] In relativistic field theories E_{Ω_0} is an ill defined quantity (usually set to zero by definition) but in nonrelativistic theories formulated in the infinite space well defined is the energy density E_{Ω_0}/V and formulae (1.34), (1.36) give then the correction due to the interaction to the ground-state energy density.

[12] Symmetries in general and their consequences for the spectrum of the Hamiltonian, when their dynamical breaking does not take place, will be discussed in Chapter 4. Breaking of symmetries in relativistic theories will be dealt with in Chapter 22.

of H (and H_0). Such a dynamical symmetry breaking cannot happen in ordinary quantum mechanics (of systems with a finite number of degrees of freedom) but is a typical phenomenon in systems having infinitely many degrees of freedom, like the systems of many interacting nonrelativistic particles studied in the limit $N \to \infty$, $V \to \infty$ (N is the number of particles and V the space volume occupied by them) with the ratio N/V kept fixed or in relativistic field theory models (the Hamiltonians of which, as will become clear in Chapters 7, 8 and 9, cannot preserve the number of particles) considered in the infinite space volume. In these cases the Hamiltonian H of the interacting system has degenerate ground-states (their number can be finite or countably or even uncountably infinite) and in the limit of infinite volume the nonseparable Hilbert space of the system splits into completely disconnected separable subspaces (matrix elements of local operators between vectors belonging to different subspaces all vanish) built on each of the degenerate ground-states of H. In such cases the Gell-Mann - Low construction can be employed either if it is possible to introduce into the Hamiltonian a small symmetry breaking interaction (removed at the end) which artificially breaks the degeneracy of the H ground-states or by starting from another free Hamiltonian (and therefore from another vector $|\Omega_0\rangle$) which can be singled out from H after an appropriate canonical transformation of the variables representing the system's degrees of freedom which implements the effects of symmetry breaking. The required transformation can be done at the operator level (it is then a sort of the Bogolyubov transformation analogous to the one employed in Section 5.5) but, if the symmetry breaking is manifested by a nonzero H ground-state expectation value of an elementary operator, it is usually much more easy to realize it in the approach based on field quantization (see Section 11.2), particularly when the quantization is done using the path integral approach (discussed in Chapter 16) in which case such a change becomes an ordinary (functional) change of integration variables.

Combining (1.34) with the relation (1.33) one obtains the formula

$$E_\Omega - E_{\Omega_0} = \frac{\langle\Omega_0|V_{\rm int}|\Psi^\varepsilon(0)\rangle_I}{\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I} \equiv \frac{\langle\Omega_0|V_{\rm int}U_I^\varepsilon(0,-\infty)|\Omega_0\rangle}{\langle\Omega_0|U_I^\varepsilon(0,-\infty)|\Omega_0\rangle}\,. \tag{1.36}$$

The formulae: (1.34), its more symmetric form, called the Sucher formula,

$$E_\Omega - E_{\Omega_0} = \frac{1}{2}\, i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\ln\langle\Omega_0|S_0^\varepsilon|\Omega_0\rangle\,, \tag{1.37}$$

in which $S_0^\varepsilon = U_I^{-\varepsilon}(\infty,0)U_I^\varepsilon(0,-\infty) = [U_I^{-\varepsilon}(0,\infty)]^\dagger U_I^\varepsilon(0,-\infty)$ and the expression (1.36) provide the practical ways (alternative to the Rayleigh - Schrödinger expansion) of computing the shift of the ground-state energy due to the interaction $V_{\rm int}$. In all of them the limit $\varepsilon \to 0^+$ is implicitly taken *after* the time argument(s) of the evolution operators are sent to (minus) infinity.

Yet another way of computing this energy shift is obtained by considering the matrix element $\langle\Omega_0|U_I^{-\varepsilon}(T,0)U_I^\varepsilon(0,-T)|\Omega_0\rangle$ and taking the limit $\varepsilon \to 0^+$ *before* the time arguments of the evolution operators are sent to infinity. Using the composition rule and the

formula (1.23) one then gets for the energy shift the formula

$$\lim_{T\to\infty}\langle\Omega_0|\mathrm{T}\exp\left\{-\frac{i}{\hbar}\int_{-T}^{T}dt\,V_{\rm int}^{I}(t)\right\}|\Omega_0\rangle=\exp\left\{-i\frac{2T}{\hbar}\left(E_\Omega-E_{\Omega_0}\right)\right\}. \tag{1.38}$$

The most straightforward justification of this formula is provided by the appropriate analytic continuation of the expression for the Canonical Ensemble statistical sum (partition function) of the considered system. While the formula (1.36) leads to the perturbative expansion of the energy shift $E_\Omega - E_{\Omega_0}$ in terms of the so called Goldstone diagrams, the last approach provides the energy shift expansion in terms of the standard Feynman diagrams (to be introduced in due course), called in this context the Hugenholtz diagrams.

Of course all these ways of computing the shift (due to the interaction $V_{\rm int}$) of the ground state energy require that $|\Omega\rangle$ is adiabatically connected to $|\Omega+0\rangle$.

1.3 An example: perturbed harmonic oscillator

As a simple illustration of the use of the Heisenberg equation of motion (1.15) and of the working of the Gell-Mann - Low prescription we consider here the one-dimensional harmonic oscillator of mass M and frequency ω perturbed with a time dependent interaction of a special form. The virtue of the considered example is that it is exactly solvable and as such can serve as the testing ground for the Gell-Mann - Low prescription and other approximate methods described in the next chapter. It will also serve to introduce the notion of the *in* and *out* states and of the S-matrix.

The Hamiltonian to be considered has the form $H = H_0 + V_{\rm int}(t)$ with ($\Delta_\omega = \hbar\omega/2$)

$$\begin{aligned} H_0 &= \hbar\omega a^\dagger a + \Delta_\omega\,,\\ V_{\rm int}(t) &= a^\dagger f(t) + a f^*(t)\,. \end{aligned} \tag{1.39}$$

