1 Time evolution in quantum mechanics

In this section we recall three ways of describing time evolution of quantum systems. The material presented here is standard (it may be found in quantum mechanics textbooks like the Schiff's one or many others) but it is a good starting point for describing the transition from ordinary quantum mechanics of a single particle to nonrelativistic and relativistic quantum mechanics of many particles and quantum field theory: it is the time evolution of systems of particles that is investigated in typical particle physics scattering experiments. Moreover, the time evolution operator (in the interacting picture), which will be introduced here, will serve to construct the lowest energy eigenvector (proportional to the ground state vector) of the full Hamiltonian out of the normalized free Hamiltonian ground state vector. This construction will be used in formulating the Dyson expansion of Green's functions in nonrelativistic many body theory and in the relativistic quantum field theory. Analysis of a simple solvable model presented in this section 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 the S-matrix which is the object of prime interest in the scattering theory together with two its representations: one in terms of the S-operator connecting the *in* and *out* states and another one in terms of the S_0-operator.

1.1 Three pictures

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

1. *The Schrödinger picture* is the basic and most natural way of describing 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 of vectors in this picture. The formal solution of the equation (1.1) can be expressed in terms of the unitary evolution operator

[1] In this section 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.

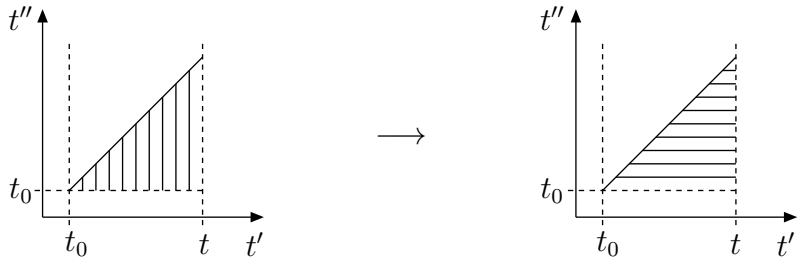

Figure 1.1: Changing the order of integrations. Solid lines in the left (right) triangle mark the range of the firstly performed integration over t'' (t') for fixed t' (t'').

$U(t,t_0)$ 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 and playing the role of the initial condition for the differential equation (1.1) is set at some arbitrary instant t_0. 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 $U(t_0,t_0)=1$ (the unit operator). Physically the following properties of $U(t,t_0)$ are obvious:

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

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 $U(t_0,t_0)=1$:

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

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

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

and so on. The iterations give 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

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, H^S(t')\, H^S(t'') = \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, H^S(t')\, H^S(t'')$$
$$+\frac{1}{2}\int_{t_0}^{t} dt' \int_{t'}^{t} dt''\, H^S(t'')\, H^S(t') \equiv \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, T\big(H^S(t')\, H^S(t'')\big)\,.$$

We have introduced the time-ordered product of time dependent operators[2] (here the Hamiltonians):

$$T(A(t')B(t'')) \equiv \theta(t'-t'')A(t')B(t'') + \theta(t''-t')B(t'')A(t')\,, \tag{1.8}$$
$$T(A(t')B(t'')B(t''')) \equiv \theta(t'-t'')\theta(t''-t''')A(t')B(t'')B(t''') + \ldots$$

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

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

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).

Computing, using the equation (1.1) and its Hermitian conjugation, the time derivative of a matrix element of an operator $O^S(t)$ (which may or may not depend on time) between the vectors $|\Psi(t)\rangle_S$ and $|\Phi(t)\rangle_S$ we get

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

[2]Time-ordering of products of "fermionic" operators (i.e. of operators which under rotations of the reference frame transform as half-integer spin representations of the rotation group - see section 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.

The last term is present only if the 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, that is its matrix elements do not change with time.

2. *The Heisenberg picture.* The physical predictions of a quantum theory are contained in matrix elements of operators, not in states 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, whose specification requires singling out a particular instant t_0, Hilbert space vectors representing states of the system do not change with time; instead, the whole time dependence of matrix elements is attributed to operators. Time independent Heisenberg picture state-vectors $|\Psi\rangle_H$ are defined by

$$|\Psi\rangle_H \equiv U^{-1}(t,t_0)|\Psi(t)\rangle_S\,. \tag{1.11}$$

Therefore (cf. (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 operators $O^H(t)$ are defined as

$$O^H(t) = U^\dagger(t,t_0)\,O^S(t)\,U(t,t_0)\,, \tag{1.12}$$

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

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

Here

$$H^H(t) \equiv U^\dagger(t,t_0)H^S(t)U(t,t_0)\,, \tag{1.14}$$

is the Hamiltonian taken 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

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

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 example of time-dependent O^S is the Lorentz boosts generator in a relativistic quantum field theory. Going over to the Heisenberg picture is a natural step in quantizing relativistic fields because field operators depend then on both space-time variables, $\mathbf{x}$ and t; this facilitates keeping the Poincaré covariance of the theory's formalism as much manifest as it is possible.

