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BARRIER PENETRATION AND INSTANTONS

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Chapter 1

Barrier Penetration: Degenerate Classical Minima

A classical particle is always reflected by a potential barrier if its energy is lower than the potential. In contrast, a quantum particle has a non-vanishing probability to tunnel through a barrier, a property also called barrier penetration or tunnelling.

This chapter is devoted to a study of a first physical manifestation of barrier penetration. Using the path integral formalism, we evaluate, in the semi-classical limit $\hbar \to 0$, the splitting between classically degenerate energy levels corresponding to symmetric minima of a potential. In the next chapter we calculate, in the same limit, the decay rate of metastable states. Since no classical trajectory can be associated to barrier penetration, one may wonder how it is possible to evaluate such effects in the semi-classical limit. Actually, it has been noticed that, formally, barrier penetration has a semi-classical interpretation in terms of classical particles moving in imaginary time (see the discussion at the end of section 1.1). The Euclidean formalism based on calculating the density matrix at thermal equilibrium $\mathrm{e}^{-\beta H}$, describes formally an evolution in imaginary time. We verify, in this chapter, that indeed it allows evaluating barrier penetration effects.

Although the methods can be generalized, we mainly discuss properties of the ground state or close excited energy levels and, thus, for example, the partition function for $\beta \to \infty$. Our tool is the steepest descent method applied to the path integral, but in this problem the saddle points correspond to solutions of the equations of the classical motion that are no longer constants. These solutions satisfy one condition: the difference between their action and the action of the minimal constant solution remains finite when $\beta \to \infty$. One associates to such solutions the name *instanton*.

To calculate instanton contributions at leading order, one must master two problems that are increasingly difficult: find the saddle points by solving classical equations, expand the integrand around the saddle point and evaluate the path integral at leading order by integrating over Gaussian fluctuations.

Note that calculations based on the steepest descent method lead to semi-classical evaluations that can also be obtained by solving the Schrödinger equation in the WKB approximation, but the steepest descent method can be generalized much more easily to barrier penetration effects in quantum field theory.

Finally, as examples we discuss the quartic double-well potential and the periodic cosine potential.

1.1 Quantum evolution. The semi-classical limit

In this chapter, we consider the non-relativistic quantum mechanics of a particle mainly in one space dimension with a simple Hamiltonian of the form

$$H(t) = \hat{p}^2/2m + V(\hat{q})\,, \tag{1.1}$$

where the operators $\hat{p}, \hat{q}$ are d-component vectors and V is a regular function of q. The canonical commutation relations between the components of $\hat{q}$ and the d components of the momentum operator $\hat{p}$ are

$$[\hat{q}, \hat{p}] = i\mathbf{1}\,, \tag{1.2}$$

where $\mathbf{1}$ is the identity operator.

The evolution operator $U(t'', t')$ between time t' and t'' is a *unitary* operator solution of

$$i\hbar \frac{\partial U}{\partial t}(t, t') = H(t)U(t, t')\,, \quad U(t', t') = \mathbf{1}\,. \tag{1.3}$$

When H is time-independent, $U(t'', t') = \mathrm{e}^{-iH(t''-t')/\hbar}$ and the Hamiltonian is the generator of time-translations. For the matrix elements of U, in the basis in which the position operator $\hat{q}$ is diagonal, equation (1.3) takes the form of a Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \langle q \left| U(t, t') \right| q' \rangle = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{(\partial q)^2} + V(q, t) \right] \langle q \left| U(t, t') \right| q' \rangle \tag{1.4}$$

with the boundary conditions

$$\langle q \left| U(t', t') \right| q' \rangle = \delta(q - q').$$

It can be shown that this equation can be solved formally in the form of a path integral

$$\langle q \left| U(t'', t') \right| q' \rangle = \int [\mathrm{d}q(t)]\, \mathrm{e}^{i\mathcal{S}(q/\hbar)},$$

where $\mathcal{S}$ is the classical action:

$$\mathcal{S}(q) = \int_{t'}^{t''} \mathrm{d}t \left[\tfrac{1}{2} m(\dot{q})^2 - V(q, t) \right]$$

and the symbol $\int [\mathrm{d}q(t)]$ means here sum over all paths satisfying the boundary conditions $q(t') = q'$ and $q(t'') = q''$ [1, 2].

In what follows, we denote by $[\mathrm{d}q(t)]$ (with brackets) the integration measure to distinguish path integrals from ordinary integrals.

Path integral and semi-classical limit. In the limit in which the classical action is much larger than $\hbar$, the path integral can be evaluated by the stationary phase approximation. The critical path that gives the leading contribution to the path integral is then obtained by expressing that the action is stationary under a variation of the path. Thus, the critical path is exactly the classical path, that is, the path solution of the classical equations of motion. For a time-independent potential and in $d = 1$ space dimension, the classical trajectory is given by inverting the relation

$$t - t' = \pm \int_{q'}^{q} \frac{\mathrm{d}s}{\sqrt{2m\bigl(E - V(s)\bigr)}}$$

with the boundary condition

$$t'' - t' = \pm \int_{q'}^{q''} \frac{\mathrm{d}s}{\sqrt{2m\bigl(E - V(s)\bigr)}}.$$

However, in quantum mechanics, barrier penetration, or tunnelling, corresponds to the classically forbidden region where $Vq) > E$ and has no classical analogue. We then notice that, formally, the forbidden region corresponds to a classical trajectory in imaginary time. Since we will be only interested in calculating barrier penetration coefficients, we can thus study imaginary time evolution, that is, the matrix elements of the operator $\mathrm{e}^{-\tau H/\hbar}$, which is identical to the matrix density at thermal equilibrium $\mathrm{e}^{-\beta H}/\mathcal{Z}$ ($\mathcal{Z} = \operatorname{tr} \mathrm{e}^{-\beta H}$) up to a change in parametrization $\beta \mapsto \tau/\hbar$. We will work in the framework of quantum statistical physics and evaluate the matrix elements of $\mathrm{e}^{-\beta H}$ in the semi-classical limit [3]. Note that when $\beta \to \infty$, the operator $\mathrm{e}^{-\beta H}$ projects onto the ground state of the Hamiltonian and, therefore, provides also a tool to determine the structure of the ground state and the ground state energy.

1.2 Double-well potentials and instantons

We study a first family of quantum systems where tunnelling plays a role: the Hamiltonian has a discrete space symmetry, but the potential has minima at points that are not group invariant. The positions of the degenerate minima are then related by symmetry group transformations.

Classically, the minimal energy solutions correspond to particles at rest in any one of the minima of the potential. The position of the particle breaks (spontaneously) the symmetry of the system. In contrast, for a quantum system with a finite number of degrees of freedom, the ground state cannot be degenerate. Therefore, the ground state must correspond to a symmetric wave function, its modulus being maximal near each of the minima of the potential. This phenomenon is a consequence of barrier penetration, a particle initially in one of the minima having a non-vanishing probability to tunnel into the others. We evaluate here the energy splitting between the classically degenerate energy levels in the semi-classical limit.

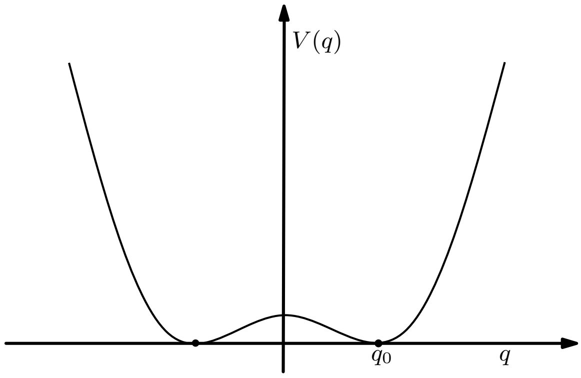

FIG. 1.1 – *Double-well potential.*

1.2.1 Double-well potentials

A simple example of such a situation is provided by a reflection-symmetric Hamiltonian with a potential of the form of a symmetric double-well (figure 1.1):

$$H = \tfrac{1}{2}\hat{p}^2 + V(\hat{q}), \tag{1.5}$$

where $\hat{p}$ and $\hat{q}$ are the momentum and position operator and the potential $V(q)$ is a regular, positive, even function; it is minimum at two symmetric points $q = \pm q_0 \neq 0$ where it vanishes:

$$V(q) = V(-q) \geq 0\,,\ V(\pm q_0) = 0\,,\ V(q_0 + x) = \tfrac{1}{2}x^2 + O(x^4).$$

The Hamiltonian (1.5) is clearly invariant under the reflection $q \mapsto -q$. To this reflection is associated an operator P that acts on wave functions as

$$[P\psi](q) = \psi(-q). \tag{1.6}$$

Reflection symmetry, then, is expressed by the commutation of the quantum Hamiltonian H with the reflection operator P:

$$[P, H] = 0\,.$$

The two operators P and H can thus be diagonalized simultaneously: the eigenfunctions ψ_n of H are even or odd functions:

$$[P\psi_{n,\pm}](q) = \psi_{n,\pm}(-q) = \pm\psi_{n,\pm}(q).$$

Below we consider the two operators $\mathrm{e}^{-\tau H/\hbar}$ and $P\,\mathrm{e}^{-\tau H/\hbar}$. The eigenvalues of $\mathrm{e}^{-\tau H/\hbar}$ and $P\,\mathrm{e}^{-\tau H/\hbar}$ corresponding to the eigenvectors $\psi_{n,\pm}(q)$ are then, respectively, $\mathrm{e}^{-\tau E_{n,\pm}/\hbar}$ and $\pm\,\mathrm{e}^{-\tau E_{n,\pm}/\hbar}$.

1.2.2 Path integral in the semi-classical limit

The properties of the ground state, in the semi-classical limit, can be inferred from the partition function $\mathcal{Z}(\tau/\hbar)$ in the limit $\hbar \to 0$ and then $\tau \to \infty$. The partition function is given by the path integral

$$\mathcal{Z}(\tau/\hbar) = \int_{q(-\tau/2)=q(\tau/2)} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}(q)/\hbar\right] \tag{1.7}$$

with

$$\mathcal{S}(q) = \int_{-\tau/2}^{\tau/2} \left[\tfrac{1}{2}\dot{q}^2(t) + V\big(q(t)\big)\right] \mathrm{d}t\,. \tag{1.8}$$

The potential has two degenerate minima at $q = \pm q_0$. Thus, the action $\mathcal{S}$ is minimum for the two constant functions $q(t) = \pm q_0$ that minimize both the kinetic and potential term. For $\hbar \to 0$, these two functions correspond to saddle points and, for symmetry reasons, they yield identical contributions. To calculate the contribution of one saddle point, for example, $q(t) = -q_0$, one can set

$$q(t) = -q_0 + x(t)\sqrt{\hbar}\,.$$

The action becomes

$$\mathcal{S}(x)/\hbar = \int_{-\tau/2}^{\tau/2} \left[\tfrac{1}{2}\dot{x}^2(t) + V\big(q_0 - x(t)\sqrt{\hbar}\big)/\hbar\right] \mathrm{d}t\,. \tag{1.9}$$

One then expands in powers of $\hbar$. The first terms are quadratic in x and correspond to a harmonic oscillator. The existence of the two symmetric saddle points yields a factor 2, which simply indicates the presence of two states of energy E_0 degenerate to all orders in $\hbar$, corresponding to two wave functions, $\psi_{n,+} \pm \psi_{n,-}$ if the functions have the same normalization, located in each of the two wells of the potential.

1.2.3 Level splitting

Notation. From now on, we restrict the discussion to the two lowest energy eigenvalues (the generalization to other levels is simple) and, thus, omit the subscript 0 on E.

Quite generally, one can show that the ground state wave function ψ_+ with energy E_+, can be chosen positive and the wave function $\psi_-(q)$ of the first excited state with energy E_-, vanishes once. The functions ψ_+ and $\psi_-(q)$ are thus even and odd, respectively.

The analysis of section 1.2.2 indicates that energy difference $E_- - E_+$ vanishes faster than any power of $\hbar$ and, thus, cannot easily be inferred from a calculation of $\operatorname{tr} \mathrm{e}^{-\tau H/\hbar}$. Indeed, in the double limit $\hbar \to 0$ then $\tau \to \infty$, one finds

$$\begin{aligned}\operatorname{tr} \mathrm{e}^{-\tau H/\hbar} &\sim \mathrm{e}^{-\tau E_+/\hbar} + \mathrm{e}^{-\tau E_-/\hbar} \\ &\sim 2\,\mathrm{e}^{-\tau(E_+ + E_-)/2\hbar} \cosh[\tau(E_+ - E_-)/2\hbar].\end{aligned} \tag{1.10}$$

The partition function is dominated by the perturbative expansion of the half-sum $E = \frac{1}{2}(E_+ + E_-)$, and depends on the non-perturbative difference between E_+ and E_- only at order $(E_+ - E_-)^2$.