The annihilation and creation operators are as usually defined as

$$a=\sqrt{\frac{M\omega}{2\hbar}}\left(x+\frac{i}{M\omega}\,p\right),\qquad a^\dagger=\sqrt{\frac{M\omega}{2\hbar}}\left(x-\frac{i}{M\omega}\,p\right), \tag{1.40}$$

and satisfy the commutation rules

$$[a,\,a^\dagger]=\hat{1}\,,\qquad [a,\,a]=[a^\dagger,\,a^\dagger]=0\,, \tag{1.41}$$

which follow from the standard commutation rule $[\hat{x},\,\hat{p}] = i\hbar$. $f(t)$ is some c-number function which can be complex. If

$$f(t)=f^*(t)=-\sqrt{\frac{\hbar}{2M\omega}}\,F(t)\,,$$

(1.39) is just the Hamiltonian $H = H_0 - xF(t)$ of the one-dimensional harmonic oscillator subjected to the action of the constant in space, but time-dependent external force $F(t)$. With $f(t) = e^{\varepsilon t}\lambda$ the model can serve to test the Gell-Mann - Low formula (1.34) for the ground-state energy of the time independent Hamiltonian

$$H = \hbar\omega a^\dagger a + \Delta_\omega + \lambda\, a^\dagger + \lambda^* a = \hbar\omega A^\dagger A + \Delta_\omega - \frac{|\lambda|^2}{\hbar\omega}\,, \tag{1.42}$$

where $A = a + b$, $A^\dagger = a^\dagger + b^*$ with $b = \lambda/\hbar\omega$, $b^* = \lambda^*/\hbar\omega$. Since the operators A and $A^\dagger$ satisfy the same commutation rules as do a and $a^\dagger$, one can use the standard algebraic argument[13] to infer that in the Hilbert space there must be a vector $|\tilde{0}\rangle$ annihilated by A and that the vectors $(A^\dagger)^n|\tilde{0}\rangle$ are the eigenvectors of $A^\dagger A$ with the eigenvalues equal n. The entire spectrum of H given by (1.42) is, therefore, simply shifted downwards, with respect to the spectrum of H_0, by $|\lambda|^2/\hbar\omega$. In particular, $E_\Omega = E_{\Omega_0} - |\lambda|^2/\hbar\omega$. We will now see how this can be recovered using the Gell-Mann - Low theorem.

In the Heisenberg picture one works with time dependent operators while state-vectors do not depend on time (Section 1.1). Since all operators can be constructed out of the annihilation and creation operators, it is sufficient to find $a_H(t)$ and $a_H^\dagger(t)$. They satisfy the equation (1.15):

$$\dot{a}_H(t) = \frac{i}{\hbar}\,[H^H(t),\, a_H(t)], \qquad \dot{a}_H^\dagger(t) = \frac{i}{\hbar}\,[H^H(t),\, a_H^\dagger(t)],$$

with $H^H(t)$ constructed in agreement with the prescription (1.12). The commutators can be easily evaluated:

$$\begin{aligned}[H^H(t),\, a_H(t)] &= U^\dagger(t,0)\,[H,\, a]\,U(t,0) \\ &= U^\dagger(t,0)\,[-\hbar\omega\, a - f(t)]\,U(t,0) = -\hbar\omega\, a_H(t) - f(t)\,.\end{aligned}$$

We have assumed that the corresponding Heisenberg and Schrödinger pictures operators coincide at $t_0 = 0$. The equation of motion of $a_H(t)$ therefore is

$$\dot{a}_H(t) = -i\omega\, a_H(t) - \frac{i}{\hbar}\, f(t)\,. \tag{1.43}$$

The equation satisfied by $a_H^\dagger(t)$ is just the Hermitian conjugate of this one. The solutions of the homogeneous part of this equation is obvious:

$$a_H(t) = e^{-i\omega t}\, a_H(0) \equiv e^{-i\omega t}\, a\,.$$

[13] Let $|\alpha\rangle$ be a normalized to unity eigenvector of the operator $A^\dagger A$ corresponding to its (real because of the Hermiticity of $A^\dagger A$) eigenvalue α. The equality $\alpha = \langle\alpha|A^\dagger A|\alpha\rangle \equiv \|A|\alpha\rangle\|^2$ shows that $\alpha \geq 0$. From the commutation rule $[A^\dagger A,\, A] = -A$, (from $[A^\dagger A,\, A^\dagger] = A^\dagger$) it readily follows that $A^n|\alpha\rangle$ (that $(A^\dagger)^n|\alpha\rangle$) is the eigenvector of $A^\dagger A$ having the eigenvalue $\alpha - n$ (the eigenvalue $\alpha + n$). Since the eigenvalues of $A^\dagger A$ have just been shown to be nonnegative, this means that that $A^{n+1}|\alpha\rangle = 0$ for some integer n. Denoting $|\alpha - n\rangle$ the normalized to unity vector $A^n|\alpha\rangle/\|A^n|\alpha\rangle\|$, one learns from the equality $\alpha - n = \langle\alpha - n|A^\dagger A|\alpha - n\rangle = 0$ that the eigenvalues of $A^\dagger A$ are (nonnegative) integer numbers. Renaming then $|\alpha - n\rangle$ to $|\tilde{0}\rangle$ one gets that the vectors $(A^\dagger)^n|\tilde{0}\rangle/\sqrt{n!}$ are the normalized to unity eigenvectors of $A^\dagger A$ with the eigenvalues n.

In order to find a solution of the full inhomogeneous equation (1.43) we substitute in it $d(t)\exp(-i\omega t)$ for $a_H(t)$. This leads to the c-number equation

$$\dot{d}(t) = -\frac{i}{\hbar}\, e^{i\omega t}\, f(t)\,.$$

Thus

$$\begin{aligned} a_H(t) &= e^{-i\omega t}\left(a - \frac{i}{\hbar}\int_0^t d\tau\, e^{i\omega\tau} f(\tau)\right) \equiv e^{-i\omega t}\,(a + h(t))\,, \\ a_H^\dagger(t) &= e^{i\omega t}\left(a^\dagger + \frac{i}{\hbar}\int_0^t d\tau\, e^{-i\omega\tau} f^*(\tau)\right) \equiv e^{i\omega t}\left(a^\dagger + h^*(t)\right). \end{aligned} \tag{1.44}$$

The lower limit of the integrals has been set to zero to secure the equalities $a_H(0) = a$, $a_H^\dagger(0) = a^\dagger$.

The simple exact form of $a_H(t)$ and $a_H^\dagger(t)$ allows to easily find an operator $\tilde{U}(t,0)$ such that

$$a_H(t) = \tilde{U}^\dagger(t,0)\, a\, \tilde{U}(t,0)\,, \qquad a_H^\dagger(t) = \tilde{U}^\dagger(t,0)\, a^\dagger\, \tilde{U}(t,0)\,. \tag{1.45}$$

It is easy to see that as $\tilde{U}(t,0)$ one can take

$$\tilde{U}(t,0) = e^{-iH_0 t/\hbar}\, e^{h(t)a^\dagger - h^*(t)a}\,. \tag{1.46}$$

This can be checked by applying twice the operator formula

$$\begin{aligned} e^B A\, e^{-B} &= A + [B,\, A] + \frac{1}{2!}[B,\, [B,\, A]] + \ldots \\ &= A - [A,\, B] + \frac{1}{2!}[[A,\, B],\, B] + \ldots \end{aligned} \tag{1.47}$$

first to find that

$$e^{iH_0 t/\hbar}\, a\, e^{-iH_0 t/\hbar} = e^{-i\omega t}\, a\,, \qquad e^{iH_0 t/\hbar}\, a^\dagger\, e^{-iH_0 t/\hbar} = e^{i\omega t}\, a^\dagger,$$

and next to check that the second exponential factor in (1.46) generates the required shifts of a and $a^\dagger$. Note that the relations (1.45) determine $\tilde{U}(t,0)$ only up to a c-number, possibly time-dependent, phase factor. As a result it may differ by such a factor from the true evolution operator $U(t,0)$, which is uniquely determined by the differential equation (1.3) and the initial condition $U(0,0) = \hat{1}$.