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 H^S 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 $V_{\rm int}^S$ which may or may not depend on time. The splitting 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

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

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

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

where $(\partial O/\partial t)_I\,(t)$ 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

$$-H^S_0 + e^{iH^S_0 t/\hbar}\, H^S e^{-iH^S_0 t/\hbar} = e^{iH^S_0 t/\hbar}\, V^S_{\rm int}\, e^{-iH^S_0 t/\hbar} \equiv V^I_{\rm int}(t) \,. \tag{1.20}$$

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

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

with the operator $U_I(t, t_0)$ satisfying the composition rules analogous to (1.4) and the differential equation analogous to (1.3) with the initial condition $U_I(t_0, t_0) = 1$. The iterative solution of this equation is given by the series

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

and can be also cast in the form

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

The iterative form of $U_I(t_2, t_1)$ turns out to be simply equivalent to the standard time dependent perturbative expansion (recalled in the next section). The form (1.23), instead, will lead to the Dyson expansion and Feynman diagrams. Applied to relativistic theories it will allow, unlike the previous one, to keep at every step relativistic covariance of amplitudes as manifest as possible.

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

$$U_I(t_2, t_1) = e^{iH^S_0 t_2/\hbar}\, U(t_2, t_1)\, e^{-iH^S_0 t_1/\hbar} \,. \tag{1.24}$$

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

1.2 The Gell-Mann - Low theorem

In many cases the ground state $|\Omega_0\rangle$, i.e. the normalized lowest energy eigenvector of the free Hamiltonian H_0 is known[3] 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[4] $H = H_0 + V_{\rm int}$. Such an expression can be obtained by using the prescription given by M. Gell-Mann and F. Low. The essential technical element of this prescription is the formula for the commutator of the free Hamiltonian H_0 with the interaction picture evolution operator $U_I^\varepsilon(t, -\infty)$ (or the $U_I^\varepsilon(t, +\infty)$ operator) corresponding to the modification of the original problem by giving the (Schrödinger picture) interaction operator $V_{\rm int}$ the explicit time dependence:

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

with $\varepsilon > 0$ (< 0). As $\varepsilon \to 0^+$ (0^-), the interaction is "adiabatically" switched on (off). At $t = 0$ the time dependent Hamiltonian $H(t) = H_0 + V_{\rm int}(t)$ is 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 described by the Hamiltonian $H(t) = H_0 + V_{\rm int}(t)$ in the three pictures 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 by (c.f. the formulae (1.23) and (1.20))

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

with

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

Although the commutator can be found without recourse to the perturbative expansion (see Appendix A), it will be computed here by using this technique because this will show how one deals 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)

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

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

[3] Some Hamiltonians do not have, however, normalizable eigenvectors.

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

τ_i and, therefore, the ordering of the operators $V^I_{\rm int}(\tau_i)$ is fixed. Alternatively, $T\left(V^I_{\rm int}(\tau_1)\dots V^I_{\rm int}(\tau_n)\right)$ can be represented as the sum over $n!$ permutations P of the terms of the form (cf. the formula (1.8))

$$\theta(\tau_{P(1)}-\tau_{P(2)})\theta(\tau_{P(2)}-\tau_{P(3)})\dots\theta(\tau_{P(n-1)}-\tau_{P(n)})\,V^I_{\rm int}(\tau_{P(1)})\dots V^I_{\rm int}(\tau_{P(n)})\,.$$

In each of these terms one gets the commutator

$$\begin{aligned}\left[H_0,\,V^I_{\rm int}(\tau_{P(1)})\dots V^I_{\rm int}(\tau_{P(n)})\right] &= \left[H_0,\,V^I_{\rm int}(\tau_{P(1)})\right]V^I_{\rm int}(\tau_{P(2)})\dots V^I_{\rm int}(\tau_{P(n)})\\ &\quad + V^I_{\rm int}(\tau_{P(1)})\left[H_0,\,V^I_{\rm int}(\tau_{P(2)})\right]\dots V^I_{\rm int}(\tau_{P(n)})+\dots\end{aligned}$$

Since the operator $V^I_{\rm int}(\tau)$ defined in (1.27) satisfies the equation

$$\frac{\hbar}{i}\,\frac{d}{d\tau}\,V^I_{\rm int}(\tau)=\left[H_0,\,V^I_{\rm int}(\tau)\right],$$

the commutator $[H_0,\,V^I_{\rm int}(\tau_{P(1)})\dots V^I_{\rm int}(\tau_{P(n)})]$ can be written in the form

$$\frac{\hbar}{i}\left(\sum_{i=1}^n\frac{d}{d\tau_{P(i)}}\right)V^I_{\rm int}(\tau_{P(1)})\dots V^I_{\rm int}(\tau_{P(n)})\,.$$