The difference $E_+ - E_-$ can more easily been inferred from the quantity $\operatorname{tr} P\, \mathrm{e}^{-\tau H/\hbar}$. Indeed, in the same limits $\hbar \to 0$ then $\tau \to \infty$, one finds

$$\begin{aligned}\operatorname{tr} P\, \mathrm{e}^{-\tau H/\hbar} &\sim \mathrm{e}^{-\tau E_+/\hbar} - \mathrm{e}^{-\tau E_-/\hbar} \\ &\sim -2\sinh[\tau(E_+ - E_-)/2\hbar]\, \mathrm{e}^{-\tau(E_+ + E_-)/2\hbar}\,. \end{aligned} \tag{1.11}$$

Since $E_+ - E_-$ vanishes to all orders in $\hbar$ (and $E_\pm \sim \frac{1}{2}\hbar$), at leading order

$$\operatorname{tr} P\, \mathrm{e}^{-\tau H/\hbar} \sim -\tau\, \mathrm{e}^{-\tau/2}\, \frac{E_+ - E_-}{\hbar}. \tag{1.12}$$

Actually, it is convenient to calculate the ratio between the quantities (1.10) and (1.11):

$$\langle P \rangle \equiv \operatorname{tr} P\, \mathrm{e}^{-\tau H/\hbar} \Big/ \operatorname{tr} \mathrm{e}^{-\tau H/\hbar} \sim -\frac{\tau}{2\hbar}(E_+ - E_-). \tag{1.13}$$

The path integral representation of $\operatorname{tr} P\, \mathrm{e}^{-\tau H/\hbar}$ differs from the representation of the partition function only in the (twisted) boundary conditions:

$$\operatorname{tr} P\, \mathrm{e}^{-\tau H/\hbar} = \int_{q(-\tau/2) = -q(\tau/2)} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}(q)/\hbar\right] \tag{1.14}$$

with the same action (1.8).

1.2.4 Instantons

Following the analysis of section 1.2.3, we calculate the twisted partition function

$$\operatorname{tr} P\, \mathrm{e}^{-\tau H/\hbar} = \int_{q(\tau/2) = -q(-\tau/2)} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}(q)/\hbar\right] \tag{1.15}$$

with

$$\mathcal{S}(q) = \int_{-\tau/2}^{\tau/2} \left[\tfrac{1}{2}\dot{q}^2(t) + V\big(q(t)\big)\right] \mathrm{d}t\,, \tag{1.16}$$

for $\hbar \to 0$ and $\tau \to \infty$.

While the path integral representing $\operatorname{tr} \mathrm{e}^{-\tau H/\hbar}$ is dominated by the constant saddle points $q(t) = \pm q_0$, these paths do not contribute to the integral (1.15) because they do not satisfy the corresponding boundary conditions. This is consistent with the property that the difference $E_+ - E_-$ vanishes faster than any power of $\hbar$. One must thus look for non-constant solutions of the equation of the Euclidean classical motion. Moreover, the action of these solutions must have a finite limit in the relevant limit $\tau \to \infty$, otherwise they do not contribute. One associates to such solutions the name *instanton*, as if they would correspond to particles.

Since both the kinetic term and the potential are positive, this condition implies that both vanish for $|t| \to \infty$. This implies

$$q(-\infty) = \pm q_0 \text{ and } q(+\infty) = \mp q_0 .$$

The splitting between the two energy levels thus depends on the existence of instanton solutions joining the two symmetric minima of the potential (Fig. 1.2).

The saddle point equation, obtained by varying the Euclidean action, is identical to the equation of the usual classical motion (*i.e.*, in real time) in the potential $-V(q)$:

$$-\ddot{q} + V'(q) = 0 . \tag{1.17}$$

In the limit $\tau \to \infty$, for finite action solutions $q_c(t)$, the integration of the equation yields

$$\tfrac{1}{2}\dot{q}_c^2(t) - V\big(q_c(t)\big) = 0 . \tag{1.18}$$

Moreover, if $q_c(t)$ is a solution, $q_c(t - t_0)$ is a solution. For τ large but finite, the parameter t_0 varies in an interval of size τ.

The integration of equation (1.18) implies that $q_c(t)$ is obtained by inverting

$$t - t_0 = \pm \int_0^{q_c} \frac{\mathrm{d}y}{\sqrt{2V(y)}} .$$

Moreover, one infers from equation (1.18) that the corresponding action can be written as

$$A = \int_{-\infty}^{+\infty} \mathrm{d}t\, \dot{q}_c^2(t) . \tag{1.19}$$

Once the saddle point is identified, the corresponding contribution to the path integral is, in general, given at leading order by a Gaussian integration. Here, the integration involves a rather subtle problem that we discuss later. However, note that we have found two families (two signs) of degenerate saddle points, which depend on the parameter t_0. Since for τ large but finite, t_0 varies in an interval of size τ, the sum over all saddle points generates a factor τ, consistent with expression (1.13).

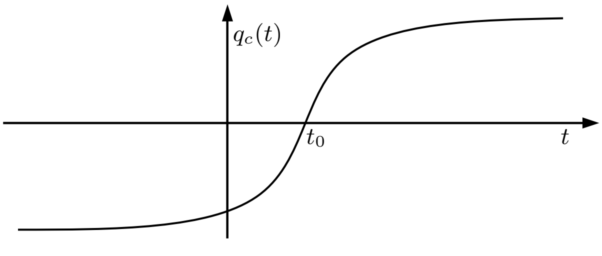

FIG. 1.2 – *Instanton-type solution.*

1.2.5 Gaussian integration and zero mode

We now expand the action $\mathcal{S}(q)$ around the saddle point, setting

$$q(t) = q_c(t) + r(t), \quad r(\tau/2) = -r(-\tau/2).$$

To second order in r, the expansion takes the form

$$\mathcal{S}(q_c + r) = A + \int_{-\tau/2}^{\tau/2} \mathrm{d}t \left[\tfrac{1}{2}\dot{r}^2(t) + V''\big(q_c(t)\big)r^2(t)\right] + O(r^3).$$

The quadratic form in r can be written as

$$\begin{aligned}\Sigma(r) &= \int_{-\tau/2}^{\tau/2} \mathrm{d}t \left[\tfrac{1}{2}\dot{r}^2(t) + \tfrac{1}{2}V''\big(q_c(t)\big)r^2(t)\right] \\ &= \frac{1}{2}\int \mathrm{d}t_1 \mathrm{d}t_2\, r(t_1)M(t_1,t_2)r(t_2),\end{aligned}$$

where

$$M(t_1,t_2) = \frac{\delta^2 \mathcal{S}}{\delta q_c(t_1)\delta q_c(t_2)} = \left[-\mathrm{d}_{t_1}^2 + V''\big(q_c(t_1)\big)\right]\delta(t_1 - t_2). \tag{1.20}$$

The differential operator M acts on a function $r(t)$ as

$$\int \mathrm{d}t'\, M(t,t')r(t') = \frac{\delta}{\delta r(t)}\Sigma(r) = -\ddot{r}(t) + V''\big(q_c(t)\big)r(t). \tag{1.21}$$

It has the form of a Hermitian quantum Hamiltonian, t playing the role of a position variable and $V''\big(q_c(t)\big)$ being the potential. All its eigenvalues are real as well as its determinant.

Note that in the limit $\tau \to \infty$, only the trajectories that satisfy $r(\pm\infty) = 0$ contribute to the path integral in such a way that the boundary conditions are automatically satisfied.

Naively, the Gaussian integral over $r(t)$ then leads to

$$\operatorname{tr} P\, \mathrm{e}^{-\tau/\hbar} \propto \mathrm{e}^{-A/\hbar} \int [\mathrm{d}r(t)] \exp\left(-\Sigma(r)/\hbar\right) \propto \frac{\mathrm{e}^{-A/\hbar}}{\sqrt{\det(M/\hbar)}},$$

an expression that must be evaluated in the limit $\tau \to \infty$.

The zero mode. Differentiating the equation of motion (1.17) with respect to t, one finds

$$\left[-\mathrm{d}_t^2 + V''\big(q_c(t)\big)\right]\dot{q}_c(t) = 0\,. \tag{1.22}$$

Comparing with equation (1.21), one recognizes the action of M on $\dot{q}_c$. Since the function $\dot{q}_c(t)$ is square integrable (equation (1.19)), the equation implies that $\dot{q}_c(t)$ is an eigenvector of M with vanishing eigenvalue:

$$M\dot{q}_c = 0\,. \tag{1.23}$$

The Gaussian integration yields a result proportional to $(\det M)^{-1/2}$, which is thus infinite!

The problem could have been anticipated: as we have already pointed out, due to time-translation invariance, one finds a one-parameter family of degenerate saddle points related by continuous time-translations. The action is thus invariant under an infinitesimal variation of $q_c(t)$, which corresponds to a variation of the parameter t_0 and, thus, is proportional to $\dot{q}_c$. The problem that we face here is by no means specific to path integrals, as the example of an ordinary integral will show. Its solution requires the introduction of collective coordinates associated to the continuous symmetries of the integrand.

Another remark is important here. One infers from the general theory of orthogonal functions that the number of zeros of eigenfunctions of the Hamiltonian M is directly related to the hierarchy of eigenvalues: the ground state of M has no zero, the first excited state has one zero... In the present example, the eigenfunction $\dot{q}_c(t)$ does not vanish (see Fig. 1.2): thus, it corresponds to the ground state, and all other eigenvalues of M are positive.

1.3 Collective coordinates and Gaussian integration

To investigate the problem of the zero mode, we first consider an ordinary integral in which the integrand is invariant under some continuous group of transformations, here rotations in the plane.

1.3.1 Zero modes in simple integrals

We consider a double integral of the general form:

$$I(g) = \int \mathrm{d}^2\mathbf{x}\ \mathrm{e}^{-S(\mathbf{x})/g},\ S(\mathbf{x}) = -\mathbf{x}^2/2 + (\mathbf{x}^2)^2/4\,, \tag{1.24}$$

where $\mathbf{x}$ is the two-component vector (x_1, x_2), and the integrand is a function only of $\mathbf{x}^2$.

For $g \to 0_+$, this integral can be calculated by the steepest descent method. A naive approach is the following: the saddle points are solutions of the equation

$$\frac{\partial S}{\partial x_\mu} = -x_\mu(1-\mathbf{x}^2) = 0\,. \tag{1.25}$$

The origin $\mathbf{x} = \mathbf{0}$, which corresponds to a relative maximum, is not a relevant saddle point. The minima correspond to

$$|\mathbf{x}| = 1\,. \tag{1.26}$$

Due to the rotation invariance of the integrand, one finds here also a one-parameter family of degenerate saddle points belonging to a circle, since only the length of the vector $\mathbf{x}$ is determined by the saddle point equation. If one chooses one particular saddle point and evaluates its contribution in the Gaussian approximation, one finds a result that involves the determinant of the matrix

$$M_{\mu\nu} = \left.\frac{\partial^2 S}{\partial x_\mu \partial x_\nu}\right|_{|\mathbf{x}|=1} = 2x_\mu x_\nu\,. \tag{1.27}$$

The matrix is a projector on the vector $\mathbf{x}$. The vector orthogonal to $\mathbf{x}$ corresponds to a flat direction for the integrand and, thus, is an eigenvector with a vanishing eigenvalue.

Here, the problem has a straightforward solution: the integral over the angular variable that parametrizes the set of all saddle points, also called the *collective coordinate*, must be calculated exactly; only the integral over the length of the vector can be evaluated by the steepest descent method. This is the strategy we want to generalize to path integrals.

1.3.2 Collective coordinates in path integrals

In the case of a path integral also, it is necessary to integrate exactly over the variables that parametrize the saddle points, the so-called *collective coordinates* [4]. In the example of the instanton solutions of equation (1.18), the time-translation parameter t_0 is the collective coordinate. To be able to integrate, one must explicitly factorize the integration over the collective coordinate in the integration measure. This is the idea of the method of collective coordinates. The problem is slightly more subtle than in the example (1.24) because the number of integration variables is infinite.

Collective coordinates and Faddeev–Popov's method. To factorize the integration over the collective time parameter (the collective coordinate), we introduce the so-called Faddeev–Popov's method.

We denote now by $q_c(t)$ a particular solution of the saddle point equation (1.18) corresponding to $t_0 = 0$ and the general solution then is $q_c(t - t_0)$.

We start from the identity

$$1 = \frac{1}{\sqrt{2\pi\xi}} \int_{-\infty}^{+\infty} \mathrm{d}\lambda\, \mathrm{e}^{-\lambda^2/2\xi},$$

where ξ is an arbitrary constant. We introduce the vector with unit $\mathcal{L}^2$ norm

$$g_0(t) = \dot{q}_c(t)/\|\dot{q}_c\| \text{ with } \|\dot{q}_c\|^2 = \int \mathrm{d}t\, \dot{q}_c^2(t).$$

We then change variables, $\lambda \mapsto t_0$, setting

$$\lambda = \int \mathrm{d}t\, g_0(t)\big(q(t + t_0) - q_c(t)\big).$$

We obtain the new identity

$$\frac{1}{\sqrt{2\pi\xi}} \int \mathrm{d}t_0 \left[\int \mathrm{d}t\, g_0(t)\dot{q}(t + t_0)\right] \exp\left\{-\frac{1}{2\xi}\left[\int \mathrm{d}t\, g_0(t)\big(q(t + t_0) - q_c(t)\big)\right]^2\right\} = 1\,. \tag{1.28}$$

The constant ξ has been introduced partially for cosmetic reasons, but is considered to be of order $\hbar$.

