TESTING METHODS OF COMPUTING CORRECTIONS TO THE GROUND-STATE ENERGY ON THE PERTURBED HARMONIC OSCILLATOR

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Received 6 February 2024, accepted 13 March 2024, published online 28 March 2024

There exist several ways of expressing the difference $E_\Omega - E_{\Omega_0}$ of the ground-state energies of the complete Hamiltonian $H = H_0 + V_{\rm int}$ and of its free part H_0. Most of them can be used to generate systematic perturbative expansions of E_Ω. In advanced applications to many-body quantum theory, the successive terms of these expansions are usually visualized in terms of diagrams (Goldstone diagrams, Feynman diagrams) and easily evaluated. Here, we recall these methods, discuss their foundations, and show how their working and their graphical representation can be simply introduced to the beginners on the harmonic oscillator example. In doing this, we will also clarify a delicate point in computing the corrections using the Goldstone diagrams which is somewhat misleadingly presented in textbooks like the one of Fetter and Walecka.

DOI:10.5506/APhysPolB.55.3-A4

1. Introduction

In typical problems of quantum mechanics, the time-independent Hamiltonian H of the system under considerations splits into a "free" part H_0 and a perturbation $V_{\rm int}$ and one wants to determine the eigenvalues of H computing corrections due to $V_{\rm int}$ (assumed to be proportional to some coupling constant λ) to the exactly known (by assumption) spectrum of eigenvalues of H_0. The simplest standard tool for this is the Rayleigh–Schrödinger perturbative expansion, presented in almost every textbook on quantum mechanics [1, 2], which allows to determine the energy E_L of a discrete eigenvector $|L\rangle$ of H connected in the (formal) limit $\lambda = 0$ to an eigenvector $|l\rangle$ (and its eigenvalue E_l) of H_0

$$E_L = E_l^{(0)} + \langle l|V_{\rm int}|l\rangle + \sum_{l'} \frac{|\langle l'|V_{\rm int}|l\rangle|^2}{E_l - E_{l'}} + \dots \tag{1}$$

In many situations, especially in discussing statistical properties at zero temperature of systems consisting of many elements (particles, nuclei, atoms, spins, *etc.*) the most important is the energy of the system's ground-state. In the course of developing more advanced methods of quantum mechanics adapted to study many body systems, one obtains several formulae allowing to determine the difference $E_\Omega - E_{\Omega_0}$ of the ground-states $|\Omega\rangle \equiv |L=0\rangle$ of H and $|\Omega_0\rangle \equiv |l=0\rangle$ of H_0. It is the purpose of this paper to illustrate these formulae on the examples which are easily accessible to beginners, namely on the harmonic oscillator subject to different types of perturbations. Some of them allow to easily write down also the exact solutions (*i.e.* the exact spectrum of $H = H_0 + V_{\rm int}$, where H_0 is the standard harmonic oscillator Hamiltonian, can be obtained) which helps to understand the working of these formulae and their origins.

The presented formulae are usually used to obtain systematic perturbative expansions of the difference $E_\Omega - E_{\Omega_0}$ in powers of the interaction strength λ. These expansions, successive terms of which are usually visualized in terms of Feynman or Goldstone diagrams, will be also illustrated here on the simple examples of the perturbed harmonic oscillator in a way which can be accessible to students. The comparison of two different ways of computing corrections to $E_\Omega - E_{\Omega_0}$ will allow to discover a subtlety in the expansion leading to Goldstone diagrams which is usually not mentioned in standard texts.

2. Advanced formulae for $E_\Omega - E_{\Omega_0}$

In the early fifties of the 20$^{\rm th}$ century, Gell-Mann and Low gave [3] (see also [4]) a prescription for constructing an eigenvector corresponding to the lowest eigenvalue E_Ω of the time-independent Hamiltonian $H = H_0 + V_{\rm int}$ out of the normalized to unity eigenvector $|\Omega_0\rangle$ of H_0. It is given by the formula

$$\lim_{\varepsilon\to 0^+} \frac{U_{\rm I}^\varepsilon(0,-\infty)|\Omega_0\rangle}{\langle\Omega_0|U_{\rm I}^\varepsilon(0,-\infty)|\Omega_0\rangle}\,, \tag{2}$$

in which $U_{\rm I}^\varepsilon(t_2,t_1)$ is the interaction picture evolution operator of the (fictitious) system with the modified, time-dependent Hamiltonian

$$H^\varepsilon(t) = H_0 + {\rm e}^{\varepsilon t} V_{\rm int}\,. \tag{3}$$

The evolution operator $U_{\rm I}^\varepsilon(t_2,t_1)$ satisfies the differential equation

$$i\hbar\,\frac{\rm d}{{\rm d}t_2}\,U_{\rm I}^\varepsilon(t_2,t_1) = {\rm e}^{\varepsilon t} V_{\rm int}^{\rm I}(t_2) U_{\rm I}^\varepsilon(t_2,t_1)\,, \tag{4}$$

with the initial condition $U_{\rm I}^\varepsilon(t,t) = \hat{1}$. In this equation,

$${\rm e}^{\varepsilon t} V_{\rm int}^{\rm I}(t) = {\rm e}^{iH_0t/\hbar}{\rm e}^{\varepsilon t} V_{\rm int}{\rm e}^{-iH_0t/\hbar} \tag{5}$$

is the interaction operator in the interaction picture. Equation (5) can be transformed into the integral equation

$$U_{\mathrm{I}}^{\varepsilon}(t_2,t_1) = \hat{1} + \frac{1}{i\hbar}\int_{t_1}^{t_2} \mathrm{d}t\, \mathrm{e}^{\varepsilon t} V_{\mathrm{int}}^{\mathrm{I}}(t)\, U_{\mathrm{I}}^{\varepsilon}(t,t_1)\,, \tag{6}$$

with the initial condition built-in and solved iteratively. In this way, $U_{\mathrm{I}}^{\varepsilon}(t_2,t_1)$ gets represented in the form of the series

$$\begin{aligned} U_{\mathrm{I}}^{\varepsilon}(t_2,t_1) = \hat{1} \;&+\; \frac{1}{i\hbar}\int_{t_1}^{t_2} \mathrm{d}t \mathrm{e}^{\varepsilon t} V_{\mathrm{int}}^{\mathrm{I}}(t) \\ &+\; \left(\frac{1}{i\hbar}\right)^2 \int_{t_1}^{t_2} \mathrm{d}t''\, \mathrm{e}^{\varepsilon t''} V_{\mathrm{int}}^{\mathrm{I}}\left(t''\right) \int_{t_1}^{t''} \mathrm{d}t'\, \mathrm{e}^{\varepsilon t'} V_{\mathrm{int}}^{\mathrm{I}}\left(t'\right) + \dots \end{aligned} \tag{7}$$

This can be formally written in the familiar form

$$U_{\mathrm{I}}^{\varepsilon}(t_2,t_1) = \mathrm{T}\exp\left\{ -\frac{i}{\hbar}\int_{t_1}^{t_2} \mathrm{d}t\, \mathrm{e}^{\varepsilon t} V_{\mathrm{int}}^{\mathrm{I}}(t) \right\}\,, \tag{8}$$

in which T stands for the operation of chronological ordering.

The Gell-Mann–Low construction (2) is based on the adiabatic principle which asserts (see *e.g.* [2]) that if a Hamiltonian undergoes a slow change in time and the system is at an initial moment in one of the instantaneous eigenstates of the Hamiltonian taken at that moment, it will, in the limit of infinitely slow change of H, pass through the corresponding sequence of the instantaneous eigenstates of the changing Hamiltonian. The requirement necessary for the validity of this statement is that the instantaneous eigenstates and eigenvalues of the changing Hamiltonian vary regularly, that is that they can be unambigously traced (*e.g.* that they do not cross with one another or merge)[1]. The factor $\mathrm{e}^{\varepsilon t}$ in (3) ensures slow (infinitely slow in the limit $\varepsilon \to 0^+$) switching on the interaction; since at $t = 0$, the instantaneous eigenstates of (3) are precisely the eigenstates of the original Hamiltonian of the system, the evolution from $t = -\infty$ to $t = 0$ of the ground-state eigenvector $|\Omega_0\rangle$ of H_0 should take it into an eigenvector H corresponding to its ground state. However, since the states of the system are in the Hilbert space represented by classes of vectors differing from one another by a phase, the vector $U_{\mathrm{I}}^{\varepsilon}(t, -\infty)|\Omega_0\rangle$ usually has no proper $\varepsilon \to 0^+$ limit: it involves a phase factor which diverges in this limit and it is the role of the denominator in (2) to remove this phase and to ensure the existence of the limit. The price is that the vector (2) is not normalized to unity.

In the formal proof that the vector (2) is the eigenvector of H crucial is the relation[2]

$$H U_{\mathrm{I}}^{\varepsilon}(0, -\infty) = U_{\mathrm{I}}^{\varepsilon}(0, -\infty) H_0 + i\hbar\varepsilon\,\lambda \frac{\partial}{\partial\lambda} U_{\mathrm{I}}^{\varepsilon}(0, -\infty)\,. \tag{9}$$

In textbooks [4], it is proven "perturbatively" by working out the commutator of H_0 with every term of the expansion of the exponent in formula (8), but recently an ingenious "nonperturbative" proof, based on manipulations done directly on the equation (6), has been given by Molinari [7].

[1] For this reason, the Gell-Mann–Low prescription fails if the interaction V_{int} induces dynamical breaking of a symmetry. This can happen in nonrelativistic many body quantum mechanics, *e.g.* in the theory of superconductivity and in relativistic quantum field theories (*e.g.* in Quantum Chromodynamics with massless quarks due to the dynamical breaking of the chiral symmetry). In such a case, the way out is to perform an appropriate transformation of the dynamical degrees of freedom and to start from another H_0 the spectrum of which has already the symmetry breaking encoded in it. In relativistic field theory models, *e.g.* in the Standard Model, symmetry breaking is frequently "parametrical", *i.e.* it is induced by taking a mass squared parameter of the Lagrangian to be negative. In this case, the naive H_0 is ill defined (has no ground state) but the problem can be cured by adding to the Lagrangian a term explicitly breaking the symmetry, proportional to a small parameter (which allows to define a H_0 with which the Gell-Mann–Low prescription can already be applied) and sending this parameter to zero at the end. Direct application of the Gell-Mann–Low construction (without bothering about the dynamical breaking of the chiral symmetry) in the perturbative Quantum Chromodynamics is possible owing to nonzero quark masses which provide the source of explicit chiral symmetry breaking.

[2] The interpretation of this relation depends on the nature of the proper Hilbert space of the system (to which only normalizable vectors belong). For instance, if H_0 and H have no normalizable eigenstates, as happens *e.g.* in the scattering theory, matrix elements of the term proportional to ε between normalizable sates all vanish and this term must be treated as the zero operator; the relation becomes then the intertwining relation usually written [5, 6] in the form $H\Omega_{\pm} = \Omega_{\pm}H_0$, where $\Omega_{\pm} = U_{\mathrm{I}}^{\varepsilon}(0, \mp\infty)$ are the so-called Møller operators.