One can now test the Gell-Mann - Low prescription by setting $f(t) = e^{\varepsilon t}\lambda$. The interaction picture evolution operator $U_I(t,0)$, which can be obtained from $U(t,0)$ with the help of the formula (1.24), has in this case the interpretation of the operator $U_I^\varepsilon(t,0)$ corresponding in the limit $\varepsilon \to 0^+$ to the adiabatic switching on the interaction $V_{\rm int} = \lambda^* a + \lambda\, a^\dagger$. If $\tilde{U}(t,0)$ given by (1.46) were the true evolution operator $U(t,0)$, the operator

$$\tilde{U}_I^\varepsilon(t,0) = e^{h(t)a^\dagger - h^*(t)a}\,, \tag{1.48}$$

with $h(t)$ given by (1.44) and $f(t) = e^{\varepsilon t}\lambda$ would be the interaction picture evolution operator $U_I^\varepsilon(t,0)$ (which is also uniquely determined by the corresponding differential equation and the initial condition $U_I^\varepsilon(0,0) = \hat{1}$) and using the property (1.4) we would then use

$$\tilde{U}_I^\varepsilon(0,-\infty) = [\tilde{U}_I^\varepsilon(-\infty,0)]^\dagger = e^{-h(-\infty)a^\dagger + h^*(-\infty)a}\,, \tag{1.49}$$

in the Gell-Mann - Low formula (1.34). Computing the relevant matrix element is straightforward (the ground-state vector of H_0 is traditionally denoted $|0\rangle$ instead of $|\Omega_0\rangle$ used in (1.34)):

$$\langle 0|\tilde{U}_I^\varepsilon(0,-\infty)|0\rangle = e^{-\frac{1}{2}|h(-\infty)|^2}\langle 0|e^{-h(-\infty)a^\dagger}e^{h^*(-\infty)a}|0\rangle = e^{-\frac{1}{2}|h(-\infty)|^2}\,.$$

We have used here the Baker-Hausdorff formula

$$e^{X+Y} = e^{-\frac{1}{2}[X,\,Y]}\,e^X\,e^Y = e^{\frac{1}{2}[X,\,Y]}\,e^Y\,e^X\,, \tag{1.50}$$

(valid for any two operators X and Y which both commute with their commutator $[X,\,Y]$) and the relations $a|0\rangle = 0 = \langle 0|a^\dagger$. But since

$$h(-\infty) \equiv -\frac{i}{\hbar}\int_0^{-\infty} d\tau\, e^{i\omega\tau} f(\tau) = \frac{i}{\hbar}\int_{-\infty}^{0} d\tau\, \lambda\, e^{(\varepsilon+i\omega)\tau} = \frac{i}{\hbar}\,\frac{\lambda}{\varepsilon+i\omega}\,, \tag{1.51}$$

it would turn out that the left hand side of the formula (1.34) for $E_\Omega - E_{\Omega_0}$ is purely imaginary (because $\langle 0|\tilde{U}_I^\varepsilon(0,-\infty)|0\rangle$ is real) and vanishes when $\varepsilon \to 0$!

It follows that $\tilde{U}_I^\varepsilon(0,-\infty)$ employed above must differ by a phase factor from the true interaction picture evolution operator $U_I^\varepsilon(0,-\infty)$. To find this phase factor we will compute $U_I^\varepsilon(t,-\infty)$ perturbatively up to the second order, using instead of the formula (1.23) the (fully equivalent to it) iterative solution analogous to (1.7):

$$\begin{aligned} U_I^\varepsilon(t,-\infty) = \hat{1} &- \frac{i}{\hbar}\int_{-\infty}^{t} d\tau\, e^{\varepsilon\tau}\left[\lambda^* a\, e^{-i\omega\tau} + \lambda\, a^\dagger\, e^{i\omega\tau}\right] \\ &- \frac{1}{\hbar^2}\int_{-\infty}^{t} d\tau_1\, e^{\varepsilon\tau_1}\left[\lambda^* a\, e^{-i\omega\tau_1} + \lambda\, a^\dagger e^{i\omega\tau_1}\right]\int_{-\infty}^{\tau_1} d\tau_2\, e^{\varepsilon\tau_2}\left[\lambda^* a\, e^{-i\omega\tau_2} + \lambda\, a^\dagger e^{i\omega\tau_2}\right] + \ldots \end{aligned}$$

It is easy to see that the first order term of this formula taken at $t = 0$:

$$-\frac{i}{\hbar}\left[\frac{\lambda^* a}{\varepsilon - i\omega}\,e^{(\varepsilon-i\omega)t} + \frac{\lambda\, a^\dagger}{\varepsilon+i\omega}\,e^{(\varepsilon+i\omega)t}\right]\Bigg|_{t=0}\,,$$

precisely equals the first order term in the expansion

$$\tilde{U}_I^\varepsilon(0,-\infty) = \hat{1} + [h^*(-\infty)\,a - h(-\infty)\,a^\dagger] + \frac{1}{2}[h^*(-\infty)\,a - h(-\infty)\,a^\dagger]^2 + \ldots$$

of the operator (1.49). The second order terms of the expansions of $U_I^\varepsilon(0,-\infty)$ and of $\tilde{U}_I^\varepsilon(0,-\infty)$ differ however:[14]

$$U_I^\varepsilon(0,-\infty) - \tilde{U}_I^\varepsilon(0,-\infty) = -\frac{|\lambda|^2}{2\hbar^2}\left[\frac{a^\dagger a}{\varepsilon\,(\varepsilon - i\omega)} + \frac{a\,a^\dagger}{\varepsilon\,(\varepsilon + i\omega)} - \frac{a^\dagger a}{\varepsilon^2+\omega^2} - \frac{a\,a^\dagger}{\varepsilon^2+\omega^2}\right] + \dots$$
$$= \frac{|\lambda|^2}{2\hbar^2}\,\frac{i\omega}{\varepsilon(\varepsilon^2+\omega^2)} + \dots \qquad (1.52)$$