We insert identity (1.28) into the path integral (1.15):

$$\operatorname{tr} P\,\mathrm{e}^{-\tau H/\hbar} = \frac{1}{\sqrt{2\pi\xi}}\int \mathrm{d}t_0 \int [\mathrm{d}q(t)] \left[\int \mathrm{d}t\, g_0(t)\dot{q}(t+t_0)\right] \exp\left[-\mathcal{S}_\xi(q)/\hbar\right],$$

where the total action

$$\mathcal{S}_\xi(q) = \mathcal{S}(q) + \frac{\hbar}{2\xi}\left[\int \mathrm{d}t\, g_0(t)\big(q(t+t_0) - q_c(t)\big)\right]^2$$

is no longer invariant under time-translations because time appears explicitly through the function $q_c(t)$ and thus $g_0(t)$.

The function $q(t+t_0)$ can now be renamed $q(t)$. This affects $\mathcal{S}(q)$, but we change variables, $t - t_0 \mapsto t$, in the action. Then, for $\tau = \infty$, one recovers the initial action because the integration domain is not modified.

The integrand then no longer depends on the variable t_0 and the integration over t_0 is immediate. For $\tau \to \infty$,

$$\operatorname{tr} P\,\mathrm{e}^{-\tau H/\hbar} \sim \frac{\tau}{\sqrt{2\pi\xi}} \int [\mathrm{d}q(t)] \left[\int \mathrm{d}t\, g_0(t)\dot{q}(t)\right] \exp\left[-\mathcal{S}_\xi(q)/\hbar\right] \tag{1.29}$$

with

$$\mathcal{S}_\xi(q) = \mathcal{S}(q) + \frac{\hbar}{2\xi}\left[\int \mathrm{d}t\, g_0(t)\big(q(t) - q_c(t)\big)\right]^2.$$

At leading order for $\hbar \to 0$, in the Jacobian $q(t)$ can be replaced by $q_c(t)$ and thus

$$\int \mathrm{d}t\, g_0(t)\dot{q}(t) \sim \int \mathrm{d}t\, g_0(t)\dot{q}_c(t) = \|\dot{q}_c\|.$$

1.3.3 Gaussian integration

The saddle point equation becomes

$$\frac{\delta \mathcal{S}}{\delta q(t)} + \frac{\hbar}{\xi} g_0(t) \int \mathrm{d}t'\, \dot{g}_0(t')\big(q(t') - q_c(t')\big) = 0\,. \tag{1.30}$$

Clearly, the solution of this equation is $q(t) = q_c(t)$. The second functional derivative of the action at the saddle point is then modified by an additional contribution:

$$\frac{\delta^2 \mathcal{S}}{\delta q_c(t_1)\delta q_c(t_2)} \mapsto M_\xi(t_1,t_2) \equiv \frac{\delta^2 \mathcal{S}}{\delta q_c(t_1)\delta q_c(t_2)} + \frac{\hbar}{\xi} g_0(t_1) g_0(t_2).$$

The additional operator is a projector on to the eigenvector of $\delta^2\mathcal{S}/\delta q_c \delta q_c$ corresponding to the vanishing eigenvalue. The modified operator, thus, has the same eigenvectors and the same eigenvalues as the initial operator $\delta^2\mathcal{S}/\delta q_c \delta q_c$, with one exception: the eigenvalue corresponding to the eigenvector $\dot{q}_c \propto g_0$ is now

$$\mu = \hbar/\xi \tag{1.31}$$

instead of 0. Therefore, the determinant of the operator M_ξ no longer vanishes and the problem of the zero mode is solved.

The normalization of the path integral can be inferred by comparing it to the partition function $\mathcal{Z}_0(\tau/\hbar)$ of the harmonic oscillator:

$$\mathcal{Z}_0(\tau/\hbar) = \int_{q(-\tau/2)=q(\tau/2)} [\mathrm{d}q(t)] \exp\left\{-\frac{1}{2\hbar}\int_{-\tau/2}^{\tau/2} \mathrm{d}t\ \left[\dot{q}^2(t) + q^2(t)\right]\right\}, \quad (1.32)$$

which for $\tau \to \infty$ reduces to $\mathrm{e}^{-\tau/2}$. In this limit, the Gaussian integral can be expressed in terms of the operator

$$M_0(t_1,t_2) = \left[-\left(\mathrm{d}_{t_1}\right)^2 + 1\right]\delta(t_1 - t_2). \quad (1.33)$$

As we indicate later, the quantity that can be easily evaluated is the determinant of the operator $(M+\varepsilon)(M_0+\varepsilon)^{-1}$, where ε is an arbitrary constant. For $\varepsilon \to 0$, this expression vanishes linearly in ε and we thus set

$$\lim_{\varepsilon\to 0} \frac{1}{\varepsilon} \det\left(M+\varepsilon\right)\left(M_0+\varepsilon\right)^{-1} \equiv \det{}' M M_0^{-1}, \quad (1.34)$$

where $\det{}' M$ means determinant in the subspace orthogonal to $\dot{q}_c$. On the other hand, what is needed here is (the factors $\hbar$ cancel in the ratio of Gaussian integrals)

$$\begin{aligned}\det M_\xi &= \det(M + \mu\,|0\rangle\,\langle 0|)M_0^{-1} \\ &= \lim_{\varepsilon\to 0} \det\left(M + \varepsilon + \mu\,|0\rangle\,\langle 0|\right)\left(M_0+\varepsilon\right)^{-1},\end{aligned}$$

where $|0\rangle$ is s shorthand notation for the vector g_0 and $\mu = \hbar/\xi$. Then, after some simple algebra,

$$\begin{aligned}\det\left(M + \varepsilon + \mu\,|0\rangle\,\langle 0|\right)\left(M_0+\varepsilon\right)^{-1} &= \det\left(M+\varepsilon\right)\left(M_0+\varepsilon\right)^{-1} \\ &\quad \times \det\left[1 + \mu\,|0\rangle\,\langle 0|\left(M+\varepsilon\right)^{-1}\right] \\ &= \left(1 + \mu/\varepsilon\right)\det\left(M+\varepsilon\right)\left(M_0+\varepsilon\right)^{-1}.\end{aligned}$$

In the limit $\varepsilon \to 0$, one thus finds

$$\det{}' M M_0^{-1}\,\hbar/\xi\,.$$

Collecting all factors, one concludes that the Gaussian integration over the configurations in the neighbourhood of the saddle point yields a factor

$$\frac{\tau}{\sqrt{2\pi\hbar}}\|\dot{q}_c\|(\det{}' M M_0^{-1})^{-1/2}\,\mathrm{e}^{-\tau/2}\,.$$

As expected, the dependence on ξ has cancelled.

Taking into account the two families of saddle points and the ratio 2 between $\mathcal{Z}_0(\tau/\hbar)$ and $\operatorname{tr} e^{-\tau H/\hbar}$ for $\tau \to \infty$, one obtains

$$\operatorname{tr} P\, e^{-\tau H/\hbar} / \operatorname{tr} e^{-\tau H/\hbar} \sim \frac{\tau}{\sqrt{2\pi\hbar}} \|\dot{q}_c\| \left[\det{}' M \left(\det M_0\right)^{-1}\right]^{-1/2} e^{-A/\hbar} \quad (1.35)$$

and, thus, using the result (1.13), the splitting of levels

$$E_- - E_+ \sim 2\sqrt{\frac{\hbar}{2\pi}} \|\dot{q}_c\| \left[\det{}' M \left(\det M_0\right)^{-1}\right]^{-1/2} e^{-A/\hbar} \quad (1.36)$$

The difference decreases exponentially for $\hbar \to 0$ and, thus, faster than any power of $\hbar$, a result consistent with the perturbative discussion of section 1.2.2.

Remark. We have calculated the instanton contribution only in the $\tau = \infty$ limit, in which the action has boundary conditions invariant under time-translations. The calculation for τ large but finite, involves a few additional subtleties.

1.4 An example: The quartic double-well potential

The simplest explicit example is provided by the quartic double-well potential corresponding to the Hamiltonian

$$H = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\left(\hat{q}^2 - \tfrac{1}{4}\right)^2 . \quad (1.37)$$

The instanton and multi-instanton contributions have been studied very thoroughly [5–8].

1.4.1 Instantons

The saddle point equation, which is the equation of the classical motion in Euclidean or imaginary time, is

$$-\ddot{q}(t) + 2q(t)\left(q^2(t) - \tfrac{1}{4}\right) = 0 . \quad (1.38)$$

In the limit $\tau \to \infty$, the equation has two families of solutions with finite action:

$$q_c^{\pm}(t) = \pm\tfrac{1}{2}\tanh\left((t - t_0)/2\right), \quad (1.39)$$

where t_0 is an integration constant, reflection of time-translation invariance for τ infinite.

The corresponding value of the action is

$$\mathcal{S}(q_c) = \tfrac{1}{6} \cdot \quad (1.40)$$

Moreover, (equation (1.19))

$$\|\dot{q}_c\| = \sqrt{A} = \frac{1}{\sqrt{6}} .$$

Finally,

$$M = -\mathrm{d}_t^2 + 1 - \frac{3}{2\cosh^2(t/2)}\,.$$

The operator M has the form of a Hamiltonian of Bargmann–Wigner's type: the corresponding Schrödinger equation can be solved explicitly. Quantum scattering is reflectionless and the poles of the S-matrix yield the spectrum of the Hamiltonian. The determinant can also be calculated explicitly. Then,

$$\det\left(M+\varepsilon\right)\left(M_0+\varepsilon\right)^{-1} \underset{\varepsilon\to 0}{\sim} \frac{\varepsilon}{12}\,.$$

Using the general result (1.36) one obtains the asymptotic behaviour of $E_+ - E_-$ for $\hbar \to 0$:

$$E_- - E_+ \underset{\hbar\to 0}{=} 2\sqrt{\frac{\hbar}{\pi}}\,\mathrm{e}^{-1/6\hbar}\left(1 + O\left(\hbar\right)\right). \tag{1.41}$$

Remark. It is possible to study the semi-classical effects to all orders in an expansion in powers of $\mathrm{e}^{-1/6\hbar}$ by a multi-instanton analysis [5--6]. This has led to a conjecture, later proved to a large extent [7], which generalizes the usual Bohr–Sommerfeld's formula to the situation of potentials with degenerate minima. The energy eigenvalues E of the Hamiltonian are solutions of a secular equation that can be written, in the case of the quartic double-well potential, as [8]

$$\Gamma^2\left(\tfrac{1}{2} - B(E,\hbar)\right)\left(-\frac{2}{\hbar}\right)^{2B(E,\hbar)} \mathrm{e}^{-A(E,\hbar)} + 2\pi = 0 \tag{1.42}$$

with

$$B(E,\hbar) = -B(E,-\hbar) = \frac{E}{\hbar} + \sum_{k=1}^{\infty} \hbar^k b_{k+1}(E/\hbar), \tag{1.43}$$

$$A(E,\hbar) = -A(E,-\hbar) = \frac{1}{3\hbar} + \sum_{k=1}^{\infty} \hbar^k a_{k+1}(E/\hbar). \tag{1.44}$$

The coefficients $a_k(s)$ and $b_k(s)$ are even or odd polynomials in s according to the degree k.

For $\hbar \to$, the perturbative expansion applies to energy eigenvalues $E = O(\hbar)$, while the semi-classical WKB expansion assumes $E = O(1)$. This amounts to summing the terms of largest degree in E to all orders in $\hbar$.

1.5 The periodic cosine potential

We now consider the slightly more complicated problem of a periodic potential. We examine the spectrum of the Hamiltonian

$$H = \tfrac{1}{2}\hat{p}^2 + g^{-1}\left(1 - \cos\hat{q}\sqrt{g}\right), \tag{1.45}$$

where the constant $g > 0$ plays the role of $\hbar$ and we thus we set $\hbar = 1$.

Since the cosine potential is periodic, it has an infinite number of degenerate classical minima. We can expand the potential in powers of g around each of the minima starting from a harmonic approximation. Correspondingly, the energy eigenvalues have an expansion in powers of g, which is independent of the chosen minimum. To all orders in g, the Hamiltonian thus has an infinite number of degenerate ground states. However, we know that the spectrum of the Hamiltonian H is continuous and has, at least for g small enough, a band structure: this property again is due to barrier penetration.

1.5.1 Eigenvalues and eigenstates

We now introduce the unitary operator T that generates an elementary translation of one period $2\pi/\sqrt{g}$. Since it commutes with the Hamiltonian,

$$[T, H] = 0\,, \tag{1.46}$$

both operators can be diagonalized simultaneously. Each eigenfunction $\psi_{N,\theta}$ of H is thus characterized by an angle θ (pseudo-momentum) eigenvalue of T:

$$T\psi_{N,\theta} = \mathrm{e}^{i\theta}\,\psi_{N,\theta}\ , \quad H\psi_{N,\theta} = E_N(g,\theta)\psi_{N,\theta}\ , \tag{1.47}$$

where the eigenvalue $E_N(g,\theta)$ is a periodic function of θ and $E_N(g,\theta) = N + 1/2 + O(g)$.