Acting directly on $|\varOmega_0\rangle$ with both sides of the relation (9), one obtains, using the fact that $H_0|\varOmega_0\rangle = E_{\varOmega_0}|\varOmega_0\rangle$, the equality

$$(H - E_{\varOmega_0})U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle = i\hbar\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle\,, \tag{10}$$

which shows that if a finite limit $\varepsilon \to 0^+$ of $U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle$ existed, the resulting vector would be in this limit the eigenvector of $H = H_0 + V_{\rm int}$ with the eigenvalue $E_{\varOmega_0}$: the interaction would not change the energy of the ground state. This means that, except for very special cases[3], the limit $\varepsilon \to 0^+$ of $U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle$ must be singular. The equality (10) can, however, be rewritten (before taking the limit $\varepsilon \to 0^+$) in the equivalent form

$$\begin{aligned}&\left(H - E_{\varOmega_0} - i\hbar\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,\ln\langle\varOmega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle\right)\frac{U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle}{\langle\varOmega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle}\\ &= i\hbar\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,\frac{U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle}{\langle\varOmega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle}\,,\end{aligned} \tag{11}$$

which shows that if the vector $U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle/\langle\varOmega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle$ is non-singular in the $\varepsilon \to 0^+$ limit (and, therefore, the right-hand side vanishes in this limit), it is an eigenvector of H with the eigenvalue

$$E_{\varOmega} = E_{\varOmega_0} + i\hbar\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,\ln\langle\varOmega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle\,. \tag{12}$$

Thus, the energy of the ground state of H can be extracted from the singular phase of the vector $U_{\rm I}^{\varepsilon}(0,-\infty)|\varOmega_0\rangle$. A more symmetric form of this formula is the so-called Sucher formula [8]

$$E_{\varOmega} - E_{\varOmega_0} = \frac{1}{2}\,i\hbar\,\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,\ln\langle\varOmega_0|S_0^{\varepsilon}|\varOmega_0\rangle\,, \tag{13}$$

in which $S_0^{\varepsilon} = U_{\rm I}^{-\varepsilon}(\infty,0)U_{\rm I}^{\varepsilon}(0,-\infty) = [U_{\rm I}^{-\varepsilon}(0,\infty)]^{\dagger}U_{\rm I}^{\varepsilon}(0,-\infty)$ is the operator which in (a class of simple) quantum field theories generates the S-matrix elements [6].

[3] This is so in the nonrelativistic scattering theory when no bound states are possible in the potential $V_{\rm int} = V(\boldsymbol{r})$ on which the scattering occurs. This is also the assumption on which the old-fashioned (largely shaped in the course of the historical development of Quantum Electrodynamics) approach to obtain S-matrix elements in (a rather narrow class of) relativistic theories is based [6]. In this case, it is enforced by modifying the interaction term $V_{\rm int}$ (by adding to it counterterms) order-by-order in the perturbative expansion and by imposing the so-called on-shell renormalization conditions.

A more practical formula, directly leading to a systematic expansion, the terms of which can be visualized by diagrams (see Sections 5, 6), is obtained by closing the relation (10) from the left with $\langle\Omega_0|$ and dividing both sides by $\langle\Omega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\Omega_0\rangle$: Since the part H_0 of H can then act on $\langle\Omega_0|$, one obtains the relation

$$\frac{\langle\Omega_0|V_{\rm int}U_{\rm I}^{\varepsilon}(0,-\infty)|\Omega_0\rangle}{\langle\Omega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\Omega_0\rangle} = i\hbar\varepsilon\,\lambda\,\frac{\partial}{\partial\lambda}\,\ln\langle\Omega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\Omega_0\rangle\,, \tag{14}$$

which, when combined with (12) leads to the expression

$$E_{\Omega}-E_{\Omega_0} = \frac{\langle\Omega_0|V_{\rm int}U_{\rm I}^{\varepsilon}(0,-\infty)|\Omega_0\rangle}{\langle\Omega_0|U_{\rm I}^{\varepsilon}(0,-\infty)|\Omega_0\rangle}\,, \tag{15}$$

for the difference of the ground-state energies.

Both expressions, (15) and (13), provide the practical means (alternative to the Rayleigh–Schrödinger expansion (1)) to compute the shift of the ground-state energy due to the interaction $V_{\rm int}$. In both of them, the limit $\varepsilon\to 0^+$ is implicitly taken *after* the time argument(s) of the evolution operator(s) are sent to infinity.

Yet another way of computing the energy shift $E_{\Omega}-E_{\Omega_0}$ is obtained by considering the "imaginary time" analog

$$\mathcal{U}_{\rm I}(\tau_2,\tau_1) = {\rm e}^{\tau_2 H_0}\,{\rm e}^{-(\tau_2-\tau_1)H}\,{\rm e}^{-\tau_1 H_0} \tag{16}$$

of the ordinary interaction picture evolution operator which satisfies the differential equation analogous to (4) with the same initial condition and can, therefore, be formally represented by the expression analogous to (8) but with $t_{1,2}$ replaced by $\tau_{1,2}$, $(i/\hbar)dt$ by $d\tau$, the chronological ordering T by the ordering T_τ with respect to the "imaginary time" τ and ${\rm e}^{\varepsilon t}V_{\rm int}^{\rm I}(t)$ defined by (4) replaced by the operator $V_{\rm int}^{\rm I}(\tau) = {\rm e}^{\tau H_0}V_{\rm int}{\rm e}^{-\tau H_0}$. Since ${\rm e}^{-\beta H} = {\rm e}^{-\beta H_0}\mathcal{U}_{\rm I}(\beta,0)$, one can write the equality

$$\frac{{\rm Tr}\big({\rm e}^{-\beta H}\big)}{{\rm Tr}({\rm e}^{-\beta H_0})} = {\rm Tr}(\hat\rho_0\,\mathcal{U}_{\rm I}(\beta,0))\,, \tag{17}$$

in which $\hat\rho_0 \equiv {\rm e}^{-\beta H_0}/{\rm Tr}({\rm e}^{-\beta H_0})$ is the Canonical Ensemble statistical operator of the free system corresponding to its equilibrium with a heat bath at the temperature $1/k_{\rm B}\beta$ and the trace Tr is taken over the Hilbert space. The right-hand side of (17) when expanded

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int\limits_{-\beta/2}^{\beta/2}{\rm d}\tau_n\ldots\int\limits_{-\beta/2}^{\beta/2}{\rm d}\tau_1{\rm Tr}\left(\hat\rho^{(0)}\,\mathrm{T}_\tau\left[V_{\rm int}^{\rm I}(\tau_n)\ldots V_{\rm int}^{\rm I}(\tau_1)\right]\right)\,, \tag{18}$$

can be evaluated using the "thermal" version of the Wick theorem [4] and, especially in the case of nonrelativistic many-body systems or relativistic field theories, represented by "vacuum" Feynman diagrams; what is, however, important here is that in the limit of $\beta \to \infty$, the analytic continuation $\beta \to (i/\hbar)T$ of the terms of this expansion give precisely the terms of the analogous expansion of the expression

$$\langle \Omega_0 | \mathrm{T} \exp\left\{ -\frac{i}{\hbar} \int\limits_{-T/2}^{T/2} \mathrm{d}t\, V^{\mathrm{I}}_{\mathrm{int}}(t) \right\} |\Omega_0\rangle \equiv \langle \Omega_0 | U_{\mathrm{I}}(T/2, -T/2) | \Omega_0 \rangle \,, \tag{19}$$

in the limit of $T \to \infty$. On the other hand, it is clear that in the zero temperature limit, $\beta \to \infty$, the left-hand side of (17) goes into $\exp(-\beta(E_\Omega - E_{\Omega_0}))$. It follows that upon analytic continuation, one obtains the formula[4]

$$\lim_{T\to\infty} \exp\left\{ -i\frac{T}{\hbar}\left(E_\Omega - E_{\Omega_0}\right) \right\} = \lim_{T\to\infty} \langle \Omega_0 | U_{\mathrm{I}}(T/2, -T/2) | \Omega_0 \rangle \,, \tag{20}$$

When the right-hand side of (20) is expanded and represented by the momentum space Feynman diagrams, the quantity $(E_\Omega - E_{\Omega_0})/V$, where V is the volume of the system, is given (because taking the logarithm of the right-hand side is equivalent to omitting disconnected diagrams) by $i\hbar$ times the sum of the connected vacuum diagrams. Moreover, since $U_{\mathrm{I}}(T/2, -T/2) = \lim_{\varepsilon\to 0^+} U_{\mathrm{I}}^{-\varepsilon}(T/2, 0) U_{\mathrm{I}}^{\varepsilon}(0, -T/2)$, it also follows that

$$\begin{aligned} &\lim_{T\to\infty} \exp\left\{ -i\frac{T}{\hbar}\left(E_\Omega - E_{\Omega_0}\right) \right\} \\ &= \lim_{T\to\infty} \left(\lim_{\varepsilon\to 0^+} \langle \Omega_0 | U_{\mathrm{I}}^{-\varepsilon}(T/2, 0) U_{\mathrm{I}}^{\varepsilon}(0, -T/2) | \Omega_0 \rangle \right), \end{aligned} \tag{21}$$

that is, the shift of the ground-state energy due to the interaction V_{int} can be read off from the exponent of the expectation value in the ground states of the free system of the product of the interaction picture evolution operators corresponding to the adiabatic switching on and off the interaction, provided the limit $\varepsilon \to 0^+$ is taken *before* the limit $T \to \infty$.

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[4] Superficially it seems, because this relies on the algebraic relation between $\mathrm{e}^{-\beta H}$ and $\mathrm{e}^{-\beta H_0}\mathcal{U}_{\mathrm{I}}(\beta, 0)$, that, unlike the formulae relying on the Gell-Mann–Low construction, this one is not invalidated if the interaction V_{int} causes spontaneous breaking of some symmetries. Yet in the limit of infinitely large system (spontaneous breaking of symmetries always require it), the Hilbert space becomes nonseparable and the trace depends on the basis in which it is performed; thus, also in this case, the tacit assumption is that the basis of the H_0 eigenvectors is chosen appropriately.

While the last approach yields the expansion of the energy shift in terms of the standard Feynman diagrams, the formula (15) leads to the perturbative expansions of the energy shift $E_\Omega - E_{\Omega_0}$ which can be encoded either in terms of the Feynman or the so-called Goldstone diagrams. All these methods will be illustrate in the following sections on the simplest possible examples based on the (familiar to every student) harmonic oscillator.

3. Harmonic oscillator with the time-dependent perturbation linear in a and $a^\dagger$

The simplest example allowing to illustrate the working of the formulae (12) and (21) is the Hamiltonian $H = H_0 + V_{\rm int}(t)$, with

$$\begin{aligned} H_0 &= \hbar\omega a^\dagger a + \varDelta_\omega \qquad \varDelta_\omega = \frac{1}{2}\hbar\omega\,, \\ V_{\rm int}(t) &= a^\dagger f(t) + a f^*(t)\,. \end{aligned} \tag{22}$$

The annihilation and creation operators are as usually defined as

$$a = \sqrt{\frac{M\omega}{2\hbar}}\left(\hat{x} + \frac{i}{M\omega}\,\hat{p}\right), \qquad a^\dagger = \sqrt{\frac{M\omega}{2\hbar}}\left(\hat{x} - \frac{i}{M\omega}\,\hat{p}\right), \tag{23}$$

and satisfy the commutation rules

$$[a,\, a^\dagger] = \hat{1}\,, \qquad [a,\, a] = [a^\dagger,\, a^\dagger] = 0\,. \tag{24}$$

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

$$f(t) = f^*(t) = -\sqrt{\frac{\hbar}{2M\omega}}\,F(t)\,, \tag{25}$$

(22) is just the Hamiltonian $H = H_0 - xF(t)$ of the one-dimensional harmonic oscillator subjected to the action of the time-dependent external force $F(t)$. With $f(t) = {\rm e}^{\varepsilon t}\lambda$, the model will serve to illustrate the Gell-Mann–Low construction of the H ground-state eigenvector and of the formulae (12) and (21) for the ground-state energy of the time-independent Hamiltonian[5] $H = \hbar\omega a^\dagger a + \varDelta_\omega + \lambda\, a^\dagger + \lambda^* a$. The exact spectrum of H can readily be found by writing

$$H = \hbar\omega a^\dagger a + \varDelta_\omega + \lambda\, a^\dagger + \lambda^* a = \hbar\omega A^\dagger A + \varDelta_\omega - \frac{|\lambda|^2}{\hbar\omega}\,, \tag{26}$$

[5] Any phase factor of the coupling λ can be absorbed into the definition of the operators a and $a^\dagger$. Hence, λ can be taken real. Still, we will keep writing λ^* to give the formulae a more symmetric form.

where $A = a + \lambda/\hbar\omega$, $A^\dagger = a^\dagger + \lambda^*/\hbar\omega$. 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 (see *e.g.* [9]) to show 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 is, therefore, simply shifted downwards, with respect to the spectrum of $H_0 = \hbar\omega a^\dagger a + \Delta_\omega$, by $|\lambda|^2/\hbar\omega$. In particular, $E_\Omega = E_{\Omega_0} - |\lambda|^2/\hbar\omega$.