Owing to the relation $a^\dagger a - a\,a^\dagger = -\hat{1}$ the difference is a purely imaginary c-number. This means that up to the second order in λ

$$U_I^\varepsilon(0,-\infty) = (1 + i\varphi + \dots)\,\tilde{U}_I^\varepsilon(0,-\infty)\,,$$

where $\varphi = (|\lambda|^2/2\hbar^2)[\omega/\varepsilon(\varepsilon^2+\omega^2)]$. Using this result, and knowing that the two operators can differ only by a phase factor, one can write[15]

$$U_I^\varepsilon(0,-\infty) = e^{i\varphi}\tilde{U}_I^\varepsilon(0,-\infty)\,.$$

The phase φ of $U_I^\varepsilon(0,-\infty)$ behaves here as $1/\varepsilon$, as expected. Therefore

$$\langle\Omega_0|U_I^\varepsilon(0,-\infty)|\Omega_0\rangle = e^{i\varphi}\,e^{-\frac{1}{2}|h(-\infty)|^2}\,,$$

and the Gell-Mann - Low formula (1.34) gives[16]

$$\lim_{\varepsilon\to 0^+} i\hbar\,\varepsilon|\lambda|\,\frac{\partial}{\partial|\lambda|}\ln\langle\Omega_0|U_I^\varepsilon(0,-\infty)|\Omega_0\rangle = -\frac{|\lambda|^2}{\hbar\omega}\,,$$

which is precisely the energy shift $E_\Omega - E_{\Omega_0}$ due to the constant perturbation of H_0 by the time-independent interaction $V_{\rm int} = \lambda\,a^\dagger + \lambda^* a$. It is also easy to check using the standard rule $[a,\,f(a^\dagger)] = f'(a^\dagger)$, that the annihilation operator $A = a + b = a + \lambda/\hbar\omega$ appearing in (1.42) annihilates the state-vector

$$\tilde{U}_I^\varepsilon(0,-\infty)|0\rangle \propto e^{-h(-\infty)a^\dagger}|0\rangle = e^{-(\lambda/\hbar\omega)a^\dagger}|0\rangle = \sum_{n=0}^{\infty}\frac{(-\lambda/\hbar\omega)^n}{\sqrt{n!}}\,|n\rangle\,,$$

(the limit $\varepsilon \to 0$ of $h(-\infty)$ has already been taken here). This demonstrates that the Gell-Mann - Low construction (1.31) indeed gives the vector proportional to the true ground-state eigenvector $|\tilde{0}\rangle$ of H.

[14]Notice that the second order term of the expansion of $U_I^\varepsilon(0,-\infty)$ is singular in the limit $\varepsilon \to 0$. Similarly singular will also be in general all higher order terms (see the formula (2.10)).

[15]We do not try here to show that the phase φ is not corrected in higher orders in λ. That at least its singular part is not, follows from the fact that its order $|\lambda|^2$ term correctly reproduces the difference $E_\Omega - E_{\Omega_0}$ of the ground-state energies of the complete and free Hamiltonians. In fact the exact phase $\varphi(t)$ can be in this case found explicitly and the conjecture used here substantiated. Knowledge of the exact evolution operator $U_I^\varepsilon(t,0)$ allows also to directly verify in this case the formula (1.38).

[16]In the derivation of the Gell-Mann - Low formulae of Section 1.2 it is assumed that λ is a real parameter; therefore here we write it as $|\lambda|$.

As another application of the exact solution (1.44) of the Heisenberg equation of motion we consider the behaviour of the harmonic oscillator subjected to the action of a time dependent force $F(t)$ which vanishes in the past and in the future: $F(t) \to 0$, when $|t| \to \infty$. One is then naturally interested in probabilities of the oscillator transitions from the H_0 eigenstate $|n\rangle$ in the remote past to another H_0 eigenstate $|k\rangle$ in the remote future. This simple and solvable example allows to introduce the S-matrix which will be the central object of interest in the context of relativistic field theory. It also will allow to test different approximations (discussed in Chapter 2) valid in different regimes.

In order to find the transition amplitudes, assuming that the function $F(t)$ vanishes sufficiently fast for $t \to \pm\infty$ (so that the integrals below are convergent), one defines two pairs of operators, $a_{\rm in}$, $a_{\rm in}^\dagger$ and $a_{\rm out}$, $a_{\rm out}^\dagger$. The operators $a_{\rm out}$ and $a_{\rm in}$ are given by

$$
\begin{aligned}
a_{\rm out} &= a + \frac{i}{\sqrt{2M\hbar\omega}} \int_0^\infty d\tau\, e^{i\omega\tau} F(\tau) \\
a_{\rm in} &= a + \frac{i}{\sqrt{2M\hbar\omega}} \int_0^{-\infty} d\tau\, e^{i\omega\tau} F(\tau) = a - \frac{i}{\sqrt{2M\hbar\omega}} \int_{-\infty}^0 d\tau\, e^{i\omega\tau} F(\tau)\,,
\end{aligned}
$$

and $a_{\rm out}^\dagger$ and $a_{\rm in}^\dagger$ are their Hermitian conjugates. From (1.44) it is clear that

$$
\begin{aligned}
a_H(t) &\to e^{-i\omega t}\, a_{\rm in} \qquad \text{for} \quad t \to -\infty\,, \\
a_H(t) &\to e^{-i\omega t}\, a_{\rm out} \qquad \text{for} \quad t \to +\infty\,,
\end{aligned}
\tag{1.53}
$$

($a_H^\dagger(t)$ analogously converges to $e^{i\omega t}\, a_{\rm in}^\dagger$ and $e^{i\omega t}\, a_{\rm out}^\dagger$ in these limits). The *in* and *out* operators defined in this way are related to each other by

$$
a_{\rm out} = a_{\rm in} + c\,, \qquad a_{\rm out}^\dagger = a_{\rm in}^\dagger + c^*.
$$

The complex number (not an operator!) $c \equiv c(\infty, -\infty)$ is the limiting value of

$$
c(t_2, t_1) = \frac{i}{\sqrt{2M\hbar\omega}} \int_{t_1}^{t_2} d\tau\, e^{i\omega\tau} F(\tau)\,. \tag{1.54}
$$

The operators $a_{\rm in}$ and $a_{\rm in}^\dagger$ as well as $a_{\rm out}$ and $a_{\rm out}^\dagger$ satisfy the same commutation relation as do the original annihilation/creation operators (1.40):

$$
\begin{aligned}
[a_{\rm in},\ a_{\rm in}^\dagger] &= \hat{1}\,, \qquad [a_{\rm in},\ a_{\rm in}] = [a_{\rm in}^\dagger,\ a_{\rm in}^\dagger] = 0\,, \\
[a_{\rm out},\ a_{\rm out}^\dagger] &= \hat{1}\,, \qquad [a_{\rm out},\ a_{\rm out}] = [a_{\rm out}^\dagger,\ a_{\rm out}^\dagger] = 0\,.
\end{aligned}
$$