The partition function in the θ-sector. We can consider the Hamiltonian in the subspace of wave functions satisfying

$$T\psi(q) = \mathrm{e}^{i\theta}\,\psi(q),$$

as a Hamiltonian H_θ on the interval $(0, 2\pi/\sqrt{g})$. It is still Hermitian but no longer real. The corresponding partition function in the sector of angle θ is then given by the sum

$$\mathcal{Z}(\beta, g, \theta) = \operatorname{tr}\mathrm{e}^{-\beta H_\theta} = \sum_N \mathrm{e}^{-\beta E_N(g,\theta)}, \tag{1.48}$$

In particular, for β large,

$$\mathcal{Z}(\beta, g, \theta) \underset{\beta\to\infty}{\sim} \mathrm{e}^{-\beta E_0(g,\theta)}\,. \tag{1.49}$$

Twisted partition functions. We also define the twisted partition function $\mathcal{Z}_l(\beta, g) = \operatorname{tr}' T^l\,\mathrm{e}^{-\beta H}$. The notation tr' has the following meaning: since the diagonal matrix elements of $\mathrm{e}^{-\beta H}$ in configuration space are periodic functions of q, we integrate only over one period. Thus,

$$\begin{aligned}\mathcal{Z}_l(\beta, g) &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \sum_N \mathrm{e}^{-\beta E_N(g,\theta)} \int \mathrm{d}q\, \psi^*_{N,\theta}(q)\psi_{N,\theta}(q + 2\pi l/\sqrt{g}) \\ &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \sum_N \mathrm{e}^{-\beta E_N(g,\theta)}\,\mathrm{e}^{il\theta} = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta\, \mathcal{Z}(\beta, g, \theta)\,\mathrm{e}^{il\theta}\,. \end{aligned} \tag{1.50}$$

Inverting this last relation, we find

$$\mathcal{Z}(\beta, g, \theta) = \sum_{l=-\infty}^{+\infty} \mathrm{e}^{-il\theta}\, \mathcal{Z}_l(\beta, g) = \sum_{l=-\infty}^{+\infty} \mathrm{e}^{-il\theta}\, \mathrm{tr}'\, T^l\, \mathrm{e}^{-\beta H} \,. \tag{1.51}$$

This is the representation we now use to calculate $\mathcal{Z}(\beta, g, \theta)$.

Path integral representation. The path integral representation of $\mathcal{Z}_l(\beta, g)$ is

$$\mathcal{Z}_l(\beta, g) = \int_{q(\beta/2)=q(-\beta/2)+2\pi l/\sqrt{g}} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}(q)\right] \tag{1.52}$$

with

$$\mathcal{S}(q) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[\tfrac{1}{2}\dot{q}^2(t) + g^{-1}\left(1 - \cos q\sqrt{g}\right)\right]. \tag{1.53}$$

Note that a factor $\mathrm{e}^{-il\theta}$ can be incorporated in the path integral. Indeed since

$$-il = -\frac{\sqrt{g}}{2\pi}\big(q(\beta/2) - q(-\beta/2)\big) = -\frac{i\sqrt{g}}{2\pi}\int_{-\beta/2}^{+\beta/2} \mathrm{d}t\, \dot{q}(t)\,,$$

this corresponds to adding to $\mathcal{S}(q)$ the integral of a local density

$$\mathcal{S}(q) \mapsto \mathcal{S}_\theta(q) = \mathcal{S}(q) + \frac{i\theta\sqrt{g}}{2\pi}\int_{-\beta/2}^{+\beta/2} \mathrm{d}t\, \dot{q}(t)\,. \tag{1.54}$$

The sum (1.51) over l then is obtained by summing over all trajectories contributing in expression (1.52). When q is considered as an angular variable, the integer l is the winding number corresponding to the number of coverings of the circle and the integral of $\dot{q}$ is a topological term that characterizes the mappings of the circle S_1 on S_1:

$$\mathcal{Z}(\beta, g, \theta) = \int [\mathrm{d}q(t)]\, \mathrm{e}^{-\mathcal{S}_\theta(q)}\,.$$

This expression has natural generalizations in the case of the θ-vacuum of the $CP(N-1)$ model and non-Abelian gauge theories (see sections 6.2,6.3).

The large β limit. We now concentrate on the large β limit and, thus, the lowest band $N = 0$. In a band, the energy eigenvalue is a periodic function of θ that can be expanded in a Fourier series:

$$E_0(g, \theta) = \sum_{-\infty}^{+\infty} \mathcal{E}_l(g)\, \mathrm{e}^{il\theta}, \quad \mathcal{E}_l = \mathcal{E}_{-l}\,. \tag{1.55}$$

All coefficients $\mathcal{E}_l$ except $\mathcal{E}_0$ vanish to all orders in a perturbative expansion in g. Like in the case of the double-well potential, we thus observe that it is difficult to determine the dependence on θ of the energy levels from the partition function.

Instead we consider

$$\mathcal{Z}_1(\beta,g)=\operatorname{tr}' T\,\mathrm{e}^{-\beta H} \underset{\beta\to\infty}{\sim} \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\theta\ \mathrm{e}^{i\theta}\,\mathrm{e}^{-\beta E_0(\theta,g)}\,. \tag{1.56}$$

For $g\to 0$, $E_0(\theta,g)-\mathcal{E}_0(g)$ vanishes faster than any power of g. Therefore, for $g\to 0$ and $\beta\to\infty$, we can expand equation (1.56):

$$\mathcal{Z}_1(\beta,g)\sim \mathrm{e}^{-\beta\mathcal{E}_0(\theta,g)}\int\frac{\mathrm{d}\theta}{2\pi}\,\mathrm{e}^{i\theta}\left[1-\beta\big(E_0(\theta,g)-\mathcal{E}_0\big)+\cdots\right]\ . \tag{1.57}$$

The integration over θ selects $\mathcal{E}_{-1}=\mathcal{E}_1$:

$$\operatorname{tr}' T\,\mathrm{e}^{-\beta H}\sim -\beta\,\mathrm{e}^{-\beta E_0(\theta,g)}\,\mathcal{E}_1(g),\quad g\to 0\,,\quad \beta\to\infty\,. \tag{1.58}$$

This equation can be more conveniently rewritten as

$$\operatorname{tr}' T\,\mathrm{e}^{-\beta H}\,/\operatorname{tr}'\mathrm{e}^{-\beta H}\sim -\beta\mathcal{E}_1(g). \tag{1.59}$$

If $\mathcal{E}_1$ does not vanish, this implies that translation symmetry is not spontaneously broken.

Remark. To evaluate the other Fourier series coefficients $\mathcal{E}_2$, $\mathcal{E}_3,\ldots$, for g small, a simple method is to consider $\operatorname{tr}' T^l\,\mathrm{e}^{-\beta H}$ for $l=2,3,\ldots$. This evaluation requires a multi-instanton analysis [5--6].

1.5.2 The instanton contributions

The path integral representations of the partition function $\operatorname{tr}' T\,\mathrm{e}^{-\beta H}$ is given by equation (1.52). We recall that $q(-\beta/2)$ varies over only one period of the potential. For β large and g small, due to the boundary conditions, the path integral is dominated by instanton configurations which connect two consecutive minima of the potential. Solving the equation of motion explicitly, one finds

$$q_c(t)=\frac{4}{\sqrt{g}}\tan^{-1}\mathrm{e}^{(t-t_0)}, \tag{1.60}$$

and the corresponding classical action, in the infinite β limit, is

$$\mathcal{S}(q_c)=8/g\,. \tag{1.61}$$

Generalizing the calculations of the double-well potential, one obtains

$$\mathcal{E}_1(g)\underset{g\to 0}{\sim}-\frac{4}{\sqrt{\pi g}}\,\mathrm{e}^{-8/g}\,. \tag{1.62}$$

Without evaluating $\mathcal{E}_l$ for $l\geq 2$ explicitly, one verifies that the corresponding boundary conditions for $\operatorname{tr}' T^l\,\mathrm{e}^{-\beta H}$ select an multi-instanton configuration which for β large has an action $8l/g$. Therefore, $\mathcal{E}_1$ gives the dominant non-perturbative contribution for g small, and

$$E_0(\theta, g) = \mathcal{E}_0(g) - \frac{8}{\sqrt{\pi g}}\, \mathrm{e}^{-8/g}\,[1 + O(g)]\cos\theta + O\left(\mathrm{e}^{-16/g}\right). \tag{1.63}$$

Discussion. We have illustrated with two examples that, as anticipated, in a theory in which, at the classical level, a discrete symmetry is spontaneously broken because the classical potential has degenerate minima, the existence of instantons implies that quantum fluctuations restore the symmetry.

Note that in the case of continuous symmetries, in contrast to discrete symmetries where quantum fluctuations lead to exponentially small effects in $1/\hbar$ or the equivalent coupling constant, the effects of quantum fluctuations show up already at first order in perturbation theory as a consequence of the Goldstone phenomenon.

While in theories in which the dynamical variables live in flat Euclidean space, instantons are always associated with a degeneracy of the classical minimum of the potential, this is no longer necessarily the case when the space has curvature or is topologically non-trivial.

An example is provided by the cosine potential with compactified space, the position q representing a point on a circle of radius $2\pi/\sqrt{g}$, corresponding to the case $\theta = 0$. The Hamiltonian then corresponds to an $O(2)$ rotator in a potential or a one-dimensional classical spin chain in a magnetic field. The classical minimum is no longer degenerate because all minima are identified to one point on the circle. The quantum ground state is equally unique since the Hilbert space consists in strictly periodic eigenfunctions. Still instanton solutions exist but they start from and return to the same classical minimum, winding around the circle. They are stable because the circle is topologically non-trivial. They generate the exponentially small corrections to the perturbative expansion that we have determined above.

General spectral equation. For the cosine potential, to all orders in the expansion parameter and the number of instantons, it has been conjectured that all energy eigenvalues are solution of the spectral equation of the form (here written for the potential $\frac{1}{16}(1 - \cos 4q)$) [8]

$$\left(\frac{2}{g}\right)^{-B(E,g)} \frac{\mathrm{e}^{A(E,g)/2}}{\Gamma[\frac{1}{2} - B(E,g)]} + \left(\frac{-2}{g}\right)^{B(E,g)} \frac{\mathrm{e}^{-A(E,g)/2}}{\Gamma[\frac{1}{2} + B(E,g)]} = \frac{2\cos\theta}{\sqrt{2\pi}}.$$

The first few terms of the perturbative expansions of the functions A and B for the periodic potential are

$$\begin{aligned} B(E,g) &= E + g\left(E^2 + \tfrac{1}{4}\right) + g^2\left(3\,E^3 + \tfrac{5}{4}\,E\right) + \mathcal{O}\left(g^3\right), \\ A(E,g) &= g^{-1} + g\left(3\,E^2 + \tfrac{3}{4}\right) + g^2\left(11\,E^3 + \tfrac{23}{4}\,E\right) + \mathcal{O}\left(g^3\right). \end{aligned}$$

1.6 Several degrees of freedom.

In general, for paths in $\mathbb{R}^N$, the equations of motion cannot be solved explicitly and the discussion is more involved. However, there is one situation where the existence of instantons can be proved, when the action takes the special form

$$\mathcal{S}(q) = \tfrac{1}{2} \int \mathrm{d}t \left\{ \dot{\mathbf{q}}^2(t) + \left[\nabla_q \mathcal{U}\bigl(\mathbf{q}(t)\bigr)\right]^2 \right\}. \tag{1.64}$$

This situation is not as artificial as it may appear since it occurs in the case of path integrals associated with the Fokker-Planck equation or supersymmetric quantum mechanics in the leading order approximation. We now assume that $\mathcal{U}(q)$ is a polynomial with at least two isolated minima where $\nabla_q \mathcal{U}(q)$ thus vanishes. Any instanton solution must start and end up at a minimum of the potential. Using a remark that will again be useful later, we start from the inequality

$$\int \mathrm{d}t \left[\dot{\mathbf{q}}(t) \pm \nabla_q \mathcal{U}\bigl(\mathbf{q}(t)\bigr)\right]^2 \geq 0\,.$$

Expanding we obtain

$$\mathcal{S}(q) \geq |\mathcal{U}(q_1) - \mathcal{U}(q_2)|,$$

where q_1 and q_2 thus are two minima of the potential. Equality corresponds to a local minimum of the action. Then, the classical solution must satisfy

$$\dot{\mathbf{q}}(t) \pm \nabla_q \mathcal{U}\bigl(\mathbf{q}(t)\bigr) = 0\,. \tag{1.65}$$

These equations, which involve only the first order derivative in time, characterize a gradient flow. Depending on the sign in equation (1.65), $\mathcal{U}(q)$ increases or decreases along the classical path.

As an exercise, it is suggested to study the example in $\mathbb{R}^2$,

$$\mathcal{U}(q_1, q_2) = -\tfrac{1}{2}\left(q_1^2 + q_2^2\right) - \alpha q_1 q_2 + \tfrac{1}{3}\left(q_1^3 + q_2^3\right) + \alpha q_1 q_2 \left(q_1 + q_2\right),$$

as a function of α.

One dimension. In one dimension, the form (1.64) is not a restriction since it contains all Hamiltonians of the form (1.5). For example, for the quartic double-well potential (1.37),

$$\mathcal{U}(q) = \tfrac{1}{3}q^3 - \tfrac{1}{4}q$$

and, thus, $|\mathcal{U}(1/2) - \mathcal{U}(-1/2)| = 1/6$.