In order to test the Gell-Mann–Low construction and formula (12), one must find the interaction picture evolution operator corresponding to the Hamiltonian (22). We will do it by first finding the Schrödinger picture evolution operator $U\left(t_2, t_1\right) = \mathrm{e}^{-(i/\hbar)H(t_2-t_2)}$ and then by using the formula

$$U_{\mathrm{I}}\left(t_2, t_1\right) = \mathrm{e}^{iH_0t_2/\hbar}\, U\left(t_2, t_1\right) \mathrm{e}^{-iH_0t_1/\hbar}\,, \tag{27}$$

relating it to the interaction picture one. Finally, we will set $f(t) = \lambda \mathrm{e}^{\varepsilon t}$.

If the Heisenberg picture is defined so that the Schrödinger (time-dependent) state-vectors coincide at $t = 0$ with their Heisenberg picture counterparts, the operators $O_{\mathrm{H}}(t)$ and O_S in these pictures are related by

$$O_{\mathrm{H}}(t) = U^\dagger(t,0) O_{\mathrm{S}} U(t,0)\,. \tag{28}$$

Therefore, any Heisenberg picture operator $O_{\mathrm{H}}(t)$ satisfies the Heisenberg equation[6]

$$\dot{O}_{\mathrm{H}}(t) = \frac{i}{\hbar}[H_{\mathrm{H}}(t),\, O_{\mathrm{H}}(t)]\,, \tag{29}$$

where $H_{\mathrm{H}}(t)$ is the Hamiltonian transformed to the Heisenberg picture according to the rule (28). The commutators arising in the equations satisfied by the Heisenberg picture counterparts $a_{\mathrm{H}}(t)$ and $a^\dagger_{\mathrm{H}}(t)$ of the creation and annihilation operators (out of which any other operator acting in the Hilbert space of the harmonic oscillator can be constructed) can be easily evaluated:

$$\begin{aligned} \left[H^H(t),\, a_{\mathrm{H}}(t)\right] &= U^\dagger(t,0)\,[H,\, a]\, U(t,0) \\ &= U^\dagger(t,0)\, \left[-\hbar\omega\, a - f(t)\right]\, U(t,0) \\ &= -\hbar\omega\, a_{\mathrm{H}}(t) - f(t)\,. \end{aligned} \tag{30}$$

The equation of motion of $a_{\mathrm{H}}(t)$, therefore, reads

$$\dot{a}_{\mathrm{H}}(t) = -i\omega\, a_{\mathrm{H}}(t) - \frac{i}{\hbar}\, f(t)\,. \tag{31}$$

[6] It readily follows by differentiating both sides of (28) with respect to t and using equation (38). As we assume that O_{S} does not depend on time, we omit the term $U^\dagger(t,0)(\partial O_S/\partial t)U(t,0)$ on the right-hand side of (29).

The equation satisfied by $a^\dagger_{\rm H}(t)$ is just the Hermitian conjugate of this one. The solutions of the homogeneous part of this equation is obvious

$$a_{\rm H}(t) = {\rm e}^{-i\omega t}\, a_{\rm H}(0) \equiv {\rm e}^{-i\omega t}\, a\,. \tag{32}$$

In order to find a solution of the full inhomogeneous equation, (31) we substitute in it ${\rm d}(t)\exp(-i\omega t)$ for $a_{\rm H}(t)$. This leads to the c-number equation

$$\dot{\rm d}(t) = -\frac{i}{\hbar}{\rm e}^{i\omega t} f(t)\,, \tag{33}$$

the solution of which can be found by a straightforward integration. Thus,

$$\begin{aligned} a_{\rm H}(t) &= {\rm e}^{-i\omega t}\left(a - \frac{i}{\hbar}\int\limits_0^t {\rm d}\tilde{t}\,{\rm e}^{i\omega\tilde{t}} f\left(\tilde{t}\right)\right) \equiv {\rm e}^{-i\omega t}\left(a + h(t)\right), \\ a^\dagger_{\rm H}(t) &= {\rm e}^{i\omega t}\left(a^\dagger + \frac{i}{\hbar}\int\limits_0^t {\rm d}\tilde{t}\,{\rm e}^{-i\omega\tilde{t}} f^*\left(\tilde{t}\right)\right) \equiv {\rm e}^{i\omega t}\Big(a^\dagger + h^*(t)\Big)\,. \end{aligned} \tag{34}$$

The lower limit of the integrals has been set to zero to secure the equalities $a_{\rm H}(0) = a$, $a^\dagger_{\rm H}(0) = a^\dagger$.

The simple exact form of $a_{\rm H}(t)$ and $a^\dagger_{\rm H}(t)$ allows to easily find an operator $\tilde{U}(t,0)$ which satisfies relations (28)

$$\tilde{U}(t,0) = {\rm e}^{-iH_0 t/\hbar}\,{\rm e}^{h(t)a^\dagger - h^*(t)a}\,. \tag{35}$$

This can be checked by applying twice the well-known operator formula

$${\rm e}^B A {\rm e}^{-B} = A + [B,\, A] + \frac{1}{2!}[B,\, [B,\, A]] + \ldots, \tag{36}$$

first, to find that

$${\rm e}^{iH_0 t/\hbar}\, a\, {\rm e}^{-iH_0 t/\hbar} = {\rm e}^{-i\omega t}\, a\,, \qquad {\rm e}^{iH_0 t/\hbar}\, a^\dagger\, {\rm e}^{-iH_0 t/\hbar} = {\rm e}^{i\omega t}\, a^\dagger\,, \tag{37}$$

and next, to check that the second exponential factor on the right-hand side of (35) generates the required shifts of a and $a^\dagger$.

Relations (28) determine $\tilde{U}(t,0)$ only up to a phase factor. As a result, Eq. (35) may differ by a c-number, possibly time-dependent phase factor $\varphi(t)$ from the true evolution operator $U(t,0)$, which is uniquely determined by the differential equation

$$i\hbar\frac{\rm d}{{\rm d}t_2}\, U(t_2,t_1) = H(t_2)\, U(t_2,t_1)\,, \tag{38}$$

and the initial condition $U(t,t) = \hat{1}$. To find $\varphi(t)$, one can insert the operator

$$U(t,0) = \mathrm{e}^{i\varphi(t)}\,\mathrm{e}^{-iH_0t/\hbar}\mathrm{e}^{h(t)a^\dagger - h^*(t)a}\,, \tag{39}$$

together with the Hamiltonian (22) into equation (38) and solve the resulting equation for $\varphi(t)$. Once the phase of $U(t,0)$ is fixed, the interaction picture evolution operator $U_\mathrm{I}(t,0)$ is obtained by applying the rule (27).

With $f(t) = \lambda \mathrm{e}^{\varepsilon t}$, the obtained operator $U_\mathrm{I}(t,0)$ acquires the interpretation of the evolution operator $U_\mathrm{I}^\varepsilon(t,0)$, corresponding to the adiabatic switching on the interaction $V_\mathrm{int} = \lambda^* a + \lambda\, a^\dagger$. Its explicit form in this case reads

$$U_\mathrm{I}^\varepsilon(t,0) = \mathrm{e}^{i\varphi(t)}\mathrm{e}^{h(t)a^\dagger - h^*(t)a}\,, \tag{40}$$

where

$$h(t) = -\frac{i}{\hbar}\,\frac{\lambda}{\varepsilon + i\omega}\left(\mathrm{e}^{(\varepsilon+i\omega)t} - 1\right), \tag{41}$$

and its phase (see Appendix A) is given by

$$\varphi(t) \equiv \varphi^\varepsilon(t) = \frac{\lambda^2}{2\hbar^2(\omega^2+\varepsilon^2)}\left\{\frac{\omega}{\varepsilon}\left(\mathrm{e}^{2\varepsilon t} - 1\right) - 2\mathrm{e}^{\varepsilon t}\sin(\omega t)\right\}. \tag{42}$$

It is, as expected, singular in the limit $\varepsilon \to 0^+$.

4. Testing the exact formulae for $E_\Omega - E_{\Omega_0}$

The results obtained in the preceding section allow to immediately test formula (12) for the shift of the ground-state energy due to the interaction as well as the Gell-Mann–Low construction (2). Indeed, the logarithm of the expectation value in the H_0 ground state $|\Omega_0\rangle$ of the operator

$$U_\mathrm{I}^\varepsilon(0,-\infty) = [U_\mathrm{I}^\varepsilon(-\infty,0)]^\dagger = \mathrm{e}^{-i\varphi(-\infty)}\,\mathrm{e}^{-h(-\infty)a^\dagger + h^*(-\infty)a}\,, \tag{43}$$

is the sum

$$-i\varphi(-\infty) + \ln\langle\Omega_0|\mathrm{e}^{-h(-\infty)a^\dagger + h^*(-\infty)a}|\Omega_0\rangle = i\,\frac{\lambda^2}{\hbar^2(\varepsilon^2+\omega^2)}\,\frac{\omega}{\varepsilon} + \ldots \tag{44}$$

in which only the first term is singular in the $\varepsilon \to 0$ limit and it is clear that performing the operations indicated in (12) one recovers the ground-state energy shift $-\lambda^2/\hbar\omega$. Moreover, using the well-known Baker–Hausdorff formula

$$\mathrm{e}^{X+Y} = \mathrm{e}^{-\frac{1}{2}[X,\,Y]}\,\mathrm{e}^X\,\mathrm{e}^Y = \mathrm{e}^{\frac{1}{2}[X,\,Y]}\,\mathrm{e}^Y\,\mathrm{e}^X\,, \tag{45}$$

(valid provided $[X,\ [X,Y]] = [Y,\ [X,Y]] = 0$), one easily finds that the vector given by (2) is proportional to

$$\mathrm{e}^{-h(-\infty)\,a^\dagger}|\Omega_0\rangle = \mathrm{e}^{-(\lambda/\hbar\omega)\,a^\dagger}|0\rangle\,, \tag{46}$$

and with the help of the standard rule $[a,\ f(a^\dagger)] = f'(a^\dagger)$, it is straightforward to check that it is annihilated by the operator $A = a + \lambda/\hbar\omega$. This proves that it is indeed the lowest energy eigenvector of $H = \hbar\omega a^\dagger a + \Delta_\omega + \lambda(a + a^\dagger)$.