One can therefore use (again) the standard algebraic argument that in the Hilbert space there must exist two vectors $|0\ {\rm in}\rangle$ and $|0\ {\rm out}\rangle$ annihilated by $a_{\rm in}$ and $a_{\rm out}$, respectively and that $a_{\rm in}^\dagger$ and $a_{\rm out}^\dagger$ acting on these vectors create the respective eigenvectors of the operators $a_{\rm in}^\dagger a_{\rm in}$ and $a_{\rm out}^\dagger a_{\rm out}$. This means that in the Hilbert space of the harmonic oscillator

(spanned by the eigenvectors $|n\rangle$ of H_0) there exist two complete sets of orthonormal vectors:

$$\begin{array}{ll} |0\text{ in}\rangle & |0\text{ out}\rangle \\ |1\text{ in}\rangle \equiv a^\dagger_{\rm in}|0\text{ in}\rangle & |1\text{ out}\rangle \equiv a^\dagger_{\rm out}|0\text{ out}\rangle \\ |2\text{ in}\rangle \equiv \dfrac{1}{\sqrt{2!}}(a^\dagger_{\rm in})^2|0\text{ in}\rangle & |2\text{ out}\rangle \equiv \dfrac{1}{\sqrt{2!}}(a^\dagger_{\rm out})^2|0\text{ out}\rangle \\ \cdots\cdots & \cdots\cdots \end{array} \tag{1.55}$$

which form two alternative (in addition to the eigenvectors $|n\rangle$ of $a^\dagger a$, i.e. of H_0) bases of the Hilbert space. The vectors (1.55) are called the *in* and *out* state-vectors, respectively. Furthermore, since

$$\begin{aligned} H^H(t) &\equiv U^\dagger(t,0)H^S(t)U(t,0) \\ &= \hbar\omega\, a^\dagger_H(t)a_H(t) + \Delta_\omega - \sqrt{\frac{\hbar}{2M\omega}}\,\Big(a_H(t) + a^\dagger_H(t)\Big)F(t)\,, \end{aligned}$$

it follows from (1.53) that $H^H(t) \to \hbar\omega a^\dagger_{\rm in}a_{\rm in} + \Delta_\omega$ for $t \to -\infty$ and, similarly, $H^H(t) \to \hbar\omega a^\dagger_{\rm out}a_{\rm out} + \Delta_\omega$ for $t \to +\infty$. The *in* state-vectors (1.55) are therefore the eigenvectors of the Heisenberg picture Hamiltonian $H^H(t)$ in the far past and the *out* state-vectors play the analogous role with respect to $H^H(t)$ in the far future. From the idea underlying the Heisenberg picture (explained in Section 1.1), it follows that the vectors $|n\text{ in}\rangle$ (the vectors $|n\text{ out}\rangle$) when treated as Schrödinger picture vectors at $t = 0$ and evolved with the help of the operator $U(t,0)$, become at $t = -\infty$ (at $t = +\infty$) the time-dependent[17] eigenvectors $|n\rangle$ of H_0:

$$H^S(t)\,U(t,0)|n\,\text{in}\rangle = U(t,0)\,H^H(t)\,|n\,\text{in}\rangle \to (n\hbar\omega + \Delta_\omega)U(-\infty,0)\,|n\,\text{in}\rangle\,.$$

That is, the constant in time state-vector $|n\text{ in}\rangle$ represents in the Heisenberg picture the whole "history" of the oscillator which in the far past (i.e. when the external force was absent) was in the n-th eigenstate of H_0. Similarly, the constant state-vector $|n\text{ out}\rangle$ represents the whole "history" of the oscillator which in the far future ends up in the n-th H_0 excited state. Therefore, the probability of the oscillator transition (under the influence of the external force $F(t)$) from the n-th excited eigenstate of H_0 in the far past to the k-th excited eigenstate of H_0 in the far future is given by

$$P(n \to k) = |S_{kn}|^2\,. \tag{1.56}$$

where

$$S_{kn} \equiv \langle k\text{ out}|n\text{ in}\rangle\,. \tag{1.57}$$

[17]Because of this, the limit in the formula does not exist in the strict sense; in contrast to $U_I(t,0)$, the Schrödinger picture evolution operator $U(t,0)$ has no $t = \mp\infty$ limits.

The (complex in general) scalar products S_{kn} - the transition amplitudes - measure the content of the state $|k\ \mathrm{out}\rangle$ in the state $|n\ \mathrm{in}\rangle$. The amplitudes S_{kn} form the so-called S-matrix which is unitary, that is such that[18] $S^\dagger \cdot S = I$:

$$(S^\dagger)_{mk}S_{kn} \equiv S^*_{km}S_{kn} = \sum_{k=0}^{\infty}\langle k\ \mathrm{out}|m\ \mathrm{in}\rangle^*\langle k\ \mathrm{out}|n\ \mathrm{in}\rangle \tag{1.58}$$
$$= \sum_{k=0}^{\infty}\langle m\ \mathrm{in}|k\ \mathrm{out}\rangle\langle k\ \mathrm{out}|n\ \mathrm{in}\rangle = \langle m\ \mathrm{in}|n\ \mathrm{in}\rangle = \delta_{mn}\,,$$

owing to the completeness of the set of vectors $|k\ \mathrm{out}\rangle$. In the similar way, using the completeness of the set of vectors $|k\ \mathrm{in}\rangle$, one shows that $S \cdot S^\dagger = I$. In view of (1.56), unitarity of the S-matrix implies that

$$\sum_k P(n \to k) = 1\,. \tag{1.59}$$

Of course,[19] $\langle k\ \mathrm{out}|n\ \mathrm{in}\rangle = \delta_{kn}$ if $F(t) \equiv 0$ (the S-matrix is then trivial).

The elements S_{kn} of the S-matrix can be computed in two different ways. One is to compute them as matrix elements of a unitary S_0 operator (to be defined in (1.71)) between the eigenvectors $|k\rangle$ and $|n\rangle$ of the free Hamiltonian H_0. Another possibility, which we are going to explain first, is to compute S_{kn} as matrix elements of another operator, called S, either between the states $|k\ \mathrm{out}\rangle$ and $|n\ \mathrm{out}\rangle$, or between the states $|k\ \mathrm{in}\rangle$ and $|n\ \mathrm{in}\rangle$.