For the cosine potential,

$$\mathcal{U}(q) = \frac{4}{g}\cos(q\sqrt{g}/2)$$

and, thus, $|\mathcal{U}(2\pi/\sqrt{g}) - \mathcal{U}(0)| = 8/g$.

Chapter 2

Instantons and Quantum Metastability

We now study another situation in which quantum tunnelling plays a role: the decay of metastable states. We assume a quantum particle initially located in the well of a potential that corresponds to a local but not absolute minimum. Due to quantum tunnelling, a quantum particle has a finite probability per unit time to leave the well and this is the probability we now want to determine in the limit $\hbar \to 0$.

As a restriction, we discuss only initial states localized deep in the well, that is close to the pseudo-ground state in the well (the equivalent of a classical particle almost at rest). We will show that, as for the perturbative calculation, one can derive the decay rate from the partition function $\mathcal{Z}(\tau/\hbar) = \operatorname{tr} e^{-\tau H/\hbar}$ for $\tau \to \infty$.

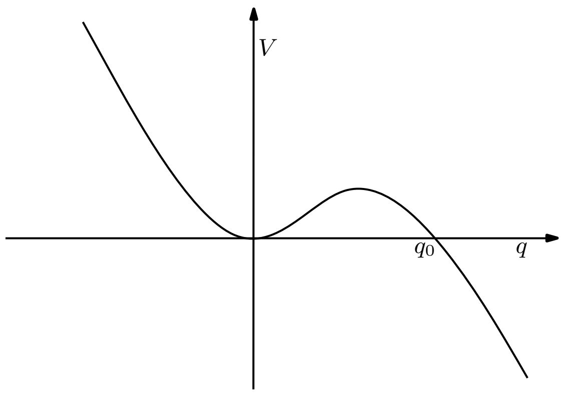

FIG. 2.1 – *Potential well leading to metastability.*

Quantum metastability. In the example of a potential of the type exhibited in Fig. 2.1, the origin is not the absolute minimum of the potential. A state corresponding to a wave function $\psi(t)$, localized at initial time $t = 0$ (t is here the *real physical time* of the Schrödinger equation) in the well of the potential around $q = 0$, decays through barrier penetration. In order to understand how to calculate the decay rate, we imagine varying a parameter in the potential in order to pass continuously from a situation where the origin is an absolute minimum to a situation where it becomes only a relative minimum. In the stable situation, the solution of the time-dependent Schrödinger equation, corresponding to the ground state energy E_0, behaves as

$$\psi_0(t) \sim \mathrm{e}^{-iE_0 t/\hbar}\,.$$

After analytic continuation, E_0 becomes complex and, thus, $\psi_0(t)$ decreases exponentially with time:

$$|\psi_0(t)| \underset{t\to+\infty}{\sim} \mathrm{e}^{-|\operatorname{Im} E_0|t/\hbar}\,.$$

The parameter $|\hbar/\operatorname{Im} E_0|$ is the lifetime of a now metastable state with wave function $\psi(t)$. Let us point out that the decay of a state receives contributions from the continuation of all excited states. However, one expects, for intuitive reasons, that when the real part of the energy increases the corresponding contribution decreases faster with time, a property that can, indeed, be verified in examples. Thus, for large times, only the component corresponding to the pseudo-ground state survives. We now show how to calculate $\operatorname{Im} E_0$ for $\hbar \to 0$.

2.1 Path integral: Steepest descent calculation and instantons

We begin with a situation, where in the Hamiltonian

$$H = \frac{1}{2m}\hat{p}^2 + V(\hat{q}),$$

the potential (assumed to be analytic) has an absolute minimum at the origin where

$$V(q) = \tfrac{1}{2}m\omega^2 q^2 + O(q^3).$$

By an analytic continuation in a parameter in V, we pass to a situation where the minimum of the potential at $q = 0$ is only relative and, thus, there exist values of q for which $V < 0$ (figure 2.1.

The imaginary part of $\mathcal{Z}(\tau/\hbar) = \operatorname{tr} \mathrm{e}^{-\tau H/\hbar}$ for $\tau \to \infty$ is expected to have to form

$$\operatorname{Im} \mathcal{Z}(\tau/\hbar) \sim \operatorname{Im} \mathrm{e}^{-\tau E_0/\hbar} \sim -\frac{\tau}{\hbar} \operatorname{Im} E_0 \, \mathrm{e}^{-\tau \operatorname{Re} E_0/\hbar}\,.$$

For $\hbar \to 0$, $\operatorname{Re} E_0$ can be replaced by the value its assumes in the harmonic approximation and, thus,

$$\operatorname{Im} \mathcal{Z}(\tau/\hbar) \sim -\frac{\omega\tau}{\hbar} \, \mathrm{e}^{-\omega\tau/2} \operatorname{Im} E_0. \tag{2.1}$$

Instantons. Since we have learned in chapter 1 that, in path integrals, tunnelling is related to instantons, we look for non-trivial saddle points of the path integral. The saddle point equation, obtained by varying the Euclidean action, is

$$-m\ddot{q}(t) + V'\big(q(t)\big) = 0 \tag{2.2}$$

with $q(-\tau/2) = q(\tau/2)$.

The functions

$$q(t) = q_{\text{ext.}} = \text{const.}\,, \tag{2.3}$$

where $q_{\text{ext.}}$ corresponds to an extremum of the potential, are clearly solutions. We do not take into account the saddle points with $V < 0$ because one can verify that the analytic continuation leads to integration domains that avoid such saddle points. On the other hand, the contributions of saddle points corresponding to extrema where $V > 0$ are of order $\mathrm{e}^{-\tau V_{\text{ext.}}/\hbar}$ and, thus, negligible for $\tau \to \infty$ and $\hbar \ll 1$ since we consider only energy eigenvalues of order $\hbar$.

Therefore, we look for solutions that have an action that has a finite limit when $\tau \to +\infty$, that is, *instanton-type* solutions.

The solutions of equation (2.2) with periodic boundary conditions correspond to periodic motions in *real time* in the potential $-V(q)$. It is clear that trajectories can be found that oscillate around the minima of $-V$. For $\tau \to \infty$, one end-point of the classical trajectory must converge toward a point where the velocity and thus $V'(q)$ vanish. Moreover, the action remains finite in this limit only if $V(q(t))$ and $\dot{q}$ vanish for $|t| \to \infty$. These conditions are compatible only the corresponding classical trajectory comes increasingly closer to the origin. Thus, the classical trajectory starts from the origin at time $-\infty$, is reflected at the zero q_0 of the potential and returns to the origin for $t \to +\infty$. This situation has to be contrasted with the situation of degenerate minima, where the instanton interpolates between different minima of the potential.

A first integration of the equation of motion (2.2) yields

$$\tfrac{1}{2}m\dot{q}^2(t) - V\big(q(t)\big) = 0\,. \tag{2.4}$$

In the limit $\tau \to \infty$, the classical solution $q_c(t)$ is thus given by (t_0 is an integration constant)

$$|t - t_0| = \sqrt{m}\int_{q_c}^{q_0} \frac{\mathrm{d}q'}{\sqrt{2V(q')}}\,.$$

The instanton action. If $q_c(t)$ is a finite action solution on the interval $t \in (-\infty, +\infty)$, then from equation (2.4) we infer

$$\tfrac{1}{2}m\int \mathrm{d}t\,\dot{q}_c^2(t) = \int \mathrm{d}t\,V\big(q_c(t)\big)$$

and, thus, the corresponding classical action

$$\mathcal{S}(q_c) \equiv A = m\int_{-\infty}^{+\infty} \mathrm{d}t\,\dot{q}_c^2(t) = 2\int_0^{q_0} \sqrt{2V(q)}\mathrm{d}q \tag{2.5}$$

is positive. The instanton thus gives a contribution of the order of $\mathrm{e}^{-A/\hbar}$, which decreases exponentially for $\hbar/A \to 0$.

Remarks.

(i) One may wonder whether it makes sense to take into account such small contributions, since E_0 is first dominated by an expansion to all orders in $\hbar$. Actually, if one starts from a stable situation and proceeds by analytic continuation, one can obtain two complex conjugate results. Each result is indeed dominated by the same trivial saddle point $q(t) \equiv 0$, from which originates the perturbation series whose terms are all real. In contrast, if one calculates the difference between the two continuations, the contribution of the leading saddle point cancels and the difference is dominated by the instanton. As a consistency check, one must thus verify that the instanton contribution is purely imaginary.

(ii) Since the Euclidean action is invariant under time-translations, the classical solution depends on an arbitrary parameter t_0, which for finite τ, varies in the interval $[-\tau/2, \tau/2]$. As in the example of section 1.2.1, one finds a one-parameter family of degenerate saddle points. In the calculation of the contribution of a saddle point the dependence on t_0 disappears, and thus all saddle points give the same contribution.

(iii) One could have also considered trajectories that oscillate n times around the maximum of the potential in a time interval τ. It is easy to verify that the corresponding action in the limit $\tau \to \infty$ becomes

$$\mathcal{S}(q_c) = nA\,, \tag{2.6}$$

and yields a contribution of order $\mathrm{e}^{-nA/\hbar}$. For $\hbar \to 0$, the $n = 1$ contribution thus dominates the imaginary part of the path integral.

Leading order contribution: Gaussian approximation. The arguments of section 1.2.1 apply also here. The naive steepest descent method with Gaussian integration involves the determinant of the operator

$$M(t_1, t_2) = \frac{\delta^2 \mathcal{S}}{\delta q_c(t_1)\delta q_c(t_2)} = \left[-m\mathrm{d}_{t_1}^2 + V''\big(q_c(t_1)\big)\right]\delta(t_1 - t_2). \tag{2.7}$$

A differentiation with respect to time of the equation of motion (2.2) yields

$$\left[-m\mathrm{d}_t^2 + V''\big(q_c(t)\big)\right]\dot q_c(t) \equiv M\dot q_c = 0\,. \tag{2.8}$$

Thus, $\dot q_c$ (which is square integrable, see equation (2.5)) is an eigenvector of the Hermitian operator M and the corresponding eigenvalue vanishes.

However, let us point out one notable difference between this situation and the situation of degenerate minima. As we have already pointed out, from the general theory of orthogonal functions one infers that the number of zeros of an eigenfunction of the Hamiltonian M is directly related to the hierarchy of eigenvalues: the ground state of M has no zero, the first excited state has one zero... Thus, the eigenfunction $\dot q_c(t)$, which vanishes exactly once, for $t = t_0$, corresponds to the first excited state, and this implies that the operator M has one negative eigenvalue. The product $\det' M$ of the non-vanishing eigenvalues of M is negative and $\sqrt{\det' M}$ is imaginary, as expected.

2.2 Collective coordinates: Alternative method

Again, due to the existence of the time zero mode, it is necessary to introduce a time collective coordinate, and one can use the Gaussian approximation only for the modes orthogonal to $\dot{q}_c$. The method of section 1.3.2 can be adapted to this new situation, but it is instructive to briefly outline an alternative solution to the same problem.

We now denote by $q_c(t)$ the particular solution of the saddle point equation (2.2) corresponding to $t_0 = 0$ and, thus, the general solution is $q_c(t - t_0)$.

To introduce an integration variable associated with time-translations, we set

$$q(t) = q_c(t - t_0) + r(t - t_0)\sqrt{\hbar}, \tag{2.9}$$

where t_0 is no longer a simple parameter, but forms, together with the path $r(t)$ a new set of integration variables. However, an infinitesimal variation of t_0 adds to $q(t)$ a contribution proportional to $\dot{q}_c$. In order for the new set $\{t_0, r(t)\}$ to include only independent variables, any variation of $r(t)$ must be orthogonal to a variation of t_0:

$$\int \dot{q}_c(t - t_0) r(t - t_0) \mathrm{d}t = 0\,. \tag{2.10}$$

After a short calculation, one then recovers the Jacobian obtained by the Faddeev–Popov method (for a general discussion see chapter 4). At leading order, the Jacobian of the transformation that relates $q(t)$ to the set $\{t_0, r(t)\}$ reduces to

$$J = \|\dot{q}_c\| / \sqrt{\hbar} = \frac{1}{\sqrt{\hbar}} \left[\int \dot{q}_c^2(t) \mathrm{d}t\right]^{1/2} = \sqrt{A/m\hbar}\,. \tag{2.11}$$

Since the integrand does not depend on t_0, the integration over the collective coordinate t_0 yields simply a factor τ (but in the case of correlation functions, the integration restores time-translation symmetry). The integration over $r(t)$ yields a factor $(\det' M)^{-1/2}$, where $\det' M$ is the product of all non-vanishing eigenvalues of M, which is also the determinant of M when restricted to the subspace orthogonal to $\dot{q}_c$.