The crucial point is now that[5]

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

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

$$\sum_{n=0}^\infty\frac{(-i/\hbar)^n}{n!}\,\frac{\hbar}{i}\int_{-\infty}^0 d\tau_1\dots\int_{-\infty}^0 d\tau_n\,e^{\varepsilon(\tau_1+\dots+\tau_n)}\left(\sum_{i=1}^n\frac{d}{d\tau_i}\right)T\left(V^I_{\rm int}(\tau_1)\dots V^I_{\rm int}(\tau_n)\right),$$

is symmetric in its n time variables τ_i, 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

$$\begin{aligned}&-\sum_{n=1}^\infty\frac{(-i/\hbar)^{n-1}}{(n-1)!}\int_{-\infty}^0 d\tau_1\dots\int_{-\infty}^0 d\tau_{n-1}\,e^{\varepsilon(\tau_1+\dots+\tau_{n-1})}\left[e^{\varepsilon\tau_n}T\left(V^I_{\rm int}(\tau_1)\dots V^I_{\rm int}(\tau_n)\right)\right]_{-\infty}^0\\ &\quad+\varepsilon\sum_{n=1}^\infty\frac{(-i/\hbar)^{n-1}}{(n-1)!}\int_{-\infty}^0 d\tau_1\dots\int_{-\infty}^0 d\tau_n\,e^{\varepsilon(\tau_1+\dots+\tau_n)}\,T\left(V^I_{\rm int}(\tau_1)\dots V^I_{\rm int}(\tau_n)\right).\end{aligned}$$

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

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

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 $V^I_{\rm int}(0) \equiv V_{\rm int}$ can be taken out of the chronological ordering and placed in front of the remaining multiple integrals. In the second term one can use the trick (we assume that the interaction operator $V_{\rm int}$ is proportional to some real coupling constant λ which at the end can be set to 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

$$[H_0,\, U^\varepsilon_I(0,-\infty)] = -V_{\rm int}\,U^\varepsilon_I(0,-\infty) + i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,U^\varepsilon_I(0,-\infty)\,, \qquad (1.28)$$

which equivalently can written in the form

$$HU^\varepsilon_I(0,-\infty) = U^\varepsilon_I(0,-\infty)H_0 + i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,U^\varepsilon_I(0,-\infty)\,, \qquad (1.29)$$

with $H = H_0 + V_{\rm int}$.

This result can be used in many ways. One possible application is the construction of the normalizable llwest energy (E_Ω) eigenvector (proportional to the normalized to unity ground state-vector $|\Omega\rangle$) of the time independent Hamiltonian $H = H_0 + V_{\rm int}$ 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 $U^\varepsilon_I(t_2,t_1)$ given by (1.26) of the particular interaction picture state-vector $|\Psi^\varepsilon(t)\rangle_I$ which in the infinite past, i.e. at $t = -\infty$, is the H_0 eigenvector $|\Omega_0\rangle$ corresponding to its lowest eigenvalue E_{Ω_0}:

$$|\Psi^\varepsilon(t)\rangle_I = U^\varepsilon_I(t,-\infty)|\Psi^\varepsilon(-\infty)\rangle_I = U^\varepsilon_I(t,-\infty)|\Omega_0\rangle\,. \qquad (1.30)$$

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

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

has the limit $\varepsilon \to 0$, it is an eigenvector of the original (time-independent) Hamiltonian. This can be understood in the following way. In general, the instantaneous eigenvalues of $H(t) = H_0 + e^{\varepsilon t}V_{\rm int}$ forming the discrete part of the spectrum evolve with time. If they are not degenerate and do not cross with one another as the time changes from $-\infty$ to 0, the evolution of the corresponding instantaneous normalizable eigenvectors can be traced uniquely. Under these conditions the adiabatic theorem ensures that if $|\Omega_0\rangle$ is the normalized ground state of H_0, the vector $|\Psi^\varepsilon(0)\rangle_I$ should be proportional

to the normalizable ground state $|\Omega\rangle$ of $H(0) = H$. If these requirements are fulfilled, applying the equality (1.29) to the vector $|\Omega_0\rangle$ one gets

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

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 the limiting vector is an eigenvector of H with the eigenvalue E_{Ω_0}, the same as the energy of the ground state of 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 sections 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 we will show on a simple example that the phase of the vector $|\Psi^\varepsilon(0)\rangle_I$ diverges as $1/\varepsilon$). It is easy to check that (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 for $\varepsilon \to 0$), this limit is the eigenvector of the complete $H = H_0 + V_{\rm int}$ and

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

This formula is consistent with the relation (1.33): if

$$(H - E_\Omega)\lim_{\varepsilon\to 0}\frac{|\Psi^\varepsilon(0)\rangle_I}{\langle\Omega_0|\Psi^\varepsilon(0)\rangle_I} = 0\,,$$

then closing this relation from the left with $\langle\Omega_0|$ one finds that in the limit $\varepsilon \to 0$ the left hand side of (1.33) must equal $E - E_{\Omega_0}$.