The operator S is defined by the conditions

$$a_{\mathrm{out}} = a_{\mathrm{in}} + c = S^\dagger a_{\mathrm{in}} S\,,$$
$$a^\dagger_{\mathrm{out}} = a^\dagger_{\mathrm{in}} + c^* = S^\dagger a^\dagger_{\mathrm{in}} S\,. \tag{1.60}$$

Similarly as in the preceding example, the relations (1.60) determine S only up to a phase factor. One possible choice is

$$S = \exp\Big(c\,a^\dagger_{\mathrm{in}} - c^* a_{\mathrm{in}}\Big) = \exp\Big(c\,a^\dagger_{\mathrm{out}} - c^* a_{\mathrm{out}}\Big)\,. \tag{1.61}$$

The operator S is clearly unitary. Using (1.60) one sees that

$$a_{\mathrm{in}}S|0\ \mathrm{out}\rangle = SS^\dagger a_{\mathrm{in}}S|0\ \mathrm{out}\rangle = Sa_{\mathrm{out}}|0\ \mathrm{out}\rangle = 0\,, \tag{1.62}$$

etc., which shows that once the arbitrary phase between $|0\ \mathrm{in}\rangle$ and $S|0\ \mathrm{out}\rangle$ is fixed by the relation[20] $S|0\ \mathrm{out}\rangle = |0\ \mathrm{in}\rangle$, the simple relation

$$S|n\ \mathrm{out}\rangle = |n\ \mathrm{in}\rangle\,, \tag{1.63}$$

[18] The dagger on S means here Hermitian conjugation of the c-number matrix (not of a Hilbert space operator) and I stands for the unit matrix (of infinite dimension).

[19] We assume here that the vectors $|0\ \mathrm{in}\rangle$ and $|0\ \mathrm{out}\rangle$, which can be defined with arbitrary phases, are chosen so that they coincide when $F(t) \equiv 0$.

[20] The phase is a priori arbitrary because we *define* $|0\ \mathrm{in}\rangle$ and $|0\ \mathrm{out}\rangle$ as the two arbitrary vectors satisfying the conditions $a_{\mathrm{in}}|0\ \mathrm{in}\rangle = 0$ and $a_{\mathrm{out}}|0\ \mathrm{out}\rangle = 0$, respectively; their phases, and therefore also their relative phase, are not fixed by these conditions.

will hold for any n. Indeed,

$$\frac{1}{\sqrt{n!}}\, S(a^\dagger_{\rm out})^n|0\ {\rm out}\rangle = \frac{1}{\sqrt{n!}}\, S(a^\dagger_{\rm out})^n S^\dagger S|0\ {\rm out}\rangle = \frac{1}{\sqrt{n!}}\, (a^\dagger_{\rm in})^n|0\ {\rm in}\rangle\,.$$

The scalar products (1.57) which gives the transition probabilities $P(n\to k) = |S_{kn}|^2$, can be, therefore, computed as the corresponding matrix elements of the S-operator:

$$S_{kn} = \langle k\ {\rm out}|n\ {\rm in}\rangle = \langle k\ {\rm out}|S|n\ {\rm out}\rangle = \langle k\ {\rm in}|S|n\ {\rm in}\rangle\,. \tag{1.64}$$

The second form of S_{kn} follows directly from (1.63), while the third one from the conjugated relation $\langle k\ {\rm out}| = \langle k\ {\rm in}|S$. With the help of the Baker-Hausdorff formula (1.50) the first of the two forms (1.61) of the S operator can be written in the form

$$S = \exp\!\left(-\frac{1}{2}|c|^2\right) e^{c\,a^\dagger_{\rm in}}\, e^{-c^*a_{\rm in}}\,, \tag{1.65}$$

which is more suitable for computing its matrix elements (1.64):

$$S_{nm} = \frac{1}{\sqrt{n!\,m!}} \exp\!\left(-\frac{1}{2}|c|^2\right) \langle 0\,{\rm in}|\,(a_{\rm in})^n\, e^{ca^\dagger_{\rm in}}\, e^{-c^*a_{\rm in}}\,(a^\dagger_{\rm in})^m|0\,{\rm in}\rangle\,.$$

In this formula we can insert $\hat 1 = e^{c\,a^\dagger_{\rm in}}\, e^{-c\,a^\dagger_{\rm in}}$ between $\langle 0\ {\rm in}|$ and the leftmost operator, and $\hat 1 = e^{c^*a_{\rm in}} e^{-c^*a_{\rm in}}$ between $|0\ {\rm in}\rangle$ and the rightmost operator. Next, using the fact that $\langle 0\ {\rm in}|e^{c\,a^\dagger_{\rm in}} = \langle 0\ {\rm in}|$ and $e^{-c^*a_{\rm in}}|0\ {\rm in}\rangle = |0\ {\rm in}\rangle$, as well as the relations

$$e^{-ca^\dagger_{\rm in}}\,(a_{\rm in})^n\, e^{ca^\dagger_{\rm in}} = \left(e^{-ca^\dagger_{\rm in}} a_{\rm in} e^{ca^\dagger_{\rm in}}\right)^n = (a_{\rm in}+c)^n\,,$$
$$e^{-c^*a_{\rm in}}(a^\dagger_{\rm in})^m e^{c^*a_{\rm in}} = \left(e^{-c^*a_{\rm in}} a^\dagger_{\rm in} e^{c^*a_{\rm in}}\right)^m = (a^\dagger_{\rm in}-c^*)^m,$$

we obtain

$$\begin{aligned} S_{nm}(c,c^*) \equiv \langle n\ {\rm in}|S|m\ {\rm in}\rangle &= \frac{1}{\sqrt{n!m!}}\, e^{-\frac{1}{2}|c|^2} \langle 0\ {\rm in}|(a_{\rm in}+c)^n (a^\dagger_{\rm in}-c^*)^m|0\ {\rm m}\rangle \\ &= \frac{1}{\sqrt{n!\,m!}}\, e^{-\frac{1}{2}|c|^2} \sum_{k=0}^{n}\sum_{l=0}^{m} \binom{n}{k}\binom{m}{l} c^{n-k}(-c^*)^{m-l} \langle 0\ {\rm in}|(a_{\rm in})^k (a^\dagger_{\rm in})^l|0\ {\rm in}\rangle \\ &= \frac{1}{\sqrt{n!\,m!}} \exp\!\left(-\frac{1}{2}|c|^2\right) \sum_{k=0}^{\min(n,m)} k! \binom{n}{k}\binom{m}{k} c^{n-k}(-c^*)^{m-k}\,. \end{aligned} \tag{1.66}$$