Normalization. To normalize the path integral, we compare it to its limit at $\hbar = 0$ (a harmonic oscillator), which in the limit $\tau \to \infty$ reduces to $\mathrm{e}^{-\omega\tau/2}$. For $\hbar \to 0$, the operator M tends toward the operator

$$M_0(t_1, t_2) = \left[-m\mathrm{d}_{t_1}^2 + m\omega^2\right] \delta(t_1 - t_2). \tag{2.12}$$

In the comparison between the contribution of the instanton and the reference path integral corresponding to the harmonic oscillator, one must recall that the two path integrals differ by one Gaussian integration since in the instanton contribution one Gaussian mode has been excluded. It is thus necessary to divide the instanton contribution by the factor

$$\int_{-\infty}^{+\infty} \mathrm{e}^{-\lambda^2/2}\, \mathrm{d}\lambda = (2\pi)^{1/2}.$$

Dividing by a factor $2i$, one then obtains the imaginary part of $\mathcal{Z}(\tau/\hbar)$ in the form (2.1). Collecting all factors, one obtains [3]

$$\operatorname{Im}\mathcal{Z}(\tau/\hbar) \sim \frac{1}{2i}\left[\det{}'(MM_0^{-1})\right]^{-1/2}\sqrt{\frac{A}{m\hbar}}\frac{\tau}{\sqrt{2\pi}}\,\mathrm{e}^{-\omega\tau/2}\,\mathrm{e}^{-A/\hbar},$$

and, finally,

$$\operatorname{Im}E_0 \sim \frac{1}{2i}\left[\det{}'(MM_0^{-1})\right]^{-1/2}\sqrt{\frac{A\hbar}{2\pi m}}\,\mathrm{e}^{-A/\hbar}. \tag{2.13}$$

The result is finite and real since, as we have pointed out, M has one negative eigenvalue.

2.3 The quartic anharmonic oscillator for negative coupling

We now apply the preceding results to the example of the quartic anharmonic potential in which the sign of the quartic term is changed from positive to negative values. The corresponding Hamiltonian is

$$H = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\hat{q}^2 + \tfrac{1}{4}g\hat{q}^4. \tag{2.14}$$

We can infer the eigenvalues of H from a calculation of the partition function

$$\mathcal{Z}(\beta) = \operatorname{tr}\mathrm{e}^{-\beta H} = \int_{q(-\beta/2)=q(\beta/2)} [\mathrm{d}q(t)]\exp\left[-\mathcal{S}(q)\right], \tag{2.15}$$

where $\mathcal{S}(q)$ is the Euclidean action,

$$\mathcal{S}(q) = \int_{-\beta/2}^{\beta/2}\left[\tfrac{1}{2}\dot{q}^2(t) + \tfrac{1}{2}q^2(t) + \tfrac{1}{4}gq^4(t)\right]\mathrm{d}t\,. \tag{2.16}$$

We have set $\hbar = 1$ because after the change $q(t) \mapsto q(t)g^{-1/2}$, one verifies that the parameter g plays here the role of $\hbar$.

A generalization of the arguments applicable to integrals over a finite number of variables indicates that the path integral (2.15) defines a function of g that is analytic in the half-plane $\operatorname{Re}(g) > 0$. In this domain, the integral is dominated for $g \to 0$ by the saddle point $q(t) \equiv 0$. Thus, it can be calculated by expanding the integrand in powers of g and integrating the successive terms. This generates a perturbative expansion of the partition function, from which, in the limit $\beta \to \infty$, an expansion of the ground state energy $E_0(g)$ can be inferred.

Negative coupling. For all $g < 0$, the Hamiltonian is no longer bounded from below. Therefore, the energy eigenvalues, considered as analytic functions of g, have a singularity at $g = 0$ and the perturbation series is always divergent.

To understand how to define and evaluate $E_0(g)$ for g negative, we first study a simple integral that illustrates some aspects of the problem.

2.3.1 The simple quartic integral

The expansion of the integral

$$I(g) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\left(x^2/2+gx^4/4\right)} \mathrm{d}x \,, \tag{2.17}$$

yields, order by order in g, the number of Feynman diagrams contributing to the partition function (2.15). For g positive and small, the integral is dominated by the saddle point at the origin and thus

$$I(g) = 1 + O(g) \,. \tag{2.18}$$

The function $I(g)$ is analytic in a cut plane. To continue the integral analytically to $g < 0$, it is necessary to rotate the integration contour C as one changes the phase of g, for example, like

$$C: \ \operatorname{Arg} x = -\tfrac{1}{4} \operatorname{Arg} g \pmod{\pi} \,.$$

Then, $\operatorname{Re}(gx^4)$ always remains positive. Depending on the orientation of the rotation in the g plane, one obtains two different, complex conjugate, expressions $I_\pm(g)$:

$$\begin{aligned} \text{for } g = \mp |g| + i0 : \qquad & I_\pm(g) = \frac{1}{\sqrt{2\pi}} \int_{C_\pm} \mathrm{e}^{-\left(x^2/2+gx^4/4\right)} \mathrm{d}x \\ \text{with } C_\pm : \qquad & \operatorname{Arg} x = \mp \frac{\pi}{4} \pmod{\pi} \,, \end{aligned} \tag{2.19}$$

For $g \to 0_-$, the two integrals are still dominated by the saddle point at the origin since the contributions of the other saddle points,

$$x + gx^3 = 0 \Rightarrow x^2 = -1/g \,, \tag{2.20}$$

are of order

$$\mathrm{e}^{-\left(x^2/2+gx^4/4\right)} \sim \mathrm{e}^{1/4g} \ll 1 \,. \tag{2.21}$$

However, the discontinuity of $I(g)$ across the cut is given by the difference between the two integrals:

$$I_+(g) - I_-(g) = 2i \operatorname{Im} I(g) = \frac{1}{\sqrt{2\pi}} \int_{C_+ - C_-} \mathrm{e}^{-\left(x^2/2+gx^4/4\right)} \mathrm{d}x \,. \tag{2.22}$$

It corresponds to the contour $C_+ - C_-$, which, as Fig. 2.2 shows, can be deformed into the sum of contours C_1 and C_2 that avoid the leading saddle point but contain the non-trivial saddle points S_1 and S_2: $x = \pm 1/\sqrt{-g}$. This shows that the contributions of the saddle point at the origin cancel, and that the integral is now dominated by the saddle points S_1 and S_2. Evaluating their contributions, one then finds

$$\operatorname{Im} I(g) \sim 2^{-1/2} \, \mathrm{e}^{1/4g} \,. \tag{2.23}$$

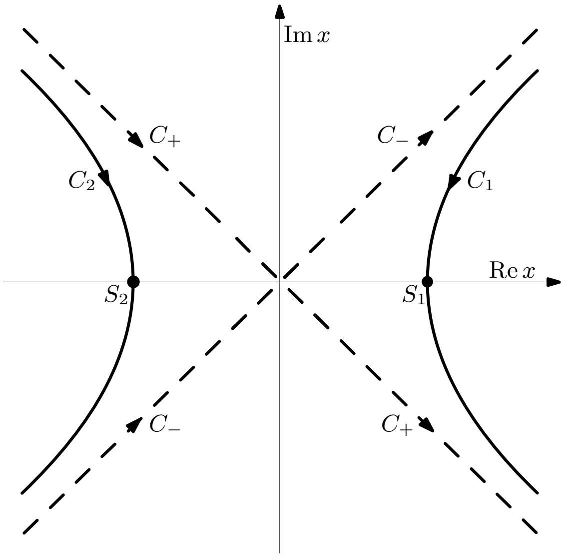

FIG. 2.2 – *The integration contours C_+, C_-, C_1 and C_2.*

As a consequence, for g negative and small, while the real part of the integral is dominated by the perturbative expansion, the leading contributions to the imaginary part come from the non-trivial saddle points and are exponentially small.

2.3.2 Path integral

We now generalize this strategy to the path integral (2.15). Inspired by the preceding example, we rotate the integration domain in functional $q(t)$ space while we change the phase of g to go from positive to negative values:

$$q(t) \mapsto q(t)\,\mathrm{e}^{-i\theta},$$

where θ is independent of time. However, there is one major difference with the case of a simple integral: the domain must satisfy $\mathrm{Re}\left[\dot{q}^2(t)\right] > 0$, because the kinetic term $\int \dot{q}^2(t)\mathrm{d}t$ determines the integration space in the path integral.

For g negative, the two conditions

$$\mathrm{Re}\left[gq^4(t)\right] > 0\,,\ \mathrm{Re}\left[\dot{q}^2(t)\right] > 0\,, \tag{2.24}$$

are satisfied if one integrates over a domain satisfying

$$\mathrm{Arg}\,q(t) = -\theta \pmod{\pi}\,,\ \pi/8 < \theta < \pi/4 \text{ or } -\pi/4 < \theta < -\pi/8\,. \tag{2.25}$$

For $g \to 0$, the two path integrals corresponding to the two analytic continuations are here also dominated by the saddle point at the origin

$$q(t) = 0\,,$$

but in the difference, this contribution cancels.

The contribution of the saddle points corresponding to the constant functions

$$q^2(t) = -1/g\,,$$

is of the order of $e^{\beta/4g}$ and is thus negligible for $\beta \to \infty$.

We then look for saddle points that are non-trivial solutions of the Euclidean equation of motion for $g < 0$:

$$-\ddot{q}(t) + q(t) + gq^3(t) = 0 \tag{2.26}$$

with

$$q(-\beta/2) = q(\beta/2). \tag{2.27}$$

We are only interested in *instanton*-type solutions, whose action remains finite when $\beta \to +\infty$.

2.3.3 Instantons

The solutions of equation (2.26) with the periodic condition (2.27) have an interpretation as describing a classical periodic motion, in real time, in the potential

$$-V(q) = -\tfrac{1}{2}q^2 - \tfrac{1}{4}gq^4. \tag{2.28}$$

It is clear that the equation of motion has solutions that correspond to oscillations around the minima of $-V$, $q = \pm\sqrt{-1/g}$. In the infinite β limit, the finite action condition implies that the equation (2.26) can be integrated once as

$$\tfrac{1}{2}\dot{q}^2 - \tfrac{1}{2}q^2 - \tfrac{1}{4}gq^4 = 0\,.$$

The classical solutions then are (t_0 is an integration constant)

$$q_c(t) = \pm\left(-\frac{2}{g}\right)^{1/2}\frac{1}{\cosh(t-t_0)}. \tag{2.29}$$

The corresponding value of the classical action is

$$\mathcal{S}(q_c) = -\frac{4}{3g} + O\left(e^{-\beta}/g\right). \tag{2.30}$$

Since the Euclidean action is time-translation invariant, the classical solution depends on one arbitrary parameter t_0, which for β finite, varies in an interval of size β. We thus find two families of degenerate saddle points that depend on one parameter.

Leading order contribution. The operator second functional derivative of the action is given by

$$M(t_1,t_2) = \frac{\delta^2\mathcal{S}}{\delta q_c(t_1)\delta q_c(t_2)} = \left[-\left(\frac{d}{dt_1}\right)^2 + 1 + 3gq_c^2(t_1)\right]\delta(t_1-t_2). \tag{2.31}$$

One verifies that the function $\dot{q}_c(t)$ is square integrable and, therefore, M has a zero mode corresponding to the eigenvector $\dot{q}_c$.

Taking into account the two families of saddle points, the zero mode and collecting all factors, one obtains

$$\operatorname{Im} \operatorname{tr} \mathrm{e}^{-\beta H} \sim \frac{2}{2i} \left[\det' M M_0^{-1}\right]^{-1/2} J \frac{\beta}{\sqrt{2\pi}} \, \mathrm{e}^{-\beta/2} \, \mathrm{e}^{4/3g}, \tag{2.32}$$

where J is the Jacobian (2.11). Moreover, it is easy to calculate the eigenvalues of M analytically because M is a Hamiltonian with a Bargmann–Wigner-type potential. One finally obtains

$$\operatorname{Im} E_0(g) = \frac{4}{\sqrt{2\pi}} \frac{\mathrm{e}^{4/3g}}{\sqrt{-g}} \left[1 + O(g)\right], \quad g \to 0_- \,. \tag{2.33}$$

Chapter 3

Metastable Vacua in Quantum Field Theory

With this chapter, we begin a semi-classical study of barrier penetration in quantum field theory [11], generalizing the methods explained in quantum mechanics. We have shown that in quantum mechanics barrier penetration is associated with classical motion in imaginary time; thus, we consider here also quantum field theory in its Euclidean formulation.

From the point of view of field integrals, in the semi-classical limit barrier penetration is also related to finite action solutions (instantons) of the Euclidean classical field equations. We first try to characterize such solutions. We then explain how to evaluate the instanton contributions at leading order, the main new problem arising from UV divergences.

In this chapter, we discuss the decay of metastable states in the case of scalar field theories [12, 13]. We have argued that the lifetime of metastable states is related to the imaginary part of the 'ground state' energy. In the case of the vacuum amplitude, we find that the instanton contribution is proportional to the space–time volume. Dividing by the volume we, therefore, obtain the probability per unit time and unit volume of a metastable pseudo-vacuum to decay.

For later purpose, we also calculate the imaginary part not only of the vacuum amplitude but also of correlation functions.

We first consider general scalar field theories. As an application, we mention the decay of the false vacuum in a cosmological context.

We then discuss a scalar field theory with a ϕ^4 interaction, generalization of the quartic anharmonic oscillator, in the dimensions in which it is super-renormalizable, that is, two and three dimensions.