It is easy to see that the same construction of the H eigenvector can be repeated by taking in (1.25) $\varepsilon < 0$ and considering time evolution of the (interction 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).[6]

Perhaps it is 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 whose true Hamiltonian 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 constructed by using the ordinary Raileigh-Schrödinger stationary perturbative expansion. The resulting formula would, however, have a form inconvenient from the point of view of formulating the Dyson expansion.

The general result (1.29) can be also applied to generalized (nonnormalizable) eigenvectors of H_0. For example, in the nonrelativistic scattering theory the free Hamiltonian H_0 has no normalizable eigenvectors and the operators $U^{\varepsilon}(0, \mp\infty)$ become in the limit $\varepsilon \to 0$ the M$\not{\rm o}$ller operators $\Omega_{\pm}$ which will be introduced in section 7.1. In this case matrix elements of the term proportional to ε on right-hand side of (1.29) between (normalizable) vectors of any arbitrarily chosen basis of the Hilbert space vanish. The left-hand side of (1.29) becomes then the intertwining relation $H\Omega_{\pm} = \Omega_{\pm}H_0$ playing an important role in the formal scattering theory (outlined in section 7).

In relativistic theory of interacting particles presented in sections 7, 8 and 9, which is simple cases can be treated as a formulation (though not the best one) of relativistic quantum field theory, the ε term 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 section 7). In the limit $\varepsilon \to 0$ the operators $U_I^{\varepsilon}(0, \mp\infty)$ become then again the M$\not{\rm o}$ller operators satisfying the intertwining relation $H\Omega_{\pm} = \Omega_{\pm}H_0$. When applied to generalized (non-normalizable) eigenvectors of H_0 the M$\not{\rm o}$ller operators yield then the corresponding (in the sense which will be explained in section 7) *in* and *out* generalized eigenvectors of H, whereas when applied to the single[7] 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 normalized to unity H eigenvector $|\Omega\rangle$.

Finally, in the approach to nonrelativistic quantum mechanics of many particles based on Green's functions and in quantum field theory formulated (in the continuum) as in section 13 (without the restrictive assumptions of

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

[7]It is the standard assumption that the Hamiltonians H_0 and H of a quantum field theory model formulated in the continuum have, in the properly selected separable Hilbert space, each only one normalizable eigenvector which is its ground state vector.

section 7) 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 formula (1.34) gives a nonzero difference of the respective ground state energies. The Gell-Mann - Low theorem constitutes in this case the cornerstone of the Dyson perturbative expansion of Green's functions which are, in some sense, the most important quantities of theoretical interest (see section 13).

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 the 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 section. It will also serve to introduce the notion of the *in* and *out* states and the S-matrix.

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

$$\begin{aligned} H_0 &= \hbar\omega a^\dagger a + \Delta_\omega \,, \\ V_{\rm int}(t) &= a^\dagger f(t) + a f^*(t) \,. \end{aligned} \tag{1.36}$$

The creation and annihilation operators are as usually defined by

$$a = \sqrt{\frac{M\omega}{2\hbar}} \left(x + \frac{i}{M\omega} p \right), \qquad a^\dagger = \sqrt{\frac{M\omega}{2\hbar}} \left(x - \frac{i}{M\omega} p \right), \tag{1.37}$$

and satisfy the commutation rules

$$[a,\, a^\dagger] = 1 \,, \qquad [a,\, a] = [a^\dagger,\, a^\dagger] = 0 \,. \tag{1.38}$$

$f(t)$ is some c-number function which can be complex. If

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

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

$$H = \hbar\omega a^\dagger a + \Delta_\omega + \lambda\, a^\dagger + \lambda^* a = \hbar\omega A^\dagger A + \Delta_\omega - \frac{|\lambda|^2}{\hbar\omega} \,, \tag{1.39}$$

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[8] to show that there must be a state $|\tilde{0}\rangle$ annihilated by A and that the vectors $(A^\dagger)^n|\tilde{0}\rangle$ are the eigenvectors of $A^\dagger A$ with the eigenvalues n. The entire spectrum of H given by (1.39) is, therefore, simply shifted downwards, with respect to the spectrum of H_0, by $|\lambda|^2/\hbar\omega$. In particular, $E_\Omega = E_{\Omega_0} - |\lambda|^2/\hbar\omega$.