From this formula it can be seen that

$$S_{nm}(c,c^*) = S_{mn}(-c^*,-c) = (-1)^{m-n}\,(S_{mn}(c,c^*))^*\,, \tag{1.67}$$

and, hence, $|S_{nm}| = |S_{mn}|$, that is $P(n\to m) = P(m\to n)$. We also see that

$$P(0\to 0) = |\langle 0\,{\rm in}|S|0\,{\rm in}\rangle|^2 = \exp\!\big(-|c|^2\big)\,,$$

that is, the factor $\exp\left(-\frac{1}{2}|c|^2\right)$ plays the role of the ground-state persistence amplitude. Furthermore, the probability of the transition from the ground-state to the n-th excited state is

$$P(0 \to n) = |\langle n \,\mathrm{in}|S|0 \,\mathrm{in}\rangle|^2 = \frac{1}{n!} \exp\left(-|c|^2\right) |c|^{2n} ,$$

which is precisely the Poisson distribution with $\bar{n} = |c|^2$ (that is, in a statistical ensemble of oscillators which are all prepared at $t = -\infty$ in the ground-state and acted upon by the force $F(t)$ the mean excitement (i.e. mean n) at $t = \infty$ is $|c|^2$). It is also interesting to compare the probability $P(n \to n+1)$ with $P(0 \to 1)$. If $|c| \ll 1$, that is always when the force $F(t)$ perturbing the oscillator is weak, restricting to the lowest power of $|c|$ in the exact expression for S_{nm} (i.e. taking only the term with $k = n$) we find

$$P(n \to n+1) \approx (n+1)|c|^2 .$$

In this approximation the probability $P(n \to n+1)$ is therefore $n+1$ times bigger than $P(0 \to 1) \approx |c|^2$. As we will be discussed in Section 5.6, by analogy with how states of many identical particles are represented in the second quantization formalism (developed in Chapter 5), the n-th excited state of the oscillator can be interpreted as the state of n particles (bosons). One sees therefore that if the perturbation is small, creating one additional boson is $n+1$ times more probable if there were already n bosons present initially. If $|c|$ is not small, this simple rule is no longer true in this model.

For completeness we will also show, how the transition amplitudes S_{kn} (1.57) can be computed using the S_0 operator. To this end we begin with the operator $\tilde{U}(t,0)$ such that

$$\begin{aligned} \tilde{U}^\dagger(t,0)\, a\, \tilde{U}(t,0) = a_H(t) &= e^{-i\omega t}\left(a + \frac{i}{\sqrt{2M\hbar\omega}} \int_0^t d\tau e^{i\omega\tau} F(\tau)\right) \\ &= e^{-i\omega t}\left(a + c(t,0)\right) , \end{aligned}$$

with $c(t_2,t_1)$ defined in (1.54) and the conjugated relation. The true Schrödinger picture evolution operator $U(t,0)$, given by (1.9), can differ from $\tilde{U}(t,0)$ only by a phase factor. It must, therefore, be of the form

$$U(t,0) = e^{-iH_0 t/\hbar}\, e^{c(t,0)\, a^\dagger - c^*(t,0)\, a}\, e^{i\varphi(t,0)} ,$$

with $c(t,0)$ given by (1.54) and some phase factor $\varphi(t,0)$, which will not be relevant. The corresponding interaction picture evolution operator can be then obtained with the help of the relation (1.24) and reads

$$U_I(t,0) = e^{c(t,0)\, a^\dagger - c^*(t,0)\, a}\, e^{i\varphi(t,0)} . \tag{1.68}$$

It is clear that

$$\begin{aligned} U_I^\dagger(-\infty,0)\, a\, U_I(-\infty,0) &= a + c(-\infty,0) = a_{\mathrm{in}} , \\ U_I^\dagger(-\infty,0)\, a^\dagger U_I(-\infty,0) &= a^\dagger + c^*(-\infty,0) = a_{\mathrm{in}}^\dagger , \end{aligned}$$

and

$$U_I^\dagger(\infty,0)\,a\,U_I(\infty,0) = a + c(\infty,0) = a_{\rm out}\,,$$
$$U_I^\dagger(\infty,0)\,a^\dagger U_I(\infty,0) = a^\dagger + c^*(\infty,0) = a_{\rm out}^\dagger\,.$$

In full analogy to (1.63) it then follows that[21]

$$U_I(-\infty,0)|n\ {\rm in}\rangle = |n\rangle\,,$$
$$U_I(\infty,0)|n\ {\rm out}\rangle = |n\rangle\,. \tag{1.69}$$

Therefore,

$$\begin{aligned} S_{nm} &\equiv \langle {\rm out}\ n|m\ {\rm in}\rangle = \langle n|U_I(\infty,0)U_I^\dagger(-\infty,0)|m\rangle \\ &= \langle n|U_I(\infty,0)U_I(0,-\infty)|m\rangle = \langle n|U_I(\infty,-\infty)|m\rangle\,. \end{aligned} \tag{1.70}$$

Thus, the transition amplitudes can be also represented as matrix elements between the free Hamiltonian eigenvectors of the operator

$$S_0 \equiv U_I(\infty,-\infty) = \lim_{t_2\to\infty}\lim_{t_1\to-\infty} U_I(t_2,t_1)\,. \tag{1.71}$$

Using (1.68), the composition rules of the evolution operators (1.4), the Baker-Hausdorff formula (1.50) and noticing that $c(t_1,0) = -c(0,t_1)$, $c(t_2,0) + c(0,t_1) = c(t_2,t_1)$, we get[22]

$$U_I(t_2,t_1) = e^{c(t_2,t_1)\,a^\dagger - c^*(t_2,t_1)\,a}\,e^{i\gamma}\,, \tag{1.72}$$

with the phase $\gamma = {\rm Im}[c(t_2,0)c^*(0,t_1)] + \varphi(t_2,0) - \varphi(t_1,0)$. Taking into account that $c(\infty,-\infty) = c$ it is clear that, up to an overall phase factor (which cannot be fixed without solving explicitly the differential equations), the matrix elements of the operator (compare the definition (7.16))

$$S_0 \equiv U_I(\infty,0)U_I^\dagger(-\infty,0) = U_I(\infty,-\infty)\,, \tag{1.73}$$

between the H_0 eigenvectors and of the S operator which in general is defined as[23]

$$S \equiv U_I^\dagger(-\infty,0)U_I(\infty,0)\,, \tag{1.74}$$

[21] This agrees with the statement already made (in the paragraph above the formula (1.56)) that the vectors $|n\ {\rm in}\rangle$ and $|n\ {\rm out}\rangle$, when treated as Schrödinger picture state-vectors at $t = 0$ and evolved with $U(t,0)$, become in the limits $t \to \mp\infty$ the eigenvectors of $H(\mp\infty) = H_0$; here they are evolved with $U_I(t,0) = e^{iH_0t/\hbar}U(t,0)$ and the factor $e^{iH_0t/\hbar}$ removes the residual time dependence, so the limits $t \to \mp\infty$ exist in the strict sense.