3.1 General scalar field theory: Instanton contributions

We consider a d-dimensional field theory for a scalar field ϕ, with a local Euclidean action of the form

$$\mathcal{S}(\phi) = \int \mathrm{d}^d x \left[\tfrac{1}{2}\left(\partial_\mu \phi(x)\right)^2 + g^{-1} V\left(\phi(x)\sqrt{g}\right)\right], \tag{3.1}$$

at tree level, in which the potential $V(\phi)$ has a relative minimum at $\phi = 0$, where

$$V(\phi) = \tfrac{1}{2} m^2 \phi^2 + O(\phi^3), \quad m > 0\,,$$

(an example is displayed in figure 3.1) and the parameter g plays a role equivalent to $\hbar$.

Assuming that at some initial time the quantum mechanical state corresponds to fields concentrated around the unstable minimum of the potential, the 'false' vacuum, we want, for example, to evaluate in the semi-classical limit $g \to 0$ the probability for the false vacuum to decay into the true vacuum of the theory.

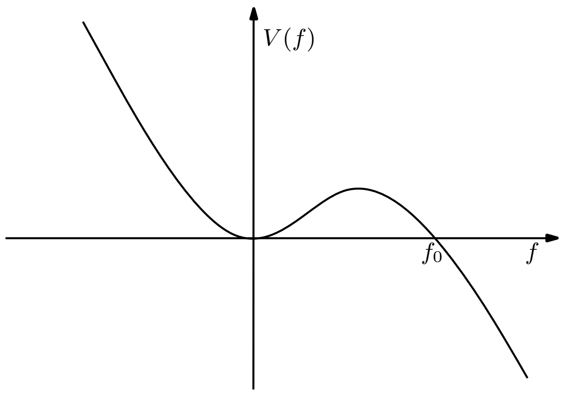

FIG. 3.1 – *Potential with a metastable minimum.*

The quantum partition function at zero temperature, or vacuum amplitude, is given by the field integral

$$\mathcal{Z} = \int [\mathrm{d}\phi(x)] \exp[-\mathcal{S}(\phi)], \tag{3.2}$$

where the field integral is normalized with respect to the free or Gaussian theory with the action

$$\mathcal{S}_0(\phi) = \tfrac{1}{2} \int \mathrm{d}^d x \left[(\partial_\mu \phi(x))^2 + m^2 \phi^2(x) \right], \tag{3.3}$$

in such a way that $\mathcal{Z}(g = 0) = 1$.

More generally, we consider also the effect of barrier penetration on correlation functions. The complete n-point correlation function can be written as

$$\langle \phi(x_1)\phi(x_2)\ldots\phi(x_n) \rangle = Z^{(n)}(x_1, \ldots, x_n)/\mathcal{Z}\,, \tag{3.4}$$

where $\mathcal{Z}$ is the partition function (or vacuum amplitude) (3.2) and

$$Z^{(n)}(x_1, \ldots, x_n) = \int [\mathrm{d}\phi(x)]\, \phi(x_1)\phi(x_2)\ldots\phi(x_n) \exp[-\mathcal{S}(\phi)]. \tag{3.5}$$

Again, we normalize field integrals with respect to the vacuum amplitude of the free field theory (3.3).

3.1.1 The instanton solution

The calculation of the barrier penetration amplitude involves the determination of instanton (finite action) solutions of the Euclidean field equation and, at leading order, a Gaussian integration around the instanton. The classical field equation reads

$$-\nabla_x^2\phi(x) + \frac{1}{\sqrt{g}}V'\big(\phi(x)\sqrt{g}\big) = 0\,. \tag{3.6}$$

A theorem establishes, under mild assumptions, that spherically symmetric solutions give the minimal action (and thus the leading contribution). Therefore, one looks for such solutions, setting

$$r = |x - x_0|\,,\quad f(r) = \sqrt{g}\phi_c(x)\,. \tag{3.7}$$

The classical equation of motion reduces to

$$\frac{\mathrm{d}^2 f}{\mathrm{d}r^2} + \frac{d-1}{r}\frac{\mathrm{d}f}{\mathrm{d}r} = V'(f). \tag{3.8}$$

Interpreting r as a time, one notes that the equation describes the motion of a particle in a potential $-V(f)$ and submitted to a viscous damping force. Since one looks for finite action solutions, one imposes the boundary condition

$$f(r) \to 0 \quad \text{for} \quad r \to \infty\,. \tag{3.9}$$

Moreover, a solution that goes to 0 goes exponentially as e^{-mr}.

The leading solution is even and is determined by its value at the origin $f(0)$. We call f_0 the non-trivial zero of the potential (figure 3.1). If we choose for $f(0)$ a value for which the potential $-V(f(0))$ is too large, $-V(f)$ will remain positive until r becomes very large. When r is large, the damping force is small so that energy is almost conserved and the particle will overshoot. By contrast, if $f(0)$ is too close to f_0, the particle will lose too much energy and, therefore, undershoot, the asymptotic value $f(r)$ then corresponding to the maximum f_+, $0 < f_+ < f_0$, of $V(f)$. Thus, somewhere in between, we expect to find a value $f(0)$, which corresponds to a solution which goes to zero at infinity and, therefore, has a finite action.

The virial theorem (see below) implies

$$\mathcal{S}(\phi_c) = \frac{1}{d}\int \left(\partial_\mu\phi_c(x)\right)^2 \mathrm{d}^d x > 0 \tag{3.10}$$

and, thus, the corresponding action is positive. We set

$$\mathcal{S}(\phi_c) = A/g \tag{3.11}$$

with

$$A = \frac{1}{d}\int \left(\partial_\mu f\right)^2 \mathrm{d}^d x = \frac{1}{d}S_d \int_0^\infty r^{d-1} f'^2(r)\mathrm{d}r\,, \tag{3.12}$$

where S_d, the area of the d-dimensional sphere, is

$$S_d = 2\pi^{d/2}/\Gamma(d/2). \tag{3.13}$$

The virial theorem. If $\phi_c(x)$ has a finite action so does $\phi_c(\lambda x)$. In the action (3.1) evaluated at $\phi_c(\lambda x)$, we then change variables $\lambda x \mapsto x$. The action then becomes

$$\mathcal{S}(\lambda, \phi_c) = \lambda^{2-d}\tfrac{1}{2}\int \mathrm{d}^d x\,\bigl(\partial_\mu \phi(x)\bigr)^2 + \lambda^{-d}\int \mathrm{d}^d x\, g^{-1} V\bigl(\phi(x)\sqrt{g}\bigr).$$

The action being stationary for $\phi_c(x)$, is stationary for $\lambda = 1$. Expressing that the derivative with respect to λ vanishes for $\lambda = 1$, we obtain

$$(d-2)\tfrac{1}{2}\int \mathrm{d}^d x\,\bigl(\partial_\mu \phi(x)\bigr)^2 + d\int \mathrm{d}^d x\, g^{-1} V\bigl(\phi(x)\sqrt{g}\bigr) = 0\,. \tag{3.14}$$

3.1.2 The problem of the Gaussian integration

In simple situations, to calculate the contribution of a saddle point one expands at the saddle point. This amounts here to setting

$$\phi(x) = \phi_c(x) + \chi(x),$$

and expanding the action in powers of χ. A leading order, one finds, for example for the partition function or vacuum amplitude,

$$\mathcal{Z} = \mathrm{e}^{-A/g}\int [\mathrm{d}\chi(x)] \exp\left[-\tfrac{1}{2}\int \mathrm{d}^d x\, \mathrm{d}^d x'\, \chi(x) M(x,x')\chi(x')\right],$$

where

$$\begin{aligned} M(x,x') &= \left.\frac{\delta^2 \mathcal{S}(\phi)}{\delta\phi(x)\delta\phi(x')}\right|_{\phi=\phi_c} \\ &= \left[-\nabla_x^2 + V''\bigl(f(r)\bigr)\right]\delta^{(d)}(x-x'). \end{aligned} \tag{3.15}$$

The Gaussian integration around the saddle point thus involves the determinant of the operator $\mathbf{M}$ with kernel $M(x,x')$.

However, differentiating the equation of motion (3.6) with respect to x_μ, one discovers that the d functions $\partial_\mu\phi_c = \partial_\mu f(r)/\sqrt{g}$ are eigenvectors of $\mathbf{M}$ with vanishing eigenvalue:

$$-\nabla_x^2 \partial_\mu \phi_c(x) + V''\bigl(f(r)\bigr)\partial_\mu\phi_c(x) = 0 \quad\Leftrightarrow\quad \mathbf{M}\,\partial_\mu\phi_c = 0\,. \tag{3.16}$$

This property is not surprising. Due to translation symmetry, one finds a family of degenerate saddle points $\phi_c(x-x_0)$ depending on d parameters $x_{0\mu}$. It is then necessary to sum over all saddle points, and thus to take the collective coordinates $x_{0\mu}$ as d of our integration variables, over which one eventually integrates exactly [14]. To change variables, $\phi(x) \mapsto (x_0, \{\chi_n\})$, we set

$$\phi(x) = \phi_c(x - x_0) + \sum_{n=1} \chi_n \psi_n(x - x_0),$$

where the functions $\psi_n(x)$ are normalized eigenfunctions of $\mathbf{M}$ orthogonal to all $\partial_\mu \phi_c(x)$.

As shown in section 4.6, the change of variables generates a Jacobian, which can be expressed in terms of determinant of $d \times d$ matrices as [10]

$$\mathcal{J}_{\text{tr.}}(\phi) = \frac{1}{J_{\text{tr.}}} \det \int \mathrm{d}^d x \, \partial_\mu \phi_c(x) \partial_\nu \phi(x), \tag{3.17}$$

with

$$J_{\text{tr.}} = \det{}^{1/2} \int \mathrm{d}^d x \, \partial_\mu \phi_c(x) \partial_\nu \phi_c(x).$$

At leading order $\phi(x) = \phi_c(x)$, and the invariance under space rotations implies

$$\int \mathrm{d}^d x \, \partial_\mu \phi_c(x) \partial_\nu \phi(x) = \frac{\delta_{\mu\nu}}{d} \int \mathrm{d}^d x \, [\nabla_x \phi_c(x)]^2 .$$

Thus, using equations (3.11, 3.12), one finds

$$\mathcal{J}_{\text{tr.}}(\phi_c) = J_{\text{tr.}} = \left[\frac{1}{d} \int \mathrm{d}^d x \big(\nabla_x \phi_c(x) \big)^2 \right]^{d/2} = \left(\frac{A}{g} \right)^{d/2} . \tag{3.18}$$

Moreover, the result must be multiplied by a factor $(2\pi)^{-1/2}$ for each collective coordinate, since to each one is associated one Gaussian integration in the normalization integral.

The integration over the variables χ_n then generates the determinant of $\mathbf{M}$ in the subspace orthogonal to the zero eigenvalue sector.

3.1.3 The determinant: A few remarks

After division by the Gaussian normalization integral (3.3), we have to evaluate the limit of the ratio of determinants

$$\Omega = \det{}' \mathbf{M} \mathbf{M}_0^{-1} \equiv \lim_{\varepsilon \to 0_+} \varepsilon^{-d} \det \mathbf{K}(\varepsilon) \tag{3.19}$$

with

$$\mathbf{K}(\varepsilon) = (\mathbf{M}_0 + \varepsilon)^{-1} (\mathbf{M} + \varepsilon)$$

and

$$\langle x | \mathbf{M}_0 | x' \rangle = \left(-\nabla_x^2 + m^2 \right) \delta^{d)}(x - x').$$

The ε contribution is, of course, only relevant in the zero-mode sector. The operator $\mathbf{K}$ can also be written as

$$\mathbf{K}(\varepsilon) = \mathbf{1} - \mathbf{\Xi}(\varepsilon)$$

with

$$\boldsymbol{\Xi}(\varepsilon) = -\left(\mathbf{M}_0 + \varepsilon\right)^{-1} \mathcal{V}(r),$$

where we have set

$$\mathcal{V}(r) = V''\big(f(r)\big) - m^2.$$

The operator $\boldsymbol{\Xi}$ is equivalent to a Hermitian operator since

$$\boldsymbol{\Xi} = \left(\mathbf{M}_0 + \varepsilon\right)^{-1/2} \mathbf{Q} \left(\mathbf{M}_0 + \varepsilon\right)^{1/2}$$

with

$$\mathbf{Q} = -\left(\mathbf{M}_0 + \varepsilon\right)^{-1/2} \mathcal{V}(r) \left(\mathbf{M}_0 + \varepsilon\right)^{-1/2}.$$

Thus, it has a real spectrum.

Traces. Denoting by ξ_n the eigenvalues of $\boldsymbol{\Xi}$, and introducing the perturbative propagator

$$\big(-\nabla_x^2 + m^2 + \varepsilon\big)\, G_2(x - x') = \delta^{(d)}(x - x') \;\Rightarrow\; G_2(x) = \frac{1}{(2\pi)^d} \int \frac{\mathrm{d}^d p \; \mathrm{e}^{ipx}}{p^2 + m^2 + \varepsilon},$$

we can calculate the successive traces of $\boldsymbol{\Xi}$.