In the Heisenberg picture one works with time dependent operators while state-vectors do not depend on time. Since all observables 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 with the help of 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 therefore is

$$\dot{a}_H(t) = -i\omega\, a_H(t) - \frac{i}{\hbar}\, f(t)\,, \tag{1.40}$$

while 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:

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

In order to find a solution of the full inhomogeneous equation (1.40) we substitute in it $d(t)\exp(-i\omega t)$ for $a_H(t)$. This leads to the c-number equation

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

[8]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 $\alpha \geq 0$. Furthermore, 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 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.

Thus

$$a_H(t) = e^{-i\omega t}\left(a - \frac{i}{\hbar}\int_0^t d\tau\, e^{i\omega\tau}\, f(\tau)\right) \equiv e^{-i\omega t}\,(a + h(t))\,,$$
$$a_H^\dagger(t) = e^{i\omega t}\left(a^\dagger + \frac{i}{\hbar}\int_0^t d\tau\, e^{-i\omega\tau}\, f^*(\tau)\right) \equiv e^{i\omega t}\left(a^\dagger + h^*(t)\right), \qquad (1.41)$$

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

$$a_H(t) = \tilde{U}^\dagger(t,0)\, a\, \tilde{U}(t,0)\,, \qquad a_H^\dagger(t) = \tilde{U}^\dagger(t,0)\, a^\dagger\, \tilde{U}(t,0)\,. \qquad (1.42)$$

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

$$\tilde{U}(t,0) = e^{-iH_0 t/\hbar}\, e^{h(t)a^\dagger - h^*(t)a}\,. \qquad (1.43)$$

This can be easily checked by applying twice the operator formula

$$e^B A\, e^{-B} = A + [B,\, A] + \frac{1}{2!}[B,\, [B,\, A]] + \ldots$$
$$= A - [A,\, B] + \frac{1}{2!}[[A,\, B],\, B] + \ldots \qquad (1.44)$$

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 (1.43) generates the required shifts of a and $a^\dagger$. Note that the relations (1.42) determine $\tilde{U}(t,0)$ only up to a c-number 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 $U(0,0) = 1$.

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

$$\tilde{U}_I^\varepsilon(t,0) = e^{h(t)a^\dagger - h^*(t)a}\,. \qquad (1.45)$$

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 $U_I^\varepsilon(0,0) = 1$) and using the property (1.4) we would then use

$$\tilde{U}_I^\varepsilon(0,-\infty) = [\tilde{U}_I^\varepsilon(-\infty,0)]^\dagger = e^{-h(-\infty)a^\dagger + h^*(-\infty)a}\,. \qquad (1.46)$$

in the Gell-Mann - Low formula (1.34). Computing the required matrix element is straightforward:

$$\langle\Omega_0|\tilde{U}_I^\varepsilon(0,-\infty)|\Omega_0\rangle = e^{-\frac{1}{2}|h(-\infty)|^2}\langle 0|e^{-h(-\infty)a^\dagger}\, e^{h^*(-\infty)a}|0\rangle = e^{-\frac{1}{2}|h(-\infty)|^2}\,.$$

We have used here the Baker-Hausdorff formula

$$e^{X+Y} = e^{-\frac{1}{2}[X,\,Y]}\, e^X\, e^Y = e^{\frac{1}{2}[X,\,Y]}\, e^Y\, e^X\,, \tag{1.47}$$

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

$$h(-\infty) = -\frac{i}{\hbar}\int_0^{-\infty} d\tau\, e^{i\omega\tau} f(\tau) = \frac{i}{\hbar}\int_{-\infty}^0 d\tau\, \lambda\, e^{(\varepsilon+i\omega)\tau} = \frac{i}{\hbar}\,\frac{\lambda}{\varepsilon+i\omega}\,, \tag{1.48}$$

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

It follows that $\tilde{U}_I^\varepsilon(0,-\infty)$ obtained 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 $U_I^\varepsilon(0,-\infty)$ perturbatively up to the second order, using instead of the formula (1.23) the (fully equivalent to it) iterative solution (1.7):

$$U_I^\varepsilon(0,-\infty) = 1 - \frac{i}{\hbar}\int_{-\infty}^0 d\tau\, e^{\varepsilon\tau}\left[\lambda^* a\, e^{-i\omega\tau} + \lambda\, a^\dagger\, e^{i\omega\tau}\right]$$
$$-\frac{1}{\hbar^2}\int_{-\infty}^0 d\tau_1\, e^{\varepsilon\tau_1}\left[\lambda^* a\, e^{-i\omega\tau_1} + \lambda\, a^\dagger e^{i\omega\tau_1}\right]\int_{-\infty}^{\tau_1} d\tau_2\, e^{-i\omega\tau_2}\left[\lambda^* a\, e^{-i\omega\tau_2} + \lambda\, a^\dagger e^{i\omega\tau_2}\right] + \dots$$