[22] The double limit of the interaction picture operator $U_I(t_2,t_1)$ exists because we assumed that the similar limit of the integral (1.54) exists. Notice that the corresponding Schrödinger picture operator $U(t_2,t_1)$ which is related to $U_I(t_2,t_1)$ by (1.24) does not have well defined operator limits $t_1 \to -\infty$ and/or $t_2 \to +\infty$ because of the exponential oscillatory factors $\exp(-iH_0t_2/\hbar)$ and $\exp(iH_0t_1/\hbar)$ present on its extremes.

[23] This definition of the S-operator readily follows by combining the relations (1.69) with the action (1.63) of S.

(compare the definition (7.20)) and in the considered case is explicitly given by (1.61), between the corresponding *in* or the corresponding *out* vectors, coincide.

The S-matrix is one of the quantities of prime interest in all variants of the scattering theory: in the nonrelativistic potential scattering theory of a single particle, in the nonrelativistic (single and multichannel) scattering theory of many particles and, finally, in the scattering theory of relativistic particles which necessarily takes the form of a relativistic quantum field theory. Because Hamiltonians of such theories are usually time independent and do not converge for $t \to \pm\infty$ in any operator sense to the corresponding free Hamiltonians, the *in* and *out* states must be defined differently than it was done here (see Section 7.3) but retain their interpretation of the states representing free "elementary excitations" of the system entering the interaction in the far past and emerging from it in the far future. The S-matrix is, however, always defined similarly as in this section, as the matrix of the scalar products (1.57) of the properly defined *in* and *out* states. In all nonrelativistic scattering theories the S-matrix elements can be computed, as here, using the unitary S_0 operator. The operator[24] S defined in (1.74) is less useful in ordinary perturbative calculations of S-matrix elements (as will be explained in Chapter 7 in the scattering theory of a single particle it is not always unitary). The S_0-operator will be also used for obtaining S-matrix elements in the simplest (perturbative) formulation (exposed in Chapters 7, 8 and 9) of quantum field theory, based on relativistic quantum mechanics of particles. This traditional approach which was largely shaped by the first theory of this kind - Quantum Electrodynamics - is however not general enough and will have to be replaced by a more general approach (formulated in Chapter 13) based on Green's functions (vacuum time ordered products of Heisenberg picture operators) which - somewhat paradoxically - is natural in applications of quantum field theory methods to nonrelativistic theory of many particle systems and in condensed matter physics. Formulation of the perturbative expansion of Green's functions relies then on the Gell-Mann - Low construction discussed in Section 1.2 of the lowest energy eigenvector of the full Hamiltonian H and the S-operator reenters the game as the one connecting true asymptotic states reconstructed from the poles of two-point Green's functions.

[24] In the case considered in this Section, due to simplicity of the dynamics, the S operator differs from the S_0 operator simply by a c-number phase factor.

A The commutator $[H_0,\, U_I^\varepsilon(0,-\infty)]$

We give here a proof, not based on the perturbative expansion, of the formula (1.29). The proof is strikingly simple.[1] One considers first the time-dependent Hamiltonian of the form

$$H(t) = H_0 + e^{\varepsilon t}\,\lambda\, V_{\rm int}\,, \tag{A.1}$$

with $\lambda = e^{\varepsilon\theta}$, where θ is a real parameter. The corresponding (Schrödinger picture) evolution operator $U^\varepsilon(t,s)$ satisfies the equation (1.6):

$$\begin{aligned} U^\varepsilon(t,\,s) &= \hat 1 + \frac{1}{i\hbar}\int_s^t d\tau\,\left(H_0 + e^{\varepsilon(\tau+\theta)}\,V_{\rm int}\right)U^\varepsilon(\tau,\,s) \\ &= \hat 1 + \frac{1}{i\hbar}\int_{s+\theta}^{t+\theta} d\tau\,\left(H_0 + e^{\varepsilon\tau}\,V_{\rm int}\right)U^\varepsilon(\tau-\theta,\,s)\,. \end{aligned} \tag{A.2}$$

Along with $H(t)$ one considers also $\tilde H(t)$ which is just $H(t)$ with $\lambda = 1$; the evolution operator $\tilde U^\varepsilon(t,\,s)$ corresponding to $\tilde H(t)$ satisfies the equation

$$\tilde U^\varepsilon(t+\theta,\,s+\theta) = 1 + \frac{1}{i\hbar}\int_{s+\theta}^{t+\theta} d\tau\,\left(H_0 + e^{\varepsilon\tau}\,V_{\rm int}\right)\tilde U^\varepsilon(\tau,\,s+\theta)\,. \tag{A.3}$$

The comparison shows that

$$U^\varepsilon(t,\,s) = \tilde U^\varepsilon(t+\theta,\,s+\theta)\,. \tag{A.4}$$

Indeed, the formula (A.2), upon substituting (A.4) in both its sides becomes identical with (A.3). Hence,[2]

$$\frac{\partial}{\partial\theta}\,U^\varepsilon(t,\,s) = \frac{\partial}{\partial t}\,U^\varepsilon(t,\,s) + \frac{\partial}{\partial s}\,U^\varepsilon(t,\,s) = \frac{1}{i\hbar}H(t)U^\varepsilon(t,\,s) - \frac{1}{i\hbar}\,U^\varepsilon(t,\,s)H(s)\,,$$

and the relation $\partial/\partial\theta = \varepsilon\,\lambda\,\partial/\partial\lambda$ leads to the formula

$$i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,U^\varepsilon(t,\,s) = H(t)\,U^\varepsilon(t,\,s) - U^\varepsilon(t,\,s)\,H(s)\,,$$

which, upon using the relation (1.24), translates into

$$i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,U_I^\varepsilon(t,\,s) = H_I(t)\,U_I^\varepsilon(t,\,s) - U_I^\varepsilon(t,\,s)\,H_I(s)\,,$$

with $H_I(t) = H_0 + e^{\varepsilon t}\,\lambda V_{\rm int}^I(t)$. Setting $t = 0$ and $s = -\infty$ one obtains the relation

$$i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{d\lambda}\,U_I^\varepsilon(0,-\infty) = H\,U_I^\varepsilon(0,-\infty) - U_I^\varepsilon(0,-\infty)\,H_0\,,$$

which is equivalent to (1.29) and which, when applied to a H_0 eigenvector $|\Omega_0\rangle$ corresponding to the eigenvalue E_{Ω_0}, yields directly the formula (1.32).

[1] L.G. Molinari, *J. Math. Phys.* **48**, 052113 (2007).

[2] The derivative $\partial U^\varepsilon(t,\,s)/\partial s$ is obtained by taking the Hermitian conjugation of the formula (1.3) written for $\partial U^\varepsilon(t,\,s)/\partial t$ and subsequent renaming the variables $t \leftrightarrow s$ after using the property $[U^\varepsilon(t,\,s)]^\dagger = U^\varepsilon(s,t)$.