The same results allow also to test formula (21). Using twice the Baker–Hausdorff identity (45): $\mathrm{e}^{A+B} = \mathrm{e}^A\mathrm{e}^B\mathrm{e}^{-[A,\,B]/2} = \mathrm{e}^B\mathrm{e}^A\mathrm{e}^{[A,\,B]/2}$, the matrix element

$$\langle\Omega_0|U_{\mathrm{I}}^{-\varepsilon}(T,0)[U_{\mathrm{I}}^{\varepsilon}(-T,0)]^\dagger|\Omega_0\rangle = \mathrm{e}^{i(\varphi_- - \varphi_+)}\langle\Omega_0|\mathrm{e}^{h_-a^\dagger - h_-^* a}\,\mathrm{e}^{-h_+a^\dagger + h_+^* a}|\Omega_0\rangle\,, \tag{47}$$

in which

$$\begin{aligned}
\varphi_- &\equiv \varphi^{-\varepsilon}(T) = \frac{|\lambda|^2}{2\hbar^2(\omega^2+\varepsilon^2)}\left\{-\frac{\omega}{\varepsilon}\left(\mathrm{e}^{-2\varepsilon T} - 1\right) - 2\mathrm{e}^{-\varepsilon T}\sin(\omega T)\right\},\\
\varphi_+ &\equiv \varphi^{\varepsilon}(-T) = \frac{|\lambda|^2}{2\hbar^2(\omega^2+\varepsilon^2)}\left\{\ \frac{\omega}{\varepsilon}\left(\mathrm{e}^{-2\varepsilon T} - 1\right) + 2\mathrm{e}^{-\varepsilon T}\sin(\omega T)\right\},\\
h_- &\equiv h^{-\varepsilon}(T) = -\frac{i}{\hbar}\,\frac{\lambda}{i\omega - \varepsilon}\left(\mathrm{e}^{(i\omega-\varepsilon)T} - 1\right),\\
h_+ &\equiv h^{\varepsilon}(-T) = -\frac{i}{\hbar}\,\frac{\lambda}{i\omega + \varepsilon}\left(\mathrm{e}^{-(i\omega+\varepsilon)T} - 1\right),
\end{aligned} \tag{48}$$

can be written first as $\mathrm{e}^{i(\varphi_- - \varphi_+)}\mathrm{e}^{-\frac{1}{2}|h_-|^2}\mathrm{e}^{-\frac{1}{2}|h_+|^2}\langle\Omega_0|\mathrm{e}^{-h_-^* a}\mathrm{e}^{-h_+a^\dagger}|\Omega_0\rangle$ and then as

$$\exp\left\{i(\varphi_- - \varphi_+) - \frac{1}{2}|h_-|^2 - \frac{1}{2}|h_+|^2 + h_-^* h_+\right\}, \tag{49}$$

upon using the rules $\mathrm{e}^{\alpha a}|\Omega_0\rangle = |\Omega_0\rangle$, $\langle\Omega_0|\mathrm{e}^{\beta a^\dagger} = \langle\Omega_0|$ and $\langle\Omega_0|\Omega_0\rangle = 1$. If the limit $\varepsilon \to 0^+$ is taken first, only the first factor in the exponent develops a term linear in T:

$$\begin{aligned}
\lim_{\varepsilon\to 0^+} i(\varphi_- - \varphi_+) &= \lim_{\varepsilon\to 0^+}\frac{i|\lambda|^2}{2\hbar^2(\omega^2+\varepsilon^2)}\left\{-2\,\frac{\omega}{\varepsilon}\left(\mathrm{e}^{-2\varepsilon T} - 1\right) - 4\mathrm{e}^{-\varepsilon T}\sin(\omega T)\right\}\\
&= -i\,\frac{2T}{\hbar}\left(-\frac{|\lambda|^2}{\hbar\omega}\right) - 2i\,\frac{|\lambda|^2}{\hbar^2\omega^2}\sin(\omega T)\,.
\end{aligned} \tag{50}$$

The remaining terms are all either constant or have the oscillatory character. Therefore,

$$\lim_{\varepsilon\to 0^+}\langle\Omega_0|U_{\mathrm{I}}^{-\varepsilon}(T,0)[U_{\mathrm{I}}^{\varepsilon}(-T,0)]^\dagger|\Omega_0\rangle = \exp\left\{-i\,\frac{2T}{\hbar}\left[-\frac{|\lambda|^2}{\hbar\omega} + \mathcal{O}\left(T^{-1}\right)\right]\right\}, \tag{51}$$

and in the limit of $T \to \infty$, the exponent is dominated by the term $-i(2T/\hbar)(E_\Omega - E_{\Omega_0})$ in agreement with formula (21).

These explicit calculations make it again clear that the order of taking the limits is crucial: in formula (12) (and hence, as will be seen again below, in formula (15)) the limit $t = -\infty$ of $U^\varepsilon(0, t)$ is taken first and the limit $\varepsilon \to 0^+$ afterwards; in formula (21) the order of taking the limits is interchanged.

5. Dyson expansions of $E_\Omega - E_{\Omega_0}$

The perturbative expansion of the difference $E_\Omega - E_{\Omega_0}$ generated by formula (15) can be illustrated by computing, up to the second order in λ, the ground-state energy E_Ω of the one-dimensional harmonic oscillator of frequency ω perturbed by the interaction $V_{\rm int} = (\lambda/4)(a^\dagger + a)^4 \equiv \lambda(\hat{x}/l)^4$, where $l = (\hbar/m\omega)^{1/2}$. This can also serve to introduce typical quantum field theory methods: Dyson expansion and the Wick theorem (see *e.g.* [4]; a very clear presentation can be found in [10]). The result obtained in this way can be checked against the one obtained using the standard Rayleigh–Schrödinger perturbative expansion (1).

It is convenient to introduce the "field" operator $\phi = a + a^\dagger$ and to write

$$V^{\rm I}_{\rm int}(t) = {\rm e}^{iH_0 t/\hbar}\, V_{\rm int}\, {\rm e}^{-iH_0 t/\hbar} = \frac{\lambda}{4}\,\phi^4_{\rm I}(t)\,, \qquad \phi_{\rm I}(t) = a\,{\rm e}^{-i\omega t} + a^\dagger\,{\rm e}^{i\omega t}\,. \tag{52}$$

It is then straightforward to find (in this case $|\Omega_0\rangle \equiv |0\rangle$ and, as usuallly, $a|0\rangle = 0$, $a^\dagger|0\rangle = |1\rangle$, *etc.*) the key object (the "propagator") in terms of which the Dyson expansion is formulated[7]

$$\begin{aligned}
\langle\Omega_0|{\rm T}\left[\phi_{\rm I}(t)\phi_{\rm I}\left(t'\right)\right]|\Omega_0\rangle \equiv\; & \theta\left(t-t'\right)\,\langle\Omega_0|\phi_{\rm I}(t)\phi_{\rm I}\left(t'\right)|\Omega_0\rangle \\
& +\theta\left(t'-t\right)\,\langle\Omega_0|\phi_{\rm I}\left(t'\right)\phi_{\rm I}(t)|\Omega_0\rangle \\
=\; & \theta\left(t-t'\right)\,{\rm e}^{-i\omega(t-t')} + \theta\left(t'-t\right)\,{\rm e}^{i\omega(t-t')} \\
=\; & \int\limits_{-\infty}^{\infty}\frac{{\rm d}\nu}{2\pi}\,\frac{2i\omega\,{\rm e}^{-i\nu(t-t')}}{\nu^2-\omega^2+i0} \equiv iG^0\left(t-t'\right) = iG^0(t'-t)\,.
\end{aligned} \tag{53}$$

[7] Because the integrals which appear in the Dyson expansion generated by formula (15) do not cover the entire t axis, the Fourier form of the function $iG^0(t-t')$ is not useful in this case. It will, however, be used in considering the Dyson expansion generated by formula (21). It also serves to define the value of the Green's function $G^0(t-t')$ at $t = t'$: it gives $G^0(0) = 1$.

In the following, formula (15) will be written as $E_{\Omega} - E_{\Omega_0}$ =NUM/DEN. Upon inserting into the numerator NUM and into the denominator DEN the representation (8) of the evolution operator one arrives at the expansions[8]

$$\begin{aligned}\mathrm{NUM} &= \langle\Omega_0|V_{\mathrm{int}}|\Omega_0\rangle + \frac{1}{i\hbar}\int\limits_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t}\, \langle\Omega_0|\mathrm{T}\left[V^{\mathrm{I}}_{\mathrm{int}}(0)\, V^{\mathrm{I}}_{\mathrm{int}}(t)\right]|\Omega_0\rangle + \dots\,, \\ \mathrm{DEN} &= 1 + \frac{1}{i\hbar}\int\limits_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t}\, \langle\Omega_0|\mathrm{T}\, V^{\mathrm{I}}_{\mathrm{int}}(t)|\Omega_0\rangle + \dots \end{aligned} \tag{54}$$

Each matrix element can be now worked out using the Wick theorem [4, 10] which (in this simple case) reduces to forming the sum of the expressions consisting of products of propagators $iG^0(t_i - t_j)$, the appropriate (corresponding to the order of the expansion) powers of the factors $\lambda/4$ and $1/i\hbar$, and some combinatoric c-number factors. The products of propagators are obtained by grouping under the symbol of the chronological ordering into pairs the "field" operators ϕ_{I} out of which the interaction operators $V^{\mathrm{I}}_{\mathrm{int}}(t)$ are composed and by replacing every pair $\phi_{\mathrm{I}}(t_i)\phi_{\mathrm{I}}(t_j)$ by the propagator $iG^0(t_i - t_i)$ given by (53); the summation is over all possible ways of grouping the available operators into distinct pairs (the pairs $\phi_{\mathrm{I}}(t_i)\phi_{\mathrm{I}}(t_j)$ and $\phi_{\mathrm{I}}(t_j)\phi_{\mathrm{I}}(t_i)$ are not treated as distinct).

The sum of terms resulting from working out in this way the matrix element

$$\left\langle\Omega_0\left|\mathrm{T}\left[V^{\mathrm{I}}_{\mathrm{int}}(t_n)\dots V^{\mathrm{I}}_{\mathrm{int}}(t_1)\right]\right|\Omega_0\right\rangle\,, \tag{55}$$

can be represented by Feynman diagrams. These are obtained by drawing n vertices (dots) with four lines (because of four ϕ_{I} operators in each interaction $V^{\mathrm{I}}_{\mathrm{int}}(t)$) attached to each of them and labeled by the times $t_1, \dots, t_n$. All these lines should be next connected pairwise in all possible ways giving rise to several diagrams. Some of these diagrams may not be connected (may consist of several disjoint subdiagrams). The analytic expression corresponding to a diagram is obtained by replacing all lines by propagators iG^0 forming a product: the line connecting the vertices labeled t_i and t_j is ascribed the propagator $iG^0(t_i - t_j)$. The combinatoric factors which should be included simply take into account that different ways of connecting lines attached to each vertex can lead to topologically identical diagrams. This will become clear below.

[8] $V_{\mathrm{int}} = V^{\mathrm{I}}_{\mathrm{int}}(0)$ can be formally put under the chronological product because the integration variables $t_1 \dots t_n$ in the integrals are never greater than 0.

The difference between matrix elements obtained in the expansions of the numerator NUM and of the denominator DEN is that in the first case, one vertex is labeled with time 0 (there are $n+1$ interaction operators $V_{\rm int}^{\rm I}$ and only n integrations). One can therefore distinguish those Feynman diagrams contributing to NUM, all vertices of which are connected (possibly by going through other, intermediate vertices) to the distinguished vertex labeled with time 0. The other diagrams are called "disconnected". In standard textbooks like [4] it is proven that in the ratio of the Dyson expansions of NUM and DEN, the contribution of the "disconnected" diagrams to NUM is precisely canceled by the denominator DEN. In computing the difference $E_\Omega - E_{\Omega_0}$, one can therefore restrict oneself to computing only the contributions of connected diagrams to the numerator NUM: $E_\Omega - E_{\Omega_0} = \mathrm{NUM}_{\rm con}$.