It is easy to see that the first order term of this formula

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

precisely equals the first order term in the expansion

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

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

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

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

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

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[9]

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

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

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

which is precisely the energy shift $E_\Omega - E_{\Omega_0}$ due to the constant perturbation of H_0 by the time-independent interaction $V_{\rm int} = \lambda\,a^\dagger + \lambda^* a$.

As another application of the exact solution (1.41) of the Heisenberg equation of motion we consider the behaviour of the harmonic oscillator subject to the action of the 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 and to test different approximations 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

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

and $a_{\rm out}^\dagger$ and $a_{\rm in}^\dagger$ are their Hermitian conjugates. It is clear that

$$\begin{aligned} a_H(t) &\to e^{-i\omega t}\,a_{\rm in} \qquad \text{for} \quad t \to -\infty\,, \\ a_H(t) &\to e^{-i\omega t}\,a_{\rm out} \qquad \text{for} \quad t \to +\infty\,. \end{aligned} \tag{1.49}$$

[9] We do not try to show here that the phase φ is not corrected in higher orders in λ.

The *in* and *out* operators defined in this way are related to each other by

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

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

$$c(t_2, t_1) = \frac{i}{\sqrt{2M\hbar\omega}} \int_{t_1}^{t_2} d\tau\, e^{i\omega\tau} F(\tau)\,. \tag{1.50}$$

The operators $a_{\rm in}$ and $a^\dagger_{\rm in}$ as well as $a_{\rm out}$ and $a^\dagger_{\rm out}$ satisfy the same commutation relation as do the ordinary annihilation/creation operators (1.37):

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

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 $a^\dagger_{\rm in}$ and $a^\dagger_{\rm out}$ acting respectively on these states create eigenvectors of the operators $a^\dagger_{\rm in}a_{\rm in}$ and $a^\dagger_{\rm out}a_{\rm out}$. This means that in the Hilbert space of the harmonic oscillator (spanned by the eigenvectors $|n\rangle$ of H_0) there exist two other complete sets of orthonormal vectors :

$$\begin{aligned} &|0\ {\rm in}\rangle && |0\ {\rm out}\rangle \\ &|1\ {\rm in}\rangle \equiv a^\dagger_{\rm in}|0\ {\rm in}\rangle && |1\ {\rm out}\rangle \equiv a^\dagger_{\rm out}|0\ {\rm out}\rangle \\ &|2\ {\rm in}\rangle \equiv \frac{1}{\sqrt{2!}}(a^\dagger_{\rm in})^2|0\ {\rm in}\rangle && |2\ {\rm out}\rangle \equiv \frac{1}{\sqrt{2!}}(a^\dagger_{\rm out})^2|0\ {\rm out}\rangle \end{aligned} \tag{1.51}$$

etc., which form two alternative (in addition to the eigenvectors $|n\rangle$ of $a^\dagger a$) bases of the Hilbert space. These vectors (1.51) are called the *in* and *out* states, respectively. Furthermore, since

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

it follows from (1.49) 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* states constructed as in (1.51) are therefore the eigenstates of the Heisenberg picture Hamiltonian $H^H(t)$ in the far past and the *out* states play the analogous role with respect to $H^H(t)$ in the far future. More precisely, from the idea underlying the Heisenberg picture (explained in section 1.1), it follows that the vectors $|n\ {\rm in}\rangle$ (the vectors $|n\ {\rm out}\rangle$) when treated as Schrödinger picture vectors at $t = 0$ and evolved with the help of the evolution operator $U(t,0)$ become at $t = -\infty$ (at $t = +\infty$) the

eigenvectors $|n\rangle$ of H_0. That is, the constant in time 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 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

$$P(n \to k) = |S_{kn}|^2 \,. \tag{1.52}$$

where

$$S_{kn} \equiv \langle k\ \text{out}|n\ \text{in}\rangle \,. \tag{1.53}$$

The (complex in general) scalar products S_{kn} - the transition amplitudes - measure the content of the state $|k\ \text{out}\rangle$ in the state $|n\ \text{in}\rangle$. The amplitudes S_{kn} form the so-called S-matrix which is unitary, that is[10] $S^\dagger \cdot S = I$:

$$\begin{aligned}(S^\dagger)_{mk}S_{kn} \equiv S^*_{km}S_{kn} &= \sum_{k=0}^{\infty}\langle k\ \text{out}|m\ \text{in}\rangle^*\langle k\ \text{out}|n\ \text{in}\rangle \\ &= \sum_{k=0}^{\infty}\langle m\ \text{in}|k\ \text{out}\rangle\langle k\ \text{out}|n\ \text{in}\rangle = \langle m\ \text{in}|n\ \text{in}\rangle = \delta_{mn}\,,\end{aligned} \tag{1.54}$$

owing to the completeness of the set of vectors $|k\ \text{out}\rangle$. (In the similar way, using the completeness of the set of vectors $|k\ \text{in}\rangle$, one shows that $S\cdot S^\dagger = I$). In view of (1.52), unitarity of the S-matrix implies that

$$\sum_k P(n \to k) = 1 \,. \tag{1.55}$$

Of course,[11] $\langle k\ \text{out}|n\ \text{in}\rangle = \delta_{kn}$ 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 between the eigenvectors $|k\rangle$ and $|n\rangle$ of the free Hamiltonian H_0. Another method, which we explain first, is to compute S_{kn} as matrix elements of another operator, called S, either between the states $|k\ \text{out}\rangle$ and $|n\ \text{out}\rangle$, or between the states $|k\ \text{in}\rangle$ and $|n\ \text{in}\rangle$.

[10] The dagger on S means here Hermitian conjugation of the c-number matrix (not of a Hilbert space operator).

[11] We assume here that the states $|0\ \text{in}\rangle$ and $|0\ \text{out}\rangle$ which can be defined with arbitrary phases, are chosen so that they coincide for $F = 0$.

The operator S is defined by the conditions

$$\begin{aligned} a_{\rm out} &= a_{\rm in} + c \, = S^\dagger a_{\rm in} S \,, \\ a^\dagger_{\rm out} &= a^\dagger_{\rm in} + c^* = S^\dagger a^\dagger_{\rm in} S \,. \end{aligned} \tag{1.56}$$

Similarly as in the preceding example, the relations (1.56) determine S only up to a phase factor. One possible choice is

$$S = \exp\Big(c\, a^\dagger_{\rm in} - c^* a_{\rm in} \Big) = \exp\Big(c\, a^\dagger_{\rm out} - c^* a_{\rm out} \Big) \,. \tag{1.57}$$

The operator S is clearly unitary here. Using (1.56) one sees that

$$a_{\rm in} S |0 \text{ out}\rangle = S S^\dagger a_{\rm in} S |0 \text{ out}\rangle = S a_{\rm out} |0 \text{ out}\rangle = 0 \,, \tag{1.58}$$

etc. which shows that once the arbitrary phase between $|0 \text{ in}\rangle$ and $S|0 \text{ out}\rangle$ is fixed by the relation[12] $S|0 \text{ out}\rangle = |0 \text{ in}\rangle$, one has

$$S|n \text{ out}\rangle = |n \text{ in}\rangle \,. \tag{1.59}$$

Indeed,

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

The scalar products (1.53), necessary to obtain the transition probabilities $P(n \to k) = |S_{kn}|^2$, can be, therefore, computed as the corresponding matrix elements of the S-operator:

$$S_{kn} = \langle k \text{ out} | n \text{ in}\rangle = \langle k \text{ out} | S | n \text{ out}\rangle = \langle k \text{ in} | S | n \text{ in}\rangle \,. \tag{1.60}$$

The first form follows directly from (1.59), while the second one from the conjugated relation $\langle k \text{ out}| = \langle k \text{ in}| S$. With the help of the Baker-Hausdorff formula (1.47) the first of the two forms (1.57) of the S operator can be written as

$$S = \exp\left(-\frac{1}{2} |c|^2 \right) e^{c\, a^\dagger_{\rm in}} \, e^{-c^* a_{\rm in}} \,, \tag{1.61}$$

which are more suitable for computing its matrix elements (1.60):

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

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

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

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

we obtain

$$\begin{aligned} S_{nm}(c, c^*) \equiv \langle n \text{ in}|S|m \text{ in}\rangle &= \frac{1}{\sqrt{n! m!}} e^{-\frac{1}{2}|c|^2} \langle 0 \text{ in}|(a_{\rm in} + c)^n (a_{\rm in}^\dagger - c^*)^m |0 \text{ m}\rangle \\ &= \frac{1}{\sqrt{n!\, m!}} e^{-\frac{1}{2}|c|^2} \sum_{k=0}^{n} \sum_{l=0}^{m} \binom{n}{k} \binom{m}{l} c^{n-k} (-c^*)^{m-l} \langle 0 \text{ in}|(a_{\rm in})^k (a_{\rm in}^\dagger)^l |0 \text{ in}\rangle \\ &= \frac{1}{\sqrt{n!\, m!}} \exp\left(-\frac{1}{2}|c|^2 \right) \sum_{k=0}^{min(n,m)} k! \binom{n}{k} \binom{m}{k} c^{n-k} (-c^*)^{m-k} \,. \end{aligned} \tag{1.62}$$