We can now illustrate this by computing the difference $E_\Omega - E_{\Omega_0}$ up to the second order (the reader may entertain himself with extending this computation to higher orders). The first term of the numerator is just the same as the first term, $\langle\Omega_0|V_{\rm int}|\Omega_0\rangle$, in the standard Rayleigh–Schrödinger formula (1) and can be evaluated using the standard method. It is, however, more instructive to evaluate it using the Wick theorem as

$$\langle\Omega_0|\,\mathrm{T}V_{\rm int}^{\rm I}(0)\,|\Omega_0\rangle = \frac{\lambda}{4}\,\langle\Omega_0|\,\mathrm{T}\phi_{\rm I}^4(0)\,|\Omega_0\rangle = \frac{\lambda}{4}\,3\,iG^0(0)\,iG^0(0) = \frac{3\lambda}{4}\,. \quad (56)$$

The combinatoric factor 3 comes from three ways of connecting the four "legs" of the interaction operator to get the diagram shown in Fig. 1 (a). Since $iG^0(0) = 1$, the standard result for $E_\Omega^{(1)}$ is immediately recovered. The second order term leads via the Wick theorem to the three diagrams

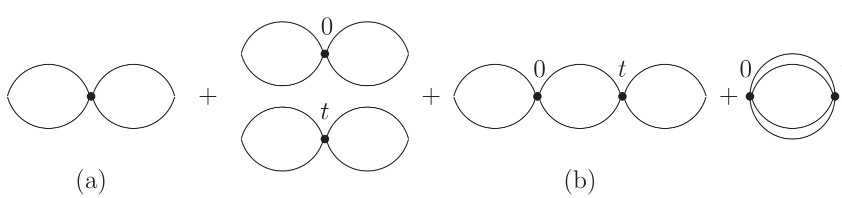


Fig. 1. Diagrams contributing in the first (a) and second (b) order in λ to the numerator of the Gell-Mann–Low formula for the ground-state energy applied to the harmonic oscillator perturbed by the interaction $\propto \hat{x}^4$. Dots mark the interaction vertices; in the second-order diagrams one of the vertices is ascribed the time 0 and the other one the time t. The connected part of the diagram is its part to which the vertex marked 0 belongs.

shown in Fig.1 (b). The first one gives the contribution

$$-\frac{i}{\hbar}\int\limits_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t}\left(\frac{\lambda}{4}\right)^2 3\left[iG^0(t-t)\right]^2\, 3\left[iG^0(0)\right]^2 = -\frac{i}{\hbar}\left(\frac{3\lambda}{4}\right)^2\frac{1}{\varepsilon}\,, \tag{57}$$

all the four propagators being taken at zero because they all arise from contracting legs attached to the same vertex. This contribution is singular as $\varepsilon \to 0$. It belongs to the class of disconnected contributions because one part of the diagram is not connected by any line with the part involving the vertex generated by $V^{\mathrm{I}}_{\mathrm{int}}(0)$. The next diagram gives rise to only two propagators taken at zero and to two others taken at t because its two lines connect two different vertices (one at time 0 and another one at t). The combinatoric factor corresponding to this diagram is

$$\binom{4}{2}\binom{4}{2}\cdot 2 = 72\,, \tag{58}$$

because there are $4!/2!2!$ ways of selecting two legs of each of the vertices which are going to be connected to the other vertex; there are also two ways of connecting the selected legs. Thus, the contribution of this diagram is

$$-\frac{i}{\hbar}\left(\frac{\lambda}{4}\right)^2\int\limits_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t}\, 72\,[iG^0(0)]^2\, iG^0(t)\, iG^0(t) = -\frac{i}{\hbar}\,\frac{9\lambda^2}{2}\,\frac{1}{\varepsilon+2i\omega}\,, \tag{59}$$

because $iG^0(0) = 1$,

$$iG^0(t)\, iG^0(t) = \theta(t)\,\mathrm{e}^{-2i\omega t} + \theta(-t)\,\mathrm{e}^{2i\omega t}\,, \tag{60}$$

and because the integral covers only the negative semi-axis so that only the second term contributes. Finally, the last diagram of Fig.1 (b) has the combinatoric factor $4\cdot 3\cdot 2 = 24$ (the number of ways of connecting the legs of the two vertices) and gives

$$-\frac{i}{\hbar}\left(\frac{\lambda}{4}\right)^2\int\limits_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t}\, 24\, iG^0(t)\, iG^0(t)\, iG^0(t)\, iG^0(t) = -\frac{i}{\hbar}\,\frac{3\lambda^2}{2}\,\frac{1}{\varepsilon+4i\omega}\,. \tag{61}$$

Combining these contributions, one has

$$\mathrm{NUM} = \frac{3}{4}\,\lambda + \lambda^2\left\{-\frac{i}{\hbar}\left(\frac{3}{4}\right)^2\frac{1}{\varepsilon} - \frac{9}{2}\,\frac{1}{2\hbar\omega - i\hbar\varepsilon} - \frac{3}{2}\,\frac{1}{4\hbar\omega - i\hbar\varepsilon} + \dots\right\}. \tag{62}$$

The second term of the denominator is represented by a diagram of the same form as that shown in Fig.1 (a) but the resulting expression is integrated. Therefore,

$$\mathrm{DEN} = 1 - \frac{i}{\hbar}\frac{3\lambda}{4}\frac{1}{\varepsilon} + \ldots \tag{63}$$

It is then clear that after multiplying the power series in λ representing the numerator by the power series

$$\mathrm{DEN}^{-1} = 1 + \frac{i}{\hbar}\frac{3\lambda}{4}\frac{1}{\varepsilon} + \ldots \tag{64}$$

the singular terms: the one coming from the first, disconnected diagram of Fig.1 (b) and the one arising from DEN^{-1} cancel out and in the limit of $\varepsilon \to 0$, one obtains the finite result

$$E_\Omega - E_{\Omega_0} = \frac{3\lambda}{4} - \frac{21\lambda^2}{8} + \ldots \tag{65}$$

In the Rayleigh–Schrödinger approach, the λ^2 contribution is given by

$$\begin{aligned} E_\Omega^{(2)} &= \sum_{l\neq 0} \frac{|\langle l|V_{\mathrm{int}}|\Omega_0\rangle|^2}{E_{\Omega_0} - E_l} \\ &= \left(\frac{\lambda}{4}\right)^2 \left\{ \frac{|\langle 2|\left(a^\dagger + a\right)^4|\Omega_0\rangle|^2}{E_{\Omega_0} - E_2} + \frac{|\langle 4|\left(a^\dagger + a\right)^4|\Omega_0\rangle|^2}{E_{\Omega_0} - E_4} \right\} . \end{aligned} \tag{66}$$

The relevant matrix elements are

$$\begin{aligned} \langle\Omega_0|\left(a^\dagger{+}a\right)^4|4\rangle &= \langle\Omega_0|a^4|4\rangle = \sqrt{4\cdot 3\cdot 2}\,, \\ \langle\Omega_0|\left(a^\dagger{+}a\right)^4|2\rangle &= \langle\Omega_0|\left(a^\dagger a^\dagger + 2a^\dagger a + \hat{1} + aa\right)\left(a^\dagger a^\dagger + 2a^\dagger a + \hat{1} + aa\right)|2\rangle \\ &= \left(\langle\Omega_0| + \sqrt{2}\,\langle 2|\right)\left(\sqrt{12}\,|4\rangle + 5|2\rangle + \sqrt{2}\,|\Omega_0\rangle\right) = 6\sqrt{2} \end{aligned} \tag{67}$$

and together with $E_{\Omega_0} - E_l = -l\hbar\omega$ lead to the same result as the Gell-Mann–Low formula.

It should be stressed that both NUM and DEN involve terms singular in the limit $\varepsilon \to 0^+$ but these cancel in the ratio (the limit $\varepsilon \to 0^+$ in formula (15) is supposed to be taken at the very end). The cancellation need not be explicitly worked out, however, because the theorem quoted ensures the cancellation of contribution of the non-connected diagrams to the numerator by the denominator.

An interesting exercise is to recover the same result using formula (20). The Dyson expansion of its right-hand side can be again encoded in the Feynman diagrams shown in Fig. 1 except that now, none of the vertices is marked with zero time — all n interaction vertices in a diagram representing a contribution arising in the n-th order of the Dyson expansion must be marked by the time variables $t_1, \ldots, t_n$ and obtaining the corresponding contribution requires integrating over all these time variables (in the $T \to \infty$ limit) from $-\infty$ to $+\infty$. But again, it can be shown that taking the logarithm of this expansion (to extract $E_\Omega - E_{\Omega_0}$) is equivalent to taking into account connected diagrams only.

The first order[9] contribution to the logarithm of the left-hand side of (21) is (the limit $\varepsilon \to 0^+$ has already been taken)

$$-\frac{i\lambda}{4\hbar}\int_{-T}^{T} \mathrm{d}t\, \langle \Omega_0|\mathrm{T}\phi_{\mathrm{I}}^4(t)|\Omega_0\rangle = -\frac{3i\lambda}{4\hbar}\int_{-T}^{T} \mathrm{d}t\, iG^0(0)\, iG^0(0)\,. \tag{68}$$

This can be evaluated directly, keeping finite T, because $iG^0(0) = 1$. It is however more in line with the procedure which will be applied to higher order contributions to evaluate it in the "frequency" space setting $T = \infty$ from the beginning. In general, since to each line ℓ connecting two interaction vertices marked, say t_i and t_j ($t_i = t_j$, *i.e.* a line which starts and ends in the same vertex, is also allowed), in a diagram there corresponds the propagator (53) involving (in its last form) the exponential factor $\mathrm{e}^{-i\nu_\ell(t_i-t_j)}$ — the frequency ν_ℓ may be then interpreted as "flowing" from the vertex marked t_j to the one marked t_i — it is easy to notice that after the integration over all times $t_1, \ldots, t_n$ labeling the vertices of the considered diagram one will obtain for each vertex one Dirac delta function

$$\int_{-\infty}^{\infty} \mathrm{d}t_i\, \exp\left\{-it_i\left(\sum_\ell \nu_\ell - \sum_{\ell'} \nu_{\ell'}\right)\right\} = 2\pi\,\delta\left(\sum_\ell \nu_\ell - \sum_{\ell'} \nu_{\ell'}\right)\,, \tag{69}$$

in which ℓ denotes labels of the frequencies "flowing" into the vertex marked t_i and ℓ' of those "flowing" out of this vertex[10]. However, these n delta functions allow to eliminate only $n-1$ integrations over frequencies — after using the equalities relating different frequencies enforced by $n-1$ delta functions, the argument of the last one can always be replaced by zero (this will be seen on examples below). This $2\pi\delta(0)$ is then to be interpreted as

[9] There is no zero-th order — the expansion of the logarithm begins from the first order term.

[10] The direction of the frequency flow ascribed to a given line of the diagram is arbitrary here because $iG^0(t_i - t_j) = iG^0(t_j - t_i)$.

$\lim_{T\to\infty}(2T)$ and will cancel out with the same factor multiplying $E_\Omega - E_{\Omega_0}$ in the right-hand side of formula (21). There remain only the integrations over independent frequencies ν, that is over those which are not fixed by the equalities enforced by the $n-1$ delta functions. Thus, $-(i/\hbar)(E_\Omega - E_{\Omega_0})$ is directly given by the sum of all connected "frequency" space Feynman diagrams shown in Fig. 2.

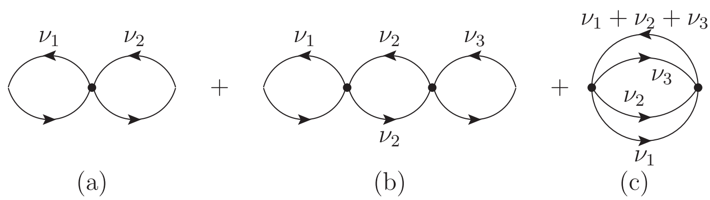


Fig. 2. Frequency space diagrams contributing in the first (a) and second (b) and (c) order in λ to $(-i/\hbar)(E_\Omega - E_{\Omega_0})$.

In agreement with these rules, the contribution to $(-i/\hbar)(E_\Omega - E_{\Omega_0})$ of the diagram of Fig. 2 (a) simply is

$$\begin{aligned}-\frac{i}{\hbar}\,(E_\Omega - E_{\Omega_0})^{(2\mathrm{a})} &= -\frac{3i\lambda}{4\hbar}\int\frac{\mathrm{d}\nu_1}{2\pi}\,\frac{2i\omega}{\nu_1^2-\omega^2+i0}\int\frac{\mathrm{d}\nu_2}{2\pi}\,\frac{2i\omega}{\nu_2^2-\omega^2+i0}\\ &= -\frac{i}{\hbar}\left(\frac{3\lambda}{4}\right). \qquad (70)\end{aligned}$$

Similarly, the contribution to $-(i/\hbar)(E_\Omega - E_{\Omega_0})$ of the first diagram of Fig. 2 (b) reads

$$\begin{aligned}&\frac{1}{2!}\left(\frac{1}{i\hbar}\,\frac{\lambda}{4}\right)^2 72\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\nu_1}{2\pi}\,\frac{2i\omega}{\nu_1^2-\omega^2+i0}\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\nu_2}{2\pi}\,\frac{(2i\omega)^2}{[\nu_2^2-\omega^2+i0]^2}\\ &\times\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\nu_3}{2\pi}\,\frac{2i\omega}{\nu_3^2-\omega^2+i0}\,. \qquad (71)\end{aligned}$$

The factor $1/2!$ comes from expansion of the exponent and 72 is the combinatoric factor already explained. The integrals over ν_1 and ν_2 are equal to unity (they just give $iG^0(0) = 1$ each). The middle integral is evaluated by the standard residue method (*e.g.* by closing the integration contour with a large semi-circle in the lower half plane and evaluating the residue of the double pole of the integrand at $\nu = \omega - i0$). In this way, one obtains

$$-\frac{i}{\hbar}\,(E_\Omega - E_{\Omega_0})^{(2\mathrm{b})} = \frac{1}{2}\left(-\frac{\lambda^2}{16\hbar^2}\right)72\,(2i\omega)^2\,\frac{2i}{(2\omega)^3} = -\frac{i}{\hbar}\left(-\frac{9\lambda^2}{4\hbar\omega}\right). \qquad (72)$$

Finally, the contribution of the diagram of Fig. 2 (c) is

$$\frac{1}{2!}\left(\frac{1}{i\hbar}\,\frac{\lambda}{4}\right)^2 24\,(2i\omega)^4\,I\,. \tag{73}$$

Again 24 is the combinatoric factor already explained and I is the "three loop" (in the language of quantum field theory) integral computed in Appendix B. It is clear that the sum of

$$-\frac{i}{\hbar}\left(E_\Omega - E_{\Omega_0}\right)^{(2\mathrm{c})} = i\left(-\frac{\lambda^2}{2\hbar^2}\right)24\,\omega^4\,\frac{-i}{32\omega^5} = -\frac{i}{\hbar}\left(-\frac{3\lambda^2}{8\hbar\omega}\right), \tag{74}$$

of (72) and of (70) reproduces the result (65) obtained using formula (15).

Although in application to the perturbed oscillator the method of computing the energy shift based on formula (15) may seem easier than the one based on the prescription (21), it is the latter that proves more practical in more advanced computations. In particular, it is formula (21) combined with the effective theory approach which allows to quite easily reproduce [11] the classic results (summarized in [4]) concerning the ground-state energy of a system of N interacting nonrelativistic fermions and to extend its calculation to yet higher orders [12] and to a nonzero polarization [13].

6. Goldstone diagrams and the cancellation of singular terms

We have illustrated how the energy difference $E_\Omega - E_{\Omega_0}$ is computed by expanding the numerator and the denominator of formula (15) in the Dyson series represented by Feynman diagrams which results from the representation (8) of the (interaction picture) evolution operator. The same formula can be, however, worked out differently, using the iterative representation (7) of this operator and inserting between the successive interaction operators $V^{\mathrm{I}}_{\mathrm{int}}$ the complete sets of eigenvectors $|l\rangle$ of the free Hamiltonian H_0. This leads to another organization of the expansion of formula (15) for $E_\Omega - E_{\Omega_0}$ which is visualized in terms of the so-called Goldstone diagrams. There is, however, a subtlety in using the representation (7) in formula (15) which is usually somewhat misleadingly presented in textbooks.

We will illustrate this point by considering the Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\left(\omega^2 + \lambda^2\right)\hat{x}^2\,, \tag{75}$$

and computing the energy of its ground state in two ways: using the Dyson expansion already introduced in Section 5 and using the Goldstone way, treating the term $\frac{1}{2}m\lambda^2\hat{x}^2$ as the perturbation V_{int}

$$V_{\mathrm{int}} = \frac{\hbar\lambda^2}{4\omega}\left(a^\dagger + a\right)^2 \equiv \alpha\,\phi^2\,. \tag{76}$$

The virtue of this example is that the exact energy levels of the Hamiltonian $H = H_0 + V_{\rm int}$ are known; in particular,

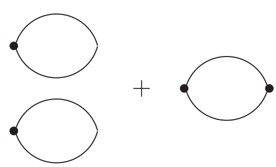
$$E_{\Omega} = \frac{1}{2}\hbar\sqrt{\omega^2+\lambda^2} = \frac{1}{2}\hbar\omega + \frac{\hbar\lambda^2}{4\omega} - \frac{\hbar\lambda^4}{16\omega^3} + \frac{\hbar\lambda^6}{32\omega^5} + \dots . \tag{77}$$

and this can be used to check the correctness of the results obtained by using the expansions generated by formula (15).

Expanded to the third order the numerator of formula (15) reads

$$\begin{aligned} \mathrm{NUM} \ &= \ \alpha + \beta\,\alpha^2 \int_{-\infty}^{0} \mathrm{d}t\,\mathrm{e}^{\varepsilon t}\,\langle\Omega_0|T\left[\phi_{\rm I}^2(0)\phi_{\rm I}^2(t)\right]|\Omega_0\rangle \\ &+\frac{1}{2}\,\beta^2\alpha^3 \int_{-\infty}^{0}\mathrm{d}t \int_{-\infty}^{0}\mathrm{d}t'\,\mathrm{e}^{\varepsilon(t+t')}\,\langle\Omega_0|T\left[\phi_{\rm I}^2(0)\phi_{\rm I}^2(t)\phi_{\rm I}^2(t')\right]|\Omega_0\rangle + \dots \end{aligned} \tag{78}$$

where $\beta = 1/i\hbar$ and the result $\langle\Omega_0|V_{\rm int}(0)|\Omega_0\rangle = \alpha$ has already been used. Evaluating the order $\beta\,\alpha^2$ contribution in the Dyson way, *i.e.* using the Wick theorem, one finds two diagrams shown in Figs. 3 (a) and (b) of which only the second one is connected (in the sense already explained in Sec. 5).



(a) (b)

Fig. 3. Second order diagrams contributing to the numerator of the formula (15) for the ground-state energy evaluated in the Dyson way, as applied to the harmonic oscillator perturbed with the interaction $\propto \hat{x}^2$.

The complete order $\beta\,\alpha^2$ contribution is (iG^0 is the propagator (53))

$$\begin{aligned} \mathrm{NUM}^{(2)} \ &= \ \beta\,\alpha^2 \int_{-\infty}^{0} \mathrm{d}t\,\mathrm{e}^{\varepsilon t}\left([iG^0(0)]^2 + 2\,iG^0(t)\,iG^0(t)\right) \\ &= \ \beta\,\alpha^2 \int_{-\infty}^{0} \mathrm{d}t\,\mathrm{e}^{\varepsilon t}\left(1 + 2\left[\theta(t)\,\mathrm{e}^{-2i\omega t} + \theta(-t)\,\mathrm{e}^{2i\omega t}\right]\right) \\ &= \ \beta\,\alpha^2\left(\frac{1}{\varepsilon} + \frac{2}{\varepsilon + 2i\omega}\right), \end{aligned} \tag{79}$$

where the term singular in the limit $\varepsilon \to 0$ comes from the disconnected diagram. The same result is obtained evaluating this contribution "in the Goldstone way"

$$\begin{aligned}
\mathrm{NUM}^{(2)} &= \beta \int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t} \sum_l \langle \Omega_0 | V_{\mathrm{int}} | l \rangle \langle l | V_{\mathrm{int}} | \Omega_0 \rangle\, \mathrm{e}^{i\omega_{n0} t} \\
&= \beta\, \alpha^2 \int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t} \left(1 + \left(\sqrt{2}\right)^2 \mathrm{e}^{2i\omega t} \right) , \qquad (80)
\end{aligned}$$

where the first term in the bracket comes from $|l\rangle = |\Omega_0\rangle \equiv |0\rangle$ and is classified as a disconnected contribution (or as a contribution of the disconnected Goldstone diagram — see Fig. 4) and the second one from $|l\rangle = |2\rangle$.

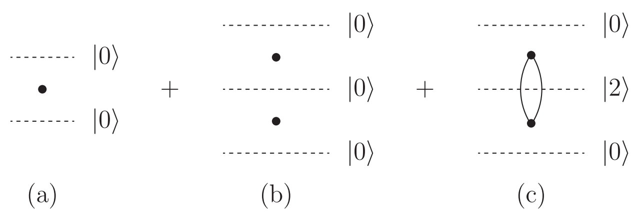


Fig. 4. Goldstone diagrams illustrating the first- and second-order terms of the expansion of the numerator of formula (15) based on the representation (7) realized in the basis formed by the H_0 eigenstates. Dots represent interactions and the horizontal dashed line represents the initial, intermediate and final states. Solid lines can be viewed as particles (bosons) created or annihilated by the interaction. Diagrams with intermediate states representing the ground state $|\Omega_0\rangle = |0\rangle$ are classified as disconnected.

Evaluating $\mathrm{NUM}^{(3)}$ — the order $\beta^2\alpha^3$ contribution to the numerator — in the Dyson way one finds the diagrams shown in Fig. 5 which give

$$\begin{aligned}
\langle \Omega_0 | T\left[\phi_{\mathrm{I}}^2(0)\phi_{\mathrm{I}}^2(t)\phi_{\mathrm{I}}^2\left(t'\right)\right] | \Omega_0 \rangle &= \left[iG^0(0)\right]^3 + 2\, iG^0(0) \left[iG^0\left(t-t'\right)\right]^2 \\
&\quad + 2\, iG^0(0)\left[iG^0(t)\right]^2 + 2\, iG^0(0)\left[iG^0\left(t'\right)\right]^2 \\
&\quad + 8\, iG^0(t)\, iG^0\left(t'\right) iG^0\left(t-t'\right) . \qquad (81)
\end{aligned}$$

The numbers in front of the successive terms are the combinatoric factors. The two terms in the middle line give equal contributions in view of the symmetry of the integration over $\mathrm{d}t\, \mathrm{d}t'$. Using the explicit form (53) of

$iG^0(t)$ this contribution is

$$
\begin{aligned}
&1+2\Big[\theta\left(t-t'\right)\mathrm{e}^{-2i\omega(t-t')}+\theta\left(t'-t\right)\mathrm{e}^{2i\omega(t-t')}\Big]+4\big[\theta(t)\,\mathrm{e}^{-2i\omega t}+\theta(-t)\,\mathrm{e}^{2i\omega t}\big]\\
&\quad+8\big[\theta(t)\,\mathrm{e}^{-i\omega t}+\theta(-t)\,\mathrm{e}^{i\omega t}\big]\Big[\theta\left(t'\right)\mathrm{e}^{-i\omega t'}+\theta\left(-t'\right)\mathrm{e}^{i\omega t'}\Big]\\
&\qquad\times\Big[\theta\left(t-t'\right)\mathrm{e}^{-i\omega(t-t')}+\theta\left(t'-t\right)\mathrm{e}^{i\omega(t-t')}\Big]\,. \qquad (82)
\end{aligned}
$$

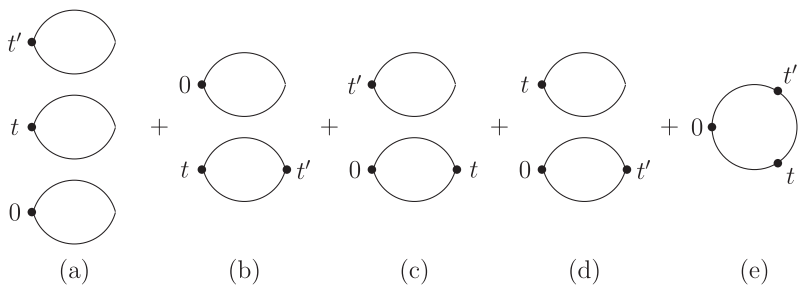


Fig. 5. Third order diagrams contributing to the numerator of the formula (15) expanded in the Dyson way, as applied to the harmonic oscillator perturbed with the interaction $\propto \hat{x}^2$. Diagrams (b), (c) and (d) have combinatoric factors 2. Diagrams (c) and (d) give equal contributions. The combinatoric factor of the last diagram is 8.