From this formula it can be seen that

$$S_{nm}(c, c^*) = S_{mn}(-c^*, -c) = (-1)^{m-n} \left(S_{mn}(c, c^*) \right)^* \,, \tag{1.63}$$

and, hence, $|S_{nm}|^2 = |S_{mn}|^2$. We also see that

$$P(0 \to 0) = |\langle 0 \text{ in}|S|0 \text{ in}\rangle|^2 = \exp\left(-|c|^2\right) \,,$$

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

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

which is precisely the Poisson distribution with $\bar{n} = |c|^2$ (that is in a statistical ensemble of oscillators all prepared at $t = -\infty$ in the ground state and subject to the force $F(t)$ the mean excitement at $t = \infty$ is $|c|^2$). It is also interesting to compare the probability $P(n \to n+1)$ with $P(0 \to 1)$. For small $|c|$, 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 $P(0 \to 1)$. As we will be discussed in section 5.5, by analogy with how states of many identical particles are represented in the second

quantization formalism (developed in section 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 ($|c| \ll 1$), creating one additional boson is $n+1$ times more probable if there were already n bosons present initially. For $|c|$ not small this simple rule is no longer true in this model.

For completeness we will also show, how the transition amplitudes S_{kn} (1.53) can be computed using the S_0 operator. To this end we begin with the operator $\tilde{U}(t,0)$ satisfying

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

and the conjugated relation. The true Schrödinger picture evolution operator $U(t,0)$, given by (1.9), can differ from $\tilde{U}(t,0)$ one 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 (1.50) and some phase factor $\varphi(t,0)$, which will not be relevant. The corresponding interaction picture evolution operator is then given by (1.24) and reads

$$U_I(t,0) = e^{c(t,0)\, a^\dagger - c^*(t,0)\, a}\, e^{i\varphi(t,0)}. \tag{1.64}$$

It is clear that

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

and

$$\begin{aligned} U_I^\dagger(\infty,0)\, a\, U_I(\infty,0) &= a + c(\infty,0) = a_{\text{out}}, \\ U_I^\dagger(\infty,0)\, a^\dagger U_I(\infty,0) &= a^\dagger + c^*(\infty,0) = a_{\text{out}}^\dagger. \end{aligned}$$

It then follows that

$$\begin{aligned} U_I^\dagger(-\infty,0)|n\rangle &= |n \text{ in}\rangle, \\ U_I^\dagger(\infty,0)|n\rangle &= |n \text{ out}\rangle. \end{aligned} \tag{1.65}$$

Therefore,

$$\begin{aligned} S_{nm} \equiv \langle \text{out } n | m \text{ in}\rangle &= \langle n | U_I(\infty,0) U_I^\dagger(-\infty,0) | m\rangle \\ &= \langle n | U_I(\infty,0) U_I(0,-\infty) | m\rangle = \langle n | U_I(\infty,-\infty) | m\rangle. \end{aligned} \tag{1.66}$$

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

$$S_0 \equiv U_I(\infty, -\infty) = \lim_{t_2 \to \infty} \lim_{t_1 \to -\infty} U_I(t_2, t_1)\,. \tag{1.67}$$

Using (1.64), the composition rules of the evolution operators (1.4), the Baker-Hausdorff formula (1.47) 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[13]

$$U_I(t_2, t_1) = e^{c(t_2,t_1)\,a^\dagger - c^*(t_2,t_1)\,a}\, e^{i\gamma}\,, \tag{1.68}$$

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

$$S_0 \equiv U_I^\dagger(0, \infty) U_I(0, -\infty)\,,$$

between the H_0 eigenstate and of the S operator which in general is defined as[14]

$$S \equiv U_I^\dagger(-\infty, 0) U_I(\infty, 0)\,, \tag{1.69}$$

between the corresponding *in* or the corresponding *out* states 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 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 7.2) but retain their interpretation as 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 of the properly defined *in* and *out* states. In all nonrelativistic scattering theories the S-matrix elements can be computed as here

[13]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 (1.50) 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.

[14]This definition of S readily follows by combining the relations (1.65) with the actionof S (1.59).

using the unitary S_0 operator. The operator[15] S is less useful (as will be explained in section 7 it is not always unitary). The S_0 operator will be also used for this purpose in the simplest formulation of quantum field theory, based on relativistic quantum mechanics of particles (exposed in sections 7, 8 and 9). This traditional formulation 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 section 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.

[15]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 phase factor.