The two terms of the first square bracket in the first line give equal contributions (again, because of the symmetry of the integration over $\mathrm{d}t\,\mathrm{d}t'$); of the second square bracket in the first line only the second term contributes (because the integral over $\mathrm{d}t$ in (15) covers only the negative semi-axis) and finally, in both brackets in the second line only the second terms contribute and the two terms of the last square bracket give equal contributions. Elementary integrations then yield

$$
\mathrm{NUM}^{(3)}_{\mathrm{Dyson}}=\frac{1}{2}\beta^2\alpha^3\left\{\frac{1}{\varepsilon^2}+\frac{4}{2\varepsilon(\varepsilon+2i\omega)}+\frac{4}{\varepsilon(\varepsilon+2i\omega)}+\frac{16}{(2\varepsilon+2i\omega)(\varepsilon+2i\omega)}\right\}. \qquad (83)
$$

Only the third term comes from the connected Feynman diagram, so if it is taken for granted that the singular (in the limit $\varepsilon\to 0$) contributions of the disconnected diagrams 5 (a)–(d) are exactly canceled by the contributions of the denominator DEN, one can write

$$
\left(\mathrm{NUM}^{(2)}_{\mathrm{con}}+\mathrm{NUM}^{(3)}_{\mathrm{con}}\right)_{\varepsilon=0}=\beta\,\alpha^2\,\frac{2}{2i\omega}+\frac{1}{2}\,\beta^2\alpha^3\,\frac{16}{(2i\omega)^2}=-\frac{\hbar\lambda^4}{16\omega^3}+\frac{\hbar\lambda^6}{32\omega^5}\,, \qquad (84)
$$

which is the correct result.

Evaluating the order $\beta^2\alpha^3$ contribution to the numerator in the Goldstone way instead, one gets ($\omega_{l'l} = (E_{l'} - E_l)/\hbar$)

$$\begin{aligned}\mathrm{NUM}^{(3)} &= \beta^2 \int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t} \int_{-\infty}^{t} \mathrm{d}t' \mathrm{e}^{\varepsilon t'} \langle \Omega_0 | V^{\mathrm{I}}_{\mathrm{int}}(0) V^{\mathrm{I}}_{\mathrm{int}}(t) V^{\mathrm{I}}_{\mathrm{int}}\left(t'\right) | \Omega_0 \rangle \\ &= \beta^2 \int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\varepsilon t} \int_{-\infty}^{t} \mathrm{d}t' \mathrm{e}^{\varepsilon t'} \sum_{l'} \sum_{l} \langle \Omega_0 | V_{\mathrm{int}} | l' \rangle \langle l' | V_{\mathrm{int}} | l \rangle \langle l | V_{\mathrm{int}} | \Omega_0 \rangle\, \mathrm{e}^{i\omega_{l'l} t}\, \mathrm{e}^{i\omega_{l0} t'} . \end{aligned} \tag{85}$$

The integrations are elementary and give ($\omega_{l'l} + \omega_{l0} = \omega_{l'0}$)

$$\mathrm{NUM}^{(3)} = \beta^2 \sum_{l'} \sum_{l} \frac{\langle \Omega_0 | V_{\mathrm{int}} | l' \rangle \langle l' | V_{\mathrm{int}} | l \rangle \langle l | V_{\mathrm{int}} | \Omega_0 \rangle}{(2\varepsilon + i\omega_{l'0})(\varepsilon + i\omega_{l0})} . \tag{86}$$

Because $V_{\mathrm{int}} = \alpha(a^\dagger a^\dagger + 2a^\dagger a + \hat{1} + aa)$, the double summation reduces to four terms only: $(l', l) = (0,0)$, $(0,2)$, $(2,0)$ and $(2,2)$ of which only the last one would be classified as "connected". The relevant matrix elements are

$$\langle \Omega_0 | V_{\mathrm{int}} | \Omega_0 \rangle = \alpha\,, \quad \langle \Omega_0 | V_{\mathrm{int}} | 2 \rangle = \langle 2 | V_{\mathrm{int}} | \Omega_0 \rangle = \sqrt{2}\, \alpha\,, \quad \langle 2 | V_{\mathrm{int}} | 2 \rangle = 5\, \alpha\,. \tag{87}$$

This leads to (the corresponding Goldstone diagrams are shown in Fig. 6)

$$\mathrm{NUM}^{(3)}_{\mathrm{Goldstone}} = \\ \beta^2\alpha^3 \left\{ \frac{1}{2\varepsilon^2} + \frac{2}{2\varepsilon(\varepsilon + 2i\omega)} + \frac{2}{\varepsilon(2\varepsilon + 2i\omega)} + \frac{10}{(2\varepsilon + 2i\omega)(\varepsilon + 2i\omega)} \right\} . \tag{88}$$

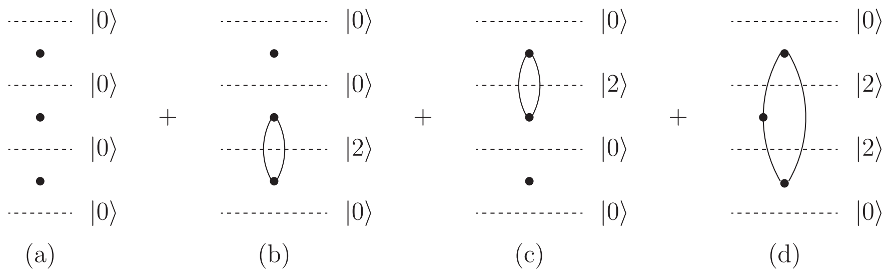


Fig. 6. Goldstone diagrams illustrating the third order terms of the expansion based on the representation (7) realized in the basis of H_0 eigenstates of the numerator of formula (15). Only the diagram (d) is classified as connected.

Comparison with $\mathrm{NUM}^{(3)}_{\mathrm{Dyson}}$ given in (83) reveals that there is a subtle difference: in the denominator of the third term, there is now 2ε in the expression in the bracket and the coefficient of the last term is now 10 instead of 8. Nevertheless, as can be straightforwardly checked, the two results, $\mathrm{NUM}^{(3)}_{\mathrm{Dyson}}$ and $\mathrm{NUM}^{(3)}_{\mathrm{Goldstone}}$, are perfectly equal as they should be (this is the same expression evaluated in two different but equally consistent ways). If, however, in the Goldstone approach, the contributions of the ground state $|\Omega_0\rangle$ as the intermediate states l' and/or l, *i.e.* of the disconnected Goldstone diagrams, are rejected, the resulting contribution to the ground-state energy of H will come out wrong! Notice that both "connected" third order contributions to the numerator of formula (15), the one obtained in the Dyson way and the one obtained *à la* Goldstone, have perfectly well defined finite limits $\varepsilon \to 0$. That the first one is the right answer is here obvious because we have the exact expression (77) for the ground-state energy. In the absence of the exact result to establish which one of the two "connected" contributions is correct, one would be forced to work out the denominator of formula (15) and carefully obtain the expansion of the ratio NUM/DEN. Let us see this on the considered example: evaluation of the denominator up to the second order in both ways gives the same result

$$\mathrm{DEN} = 1 + \beta\alpha\,\frac{1}{\varepsilon} + \frac{1}{2}\,\beta^2\alpha^2\left(\frac{1}{\varepsilon^2} + \frac{4}{2\varepsilon(\varepsilon+2i\omega)}\right) + \dots \tag{89}$$

Therefore,

$$\mathrm{DEN}^{-1} = 1 - \beta\alpha\,\frac{1}{\varepsilon} + \frac{1}{2}\,\beta^2\alpha^2\left(\frac{1}{\varepsilon^2} - \frac{4}{2\varepsilon(\varepsilon+2i\omega)}\right) + \dots \tag{90}$$

and, multiplying the two series, one obtains

$$\begin{aligned}\frac{\mathrm{NUM}}{\mathrm{DEN}} &= \alpha + \beta\alpha^2\left(\frac{1}{\varepsilon} + \frac{2}{\varepsilon+2i\omega}\right) + \mathrm{NUM}^{(3)} \\ &-\beta\alpha^2\frac{1}{\varepsilon} - \beta^2\alpha^3\left(\frac{1}{\varepsilon^2} + \frac{2}{\varepsilon(\varepsilon+2i\omega)}\right) + \frac{1}{2}\beta^2\alpha^3\left(\frac{1}{\varepsilon^2} - \frac{2}{\varepsilon(\varepsilon+2i\omega)}\right)\,,\end{aligned} \tag{91}$$

where the first line is just the numerator ($\mathrm{NUM}^{(3)}$ is the order $\beta^2\alpha^3$ contribution to it) and all the remaining terms of the expansion of the ratio have been put in the second line. It is clear that the singular terms of order $\beta\alpha^2$ cancel out directly. It is also seen that the order $\beta^2\alpha^3$ terms of the second line directly remove the singular terms of $\mathrm{NUM}^{(3)}_{\mathrm{Dyson}}$ (83), so that indeed, what remains is the last term contributed by the connected Dyson diagram 5 (e). In contrast, the singular terms of $\mathrm{NUM}^{(3)}_{\mathrm{Goldstone}}$ (88) do not match exactly the order $\beta^2\alpha^3$ terms of the second line of (91): the sum of all singular terms is in this case

$$-\frac{2}{\varepsilon(\varepsilon+2i\omega)}+\frac{2}{\varepsilon(2\varepsilon+2i\omega)}=-\frac{2}{(\varepsilon+2i\omega)(2\varepsilon+2i\omega)}\,, \qquad (92)$$

and is finite in the $\varepsilon\to 0$ limit. This finite contribution corrects the coefficient of the "connected" third order contribution to the ground-state energy computed in the Goldstone way.

It is instructive to compare the calculation of the contribution to $\mathrm{NUM}^{(3)}$ done à la Goldstone with the third order correction to the ground-state energy

$$\begin{aligned} E^{(3)}_{\Omega} &= \sum_{l'\neq\Omega_0}\sum_{l\neq\Omega_0}\frac{\langle\Omega_0|V_{\rm int}|l'\rangle\langle l'|V_{\rm int}|l\rangle\langle l|V_{\rm int}|\Omega_0\rangle}{(E_{\Omega_0}-E_{l'})(E_{\Omega_0}-E_l)} \\ &\quad -\langle\Omega_0|V_{\rm int}|\Omega_0\rangle\sum_{l\neq\Omega_0}\frac{|\langle\Omega_0|V_{\rm int}|l\rangle|^2}{(E_{\Omega_0}-E_l)^2}\,, \end{aligned} \qquad (93)$$

given by the ordinary Rayleigh–Schrödinger series[11]. It is clear that taking into account only the contributions of connected Goldstone diagrams in evaluating $\mathrm{NUM}^{(3)}$ is equivalent to omitting the second, "non-connected", term in this formula, which is necessary to reproduce correctly the third order correction to the ground-state energy. In higher orders, the Rayleigh–Schrödindger formula has even more such "non-connected" terms which are potentially missed if only connected Goldstone diagrams are taken into account in computing the numerator taking for granted the statements to this effect which can be found in renowned textbooks [4, 9][12].

7. Summary

We have recalled several advanced methods of expressing the difference $E_\Omega - E_{\Omega_0}$ of the energies of ground-states $|\Omega\rangle$ and $|\Omega_0\rangle$ of the complete $H = H_0 + V_{\rm int}$ and free H_0 Hamiltonians. We have illustrated their working on a simple completely solvable example which requires only standard methods of quantum mechanics and is, therefore, accessible to students. We have also discussed systematic perturbative expansions of the difference $E_\Omega -$

[11] The third order term of this expansion is rarely displayed in textbooks.

[12] It seems that the proof that the denominator DEN exactly cancels the contribution of the disconnected diagrams, correct in the Dyson approach, has been in [4] extended to the Goldstone expansion witout any justification. Feynman [9] in reproducing the result of [14] sums only a class of Goldstone diagrams so the omission of "disconnected" contributions is of no consequence.

E_{Ω_0} in terms of Feynman and Goldstone diagrams and illustrated them on simple examples which can also serve to introduce diagrammatic techniques to beginners. The comparison of the results obtained with the help of the Dyson and Goldstone expansions allowed to point out the subtlety in the latter approach which is not taken into account in standard presentations of this method.

Appendix A

Phase of the evolution operator $U(t,0)$

Inserting into both sides of the equation (38) the operator

$$U(t,0) = \mathrm{e}^{i\varphi(t)}\,\mathrm{e}^{-iH_0t/\hbar}\,\mathrm{e}^{h(t)\,a^\dagger - h^*(t)\,a}\,, \tag{A.1}$$

together with $H(t) = \hbar\omega a^\dagger a + \varDelta_\omega + f(t)\,a^\dagger + f^*(t)\,a$, one obtains the equation

$$-\hbar\dot\varphi(t)\,U^\varepsilon(t,0) + i\hbar\,U(t,0)\,\mathrm{e}^{-B(t)}\,\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{B(t)} = \Big(f(t)\,a^\dagger + f^*(t)\,a\Big)\,U(t,0)\,, \tag{A.2}$$

in which $B(t) \equiv h(t)\,a^\dagger - h^*(t)\,a$. The terms with $H_0\,U(t,0)$ on both sides have canceled. One has now to work out the derivative

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^B = \dot B + \frac{1}{2}\,\dot B\,B + \frac{1}{2}\,B\,\dot B + \frac{1}{6}\,\dot B\,B\,B + \frac{1}{6}\,B\,\dot B\,B + \frac{1}{6}\,B\,B\,\dot B + \ldots\,, \tag{A.3}$$

by moving in each term $\dot B$ to the right. Since $[\dot B,\,B] = h^*\dot h - \dot h^* h$ is a c-number, this is easy and after writing down a few terms, one sees that the result is

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^B = \mathrm{e}^B\left[\dot B + \frac{1}{2}\Big(h^*\dot h - \dot h^* h\Big)\right]. \tag{A.4}$$

The equation determining φ can be therefore written in the form

$$\begin{aligned}&-\hbar\dot\varphi(t) + \frac{i}{2}\,\hbar\Big(h^*\dot h - \dot h^* h\Big) + i\hbar\,U(t,0)\Big(\dot h\,a^\dagger - \dot h^* a\Big)\,[U(t,0)]^\dagger\\ &= \mathrm{e}^{\varepsilon t}\Big(f(f)\,a^\dagger + f^*(t)\,a\Big)\,.\end{aligned} \tag{A.5}$$

Using formula (36), one works then out the last term on the left-hand side

$$\begin{aligned}&\mathrm{e}^{-iH_0t/\hbar}\,\mathrm{e}^{h\,a^\dagger - h^* a}\Big(\dot h\,a^\dagger - \dot h^* a\Big)\\ &\mathrm{e}^{-h\,a^\dagger + h^* a}\,\mathrm{e}^{iH_0t/\hbar} = \dot h\,\mathrm{e}^{-i\omega t}\,a^\dagger - \dot h^*\,\mathrm{e}^{i\omega t}\,a - h^*\dot h + \dot h^* h\,.\end{aligned} \tag{A.6}$$

Inserting this in the preceding formula after taking into account that

$$\dot{h} = -\frac{i}{\hbar}\, f(t)\, \mathrm{e}^{i\omega t}\,, \tag{A.7}$$

one finds that the terms with the operators $a^\dagger$ and a cancel out as they should and one obtains the c-number equation

$$\dot{\varphi} = -\frac{i}{2}\left(h^*\,\dot{h} - \dot{h}^*\,h\right)\,, \tag{A.8}$$

which determines the phase $\varphi(t)$.

Specifying now to $f(t) = \lambda\,\mathrm{e}^{\varepsilon t}$, *i.e.* setting

$$h = -\frac{i}{\hbar}\,\frac{\lambda}{\varepsilon + i\omega}\left(\mathrm{e}^{(\varepsilon+i\omega)t} - 1\right), \tag{A.9}$$

one gets

$$\dot{\varphi} = \frac{|\lambda|^2}{2\hbar^2(\omega^2+\varepsilon^2)}\left\{2\omega\,\mathrm{e}^{2\varepsilon t} + i\,(\varepsilon + i\omega)\,\mathrm{e}^{(\varepsilon+i\omega)t} - i\,(\varepsilon - i\omega)\,\mathrm{e}^{(\varepsilon-i\omega)t}\right\}. \tag{A.10}$$

Integrating (the integration constant is fixed by the requirement $\varphi(0) = 0$ which stems from the initial condition $U(0,0) = \hat{1}$) one finds

$$\varphi(t) \equiv \varphi^{\varepsilon}(t) = \frac{|\lambda|^2}{2\hbar^2(\omega^2+\varepsilon^2)}\left\{\frac{\omega}{\varepsilon}\left(\mathrm{e}^{2\varepsilon t} - 1\right) + i\,\mathrm{e}^{(\varepsilon+i\omega)t} - i\,\mathrm{e}^{(\varepsilon-i\omega)t}\right\}. \tag{A.11}$$

Appendix B

Computation of the integral I

Here, we compute the integral I. The computation is rudimentary (it uses the residue method) but somewhat tedious. It is convenient to do it in steps

$$\begin{aligned}
I &= \int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\nu_1}{2\pi}\,\frac{1}{[\nu_1^2 - \omega^2 + i0]}\,J(\nu_1)\,,\\
J(\nu_1) &= \int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\nu_2}{2\pi}\,\frac{1}{[\nu_2^2 - \omega^2 + i0]}\,K(\nu_1,\nu_2)\,,\\
K(\nu_1,\nu_2) &= \int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\nu_3}{2\pi}\,\frac{1}{[\nu_3^2 - \omega^2 + i0][(\nu_1+\nu_2+\nu_3)^2 - \omega^2 + i0]}\,.
\end{aligned} \tag{B.1}$$

The integrand of the last integral has four simple poles: two below the real axis, at $\nu_3 = \omega - i0$ and at $\nu_3 = \omega - \nu_1 - \nu_2 - i0$, and two above the real axis at $\nu_3 = -\omega + i0$ and at $\nu_3 = -\omega + \nu_1 + \nu_2 + i0$. Closing the contour in the lower half plane, *i.e.* picking the poles below the real axis, one finds that

$$\begin{aligned} K(\nu_1, \nu_2) &= \frac{-i}{2\omega(\nu_1 + \nu_2)} \left[\frac{1}{2\omega + \nu_1 + \nu_2 - 2i0} - \frac{1}{2\omega - \nu_1 - \nu_2 - 2i0} \right] \\ &= \frac{-i}{\omega} \frac{1}{(\nu_1 + \nu_2)^2 - (2\omega - 2i0)^2} \, . \end{aligned} \tag{B.2}$$

The next integral

$$J(\nu_1) = \frac{-i}{\omega} \int_{-\infty}^{\infty} \frac{d\nu_2}{2\pi} \frac{1}{[\nu_2^2 - \omega^2 + i0][(\nu_1 + \nu_2)^2 - (2\omega - 2i0)^2]} \, , \tag{B.3}$$

has also two simple poles below the real axis, at $\nu_2 = \omega - i0$ and at $\nu_2 = 2\omega - \nu_1 - 2i0$, and two above it, $\nu_2 = -\omega + i0$ and at $\nu_2 = -2\omega + \nu_1 - 2i0$. Picking those below (or those above) one finds that

$$\begin{aligned} J(\nu_1) &= \left(\frac{-i}{\omega} \right) \left(\frac{-i}{2\omega} \right) \\ &\times \left[\frac{1}{(\nu_1 + \omega - i0)^2 - (2\omega - 2i0)^2} + \frac{1}{2} \frac{1}{(\nu_1 - 2\omega + 2i0)^2 - \omega^2 + i0} \right] . \end{aligned} \tag{B.4}$$

Therefore, I splits into two parts $I = I_1 + I_2$. The integrand of I_1,

$$I_1 = -\frac{1}{2\omega^2} \int_{-\infty}^{\infty} \frac{d\nu_1}{2\pi} \frac{1}{[\nu_1 - \omega + i0]^2 [\nu_1 + \omega - i0][\nu_1 + 3\omega - 3i0]} \, , \tag{B.5}$$

has three poles. Either way, *i.e.* either picking the single double pole below the real axis at $\nu_1 = \omega - i0$, or picking the two simple poles at $\nu_1 = -\omega + i0$ and at $\nu_1 = -3\omega + 3i0$, one finds that $I_1 = -3i/64\omega^5$. The integrand of I_2,

$$I_2 = -\frac{1}{4\omega^2} \int_{-\infty}^{\infty} \frac{d\nu_1}{2\pi} \frac{1}{[\nu_1 - \omega + i0]^2 [\nu_1 + \omega - i0][\nu_1 - 3\omega + 3i0]} \, , \tag{B.6}$$

has also three poles but now there is only one simple pole above the real axis at $\nu_1 = -\omega + i0$ and two, one simple at $\nu_1 = 3\omega - 3i0$ and one double at $\nu_1 = \omega - i0$. It is therefore easier to pick the pole above the axis. The result is $I_2 = i/64\omega^5$. In all, therefore, $I = -i/32\omega^5$.

REFERENCES

[1] L. Schiff, «Quantum Mechanics», 3rd Ed., *McGraw-Hill Book Company*, 1968; L.D. Landau, E.M. Lifshitz, «Kwantovaja Mechanika», *Fizmatlit*, 2002.

[2] A. Messiah, «Quantum Mechanics», *Dover Books on Physics*, 2014.

[3] M. Gell-Mann, F. Low, «Bound States in Quantum Field Theory», *Phys. Rev.* **84**, 350 (1951).

[4] A.L. Fetter, J.D. Walecka, «Quantum Theory of Many Particle Systems», *McGraw Hill*, 1971.

[5] J.R. Taylor, «The Quantum Scattering Theory of Nonrelativistic Collisions», *John Wiley and Sons, Inc.*, 1972.

[6] S. Weinberg, «The Quantum Theory of Fields, Volume 1: Foundations», *Cambridge University Press*, 1995.

[7] L.G. Molinari, «Another proof of Gell-Mann and Low's theorem», *J. Math. Phys.* **48**, (2007).

[8] J. Sucher, «S-Matrix Formalism for Level-Shift Calculations», *Phys. Rev.* **107**, 1448 (1957).

[9] R.P. Feynman, «Statistical Mechanics. A Set of Lectures», *W.A. Benjamin, Inc.*, 1972.

[10] L.G. Molinari, «Notes on Wick's theorem in many-body theory» `arXiv:1710.09248 [math-phys]`.

[11] H.-W. Hammer, R.J. Furnstahl, «Effective field theory for dilute Fermi systems», *Nucl. Phys. A* **678**, 277 (2000), `arXiv:nucl-th/0004043`.

[12] C. Wellenhofer, C. Drischler, A. Schwenk, «Dilute Fermi gas at fourth order in effective field theory», *Phys. Lett. B* **802**, 135247 (2020).

[13] P.H. Chankowski, J. Wojtkiewicz, «Ground-state energy of the polarized dilute gas of interacting spin-$\frac{1}{2}$ fermions», *Phys. Rev. B* **104**, 144425 (2021); P.H. Chankowski, J. Wojtkiewicz, R. Bakhshizada, «Third-order Corrections to the Ground-state Energy of the Polarized Diluted Gas of spin-$\frac{1}{2}$ Fermions», *Acta Phys. Pol. B* **53**, 9-A4 (2022); P.H. Chankowski, J. Wojtkiewicz, S. Augustynowicz, «Third-order corrections to the ground-state energy of the gas of spin-s fermions with arbitrary densities of different spin projections» *Phys. Rev. A* **107**, 063311 (2023).

[14] M. Gell-Mann, K.A. Brueckner, «Correlation Energy of an Electron Gas at High Density», *Phys. Rev.* **106**, 364 (1957).