First,

$$\operatorname{tr} \boldsymbol{\Xi} = \sum_{n=0} \xi_n = -G_2(0) \int \mathrm{d}^d x \, \mathcal{V}(r).$$

This trace is divergent for $d \geq 2$, a problem we will have to solve by introducing the corresponding renormalization (see section 3.1.5). Next,

$$\operatorname{tr} \boldsymbol{\Xi}^2 = \sum_{n=0} \xi_n^2 = \int \mathrm{d}^d x \, \mathrm{d}^d x' \, \mathcal{V}(r) G_2^2(x - x') \mathcal{V}(r'),$$

which is UV finite for $d < 4$. For $d > 4$, this confirms that the spectrum is discrete and accumulates to 0. For $d = 4$, an additional renormalization is required but the other traces are finite.

Successive traces of $\boldsymbol{\Xi}$ are related to successive one-loop diagrams.

Eigenvalues. The corresponding spectral equation

$$\boldsymbol{\Xi} \psi_n = \xi_n \psi_n$$

can be rewritten as

$$\left[-\nabla_x^2 + m^2 + \varepsilon + \mathcal{V}(r)/\xi_n\right] \psi_n(x) = 0\,. \tag{3.20}$$

In the limit $\varepsilon \to 0$, $\boldsymbol{\Xi}$ has one eigenvalue ξ_0 larger than 1 (because $\partial_\mu \phi_c$ vanishes once) and the eigenvalue $\xi_1 = 1$ d times degenerate (corresponding to $\partial_\mu \phi_c$). All other eigenvalues are smaller than 1.

Then, Ω can be written formally as the product

$$\Omega = \lim_{\varepsilon\to 0_+} (1-\xi_0)\left(\frac{1-\xi_1}{\varepsilon}\right)^d \prod_{n>1}(1-\xi_n).$$

The equation (3.20) has the form of a Schrödinger equation. Thus, the relevant ratio $(1-\xi_1)/\varepsilon$ can be evaluated by first order perturbation theory, $(1-\xi_1)$ inducing a variation of the potential,$-\varepsilon$ being the corresponding energy shift and $\partial_\mu\phi_c$ the unperturbed eigenfunction. One finds

$$\frac{1-\xi_1}{\varepsilon} \sim \left[\int_0^\infty f'^2(r)r^{d-1}\mathrm{d}r\right]\left[\int_0^\infty \mathcal{V}(r)f'^2(r)r^{d-1}\mathrm{d}r\right]^{-1} \equiv R\,.$$

Thus,

$$\Omega = (1-\xi_0)R^d\prod_{n>1}(1-\xi_n).$$

Also, using $\ln\det = \operatorname{tr}\ln$, formally

$$\Omega = R^d \exp\left[-\sum_{k=1}\frac{1}{k}\left(\operatorname{tr}\boldsymbol{\Xi}^k(0) - d\right)\right]. \tag{3.21}$$

In fact, to ensure the convergence of the sum, one must first separate all eigenvalues with $|\xi_n - 1| \geq 1$ and factorize their contributions.

3.1.4 The unrenormalized instanton contribution at leading order

The instanton contribution yields the discontinuity of the function across its cut. The imaginary part is obtained by dividing by a factor $2i$. The imaginary part of the ground state energy density is then obtained from equation (3.28). At leading order, the real part of the partition function is 1. Collecting all factors, one finds

$$\operatorname{Im}\mathcal{E} \equiv -\operatorname{Im}\ln(\operatorname{Re}\mathcal{Z} + i\operatorname{Im}\mathcal{Z})/\text{volume} \underset{g\to 0}{\sim} -\frac{1}{2i}\left(\frac{A}{2\pi}\right)^{d/2}(\Omega)^{-1/2}\frac{\mathrm{e}^{-A/g}}{g^{d/2}}.$$

Moreover, $\delta^2\mathcal{S}/(\delta\phi_c)^2$ has one and only one negative eigenvalue so that the final result is real, as expected.

For correlation functions, in expression (3.5) one can replace at leading order the field $\phi(x)$ by $\phi_c(x)$ in the product $\prod_{i=1}^n \phi(x_i)$. One finds

$$\operatorname{Im} Z^{(n)}(x_1,\ldots,x_n) = \frac{1}{2i}\left(\frac{A}{2\pi}\right)^{d/2}(\Omega)^{-1/2}\frac{\mathrm{e}^{-A/g}}{g^{(d+n)/2}}F_n(x_1,\ldots,x_n) \tag{3.22}$$

with

$$F_n(x_1,\ldots,x_n) = \int \mathrm{d}^d x_0 \prod_{i=1}^n f(x_i - x_0). \tag{3.23}$$

Note one important feature of this expression: each component of x_0 generates a factor $g^{-1/2}$. While for the vacuum amplitude the integration over x_0 generates a factor proportional to the volume, for non-trivial correlation functions the integration restores translation invariance.

3.1.5 Renormalization

As we have already noticed, the determinant of the operator $\mathbf{M}$ is actually UV divergent for $d > 1$ and we have to deal with this new problem. To define properly the field theory in two and three dimensions, one first introduces a UV cut-off, for example by modifying the action in the form

$$\mathcal{S}_\Lambda(\phi) = \int \mathrm{d}^d x \left[\tfrac{1}{2}\phi(x)\left(-\nabla^2 + \nabla^4/\Lambda^2 + \cdots\right)\phi(x) + g^{-1}V\left(\phi(x)\sqrt{g}\right)\right].$$

For large cut-off Λ the modification of the instanton contribution is negligible. One then adds to the classical action counter-terms that cancel the divergences in the perturbative expansion, order by order in a loop expansion, that is, here an expansion in powers of g. Finally, one takes the infinite cut-off limit. The renormalized action has the form

$$\mathcal{S}_\mathrm{r}(\phi) = \frac{1}{g}\mathcal{S}_\Lambda(\phi\sqrt{g}) + \delta\mathcal{S}_1(\phi\sqrt{g}) + \cdots + g^{L-1}\delta\mathcal{S}_L(\phi\sqrt{g}) + \cdots .$$

At leading order, only the one-loop counter-terms contribute in the instanton calculation. To render correlation functions finite, one has to subtract to the regularized action the divergent part of the one-loop term:

$$\delta\mathcal{S}_1(\phi\sqrt{g}) = -\frac{1}{2}\left(\operatorname{tr}\ln\frac{\delta^2\mathcal{S}}{\delta\phi\delta\phi} - \operatorname{tr}\ln\frac{\delta^2\mathcal{S}_0}{\delta\phi\delta\phi}\right)_{\mathrm{div.}}.$$

When evaluated for $\phi = \phi_c$, this contribution exactly cancels the divergence in the determinant coming from the Gaussian integration around the saddle point. At one-loop order, one can choose

$$\delta\mathcal{S}_1(\phi\sqrt{g}) = -\tfrac{1}{2}G_2(0)\int \mathrm{d}^d x\left[V''\left(\phi(x)\sqrt{g}\right) - m^2\right],$$

where $G_2(x)$ is the regularized perturbative propagator:

$$G_2(x) = \frac{1}{(2\pi)^d}\int \frac{\mathrm{d}^d p\ \mathrm{e}^{ipx}}{m^2 + p^2 + p^4/\Lambda^2 + \cdots}. \tag{3.24}$$

Evaluating the contribution of the counter-term for $\phi(x) = \phi_c(x)$, one verifies that it exactly cancels $\operatorname{tr}\Xi$ in the expression (3.21). Thus, formally, in the infinite cut-off limit

$$\Omega_{\mathrm{ren.}} = R^d \exp\left[d - \sum_{k=2}\frac{1}{k}\left(\operatorname{tr}\boldsymbol{\Xi}^k(0) - d\right)\right], \tag{3.25}$$

an expression that is indeed finite order by order for $d < 4$ (but one must still separate the eigenvalues of $\boldsymbol{\Xi}$ such that $|1-\xi| \geq 1$ to render the series convergent).

The property that counter-terms determined from the perturbative expansion render also the instanton contributions finite, can be proved to all orders. The general argument relies, in particular, on the property that the classical solutions are smooth functions.

3.2 Instanton contributions and generating functional

We now discuss the contributions of instantons to correlation functions. A generating functional of the functions $Z^{(n)}$ (equation (3.4)) is given by

$$\mathcal{Z}(J) = \int [\mathrm{d}\phi(x)] \exp\left[-\mathcal{S}(\phi) + \int \mathrm{d}^d x\, J(x)\phi(x)\right]. \tag{3.26}$$

At leading order in the instanton contribution, the generating functional $\mathcal{Z}(J)$ is the sum of a formally real expansion in powers of g and an imaginary, exponentially small for $g \to 0$, instanton contribution of order $\mathrm{e}^{-A/g}$.

We thus write the functional $\mathcal{Z}(J)$ in the form

$$\mathcal{Z}(J) = \mathcal{Z}_0(J) + \varepsilon \mathcal{Z}_1(J),$$

where $\mathcal{Z}_0$ is the perturbative contribution, $\mathcal{Z}_1$ the leading instanton contribution and the parameter ε is introduced here only as a book-keeping device to indicate that we expand in the instanton contribution.

The generating functional of connected correlation functions is given by

$$\mathcal{W}(J) = \ln \mathcal{Z}(J) = \ln \mathcal{Z}_0(J) + \varepsilon \mathcal{Z}_1(J)/\mathcal{Z}_0(J) + O\left(\varepsilon^2\right). \tag{3.27}$$

Expanding

$$\mathcal{W}(J) = \mathcal{W}_0(J) + \varepsilon \mathcal{W}_1(J) + O(\varepsilon^2),$$

we find

$$\mathcal{W}_1(J) = \mathcal{Z}_1(J)/\mathcal{Z}_0(J).$$

We set ($\iota = 0, 1$)

$$W_\iota^{(n)}(x_1, \ldots, x_n) = \left(\prod_{i=1}^{n} \frac{\delta}{\delta J(x_i)}\right) \mathcal{W}_\iota(J)\bigg|_{J=0}.$$

To simplify the explicit expressions, we now assume that $\mathcal{S}(\phi) = \mathcal{S}(-\phi)$ and thus, that correlation functions with n odd vanish, but the method is general.

Then, one finds, for example,

$$\mathcal{W}_1(J=0) = \mathcal{Z}_1(0)/\mathcal{Z}_0(0), \tag{3.28}$$

$$W_1^{(2)}(x_1, x_2) = Z_1^{(2)}(x_1, x_2)/\mathcal{Z}_0(0) - Z_0^{(2)}(x_1, x_2)\mathcal{Z}_1(0)/\mathcal{Z}_0^2(0), \tag{3.29}$$

and

$$\begin{aligned} W_1^{(4)}&(x_1, x_2, x_3, x_4) \\ &= Z_1^{(4)}(x_1, x_2, x_3, x_4)/\mathcal{Z}_0(0) - Z_0^{(2)}(x_1, x_2) Z_1^{(2)}(x_3, x_4)/\mathcal{Z}_0^2(0) + 5 \text{ terms} \\ &\quad - Z_0^{(4)}(x_1, x_2, x_3, x_4)\mathcal{Z}_1(0)/\mathcal{Z}_0^2(0) \\ &\quad + 2 Z_0^{(2)}(x_1, x_2) Z_0^{(2)}(x_3, x_4)\mathcal{Z}_1(0)/\mathcal{Z}_0^3(0) + 2 \text{ terms}. \end{aligned} \tag{3.30}$$

At leading order, $Z_1^{(n)}$ is proportional to $(\phi_c)^n$. Since the classical field ϕ_c is of order $1/\sqrt{g}$ (equation (3.7)), $Z_1^{(n)}$ of order $g^{-n/2}\mathcal{Z}_1(0)$ (see, e.g., equation (3.55)). This implies $Z_1^{(4)} \gg Z_1^{(2)} \gg \mathcal{Z}_1$ and thus, at leading order, the disconnected contributions are subleading.

Finally, from the well-known property of the Legendre transformation, if we expand the vertex (1PI) functional in the form

$$\Gamma(\phi) = \Gamma_0(\phi) + \varepsilon\Gamma_1(\phi) + O\left(\varepsilon^2\right), \tag{3.31}$$

where $\Gamma_0(\phi)$ is the Legendre transform of $\mathcal{W}_0(J)$, then

$$\Gamma_1(\phi) = -\mathcal{W}_1\big(J_0(\phi)\big)$$

with

$$J_0(\phi) = \frac{\delta\Gamma_0}{\delta\phi}\,.$$

Setting

$$\Gamma^{(n)}(x_1,\ldots,x_n) = \left(\prod_{i=1}^{n}\frac{\delta}{\delta\phi(x_i)}\right)\Gamma(\phi)\bigg|_{\phi=0}\,,$$

one finds, for example,

$$\Gamma_1^{(2)}(x_1,x_2) = -\int \mathrm{d}^d y_1\,\mathrm{d}^d y_2\,\Gamma_0^{(2)}(x_1,y_1)W_1^{(2)}(y_1,y_2)\Gamma_0^{(2)}(x_2,y_2) \tag{3.32}$$

and

$$\begin{aligned}\Gamma_1^{(4)}(\mathbf{x}) = &-\int\left(\prod_{i=1}^{4}\mathrm{d}^d y_i\Gamma_0^{(2)}(x_i,y_i)\right)W_1^{(4)}(\mathbf{y})\\ &-\int \mathrm{d}^d y\,\mathrm{d}^d z\,\Gamma_0^{(2)}(x_1,y)W_1^{(2)}(y,z)\Gamma_0^{(4)}(z,x_2,x_3,x_4) + 3\ \text{terms.}\end{aligned} \tag{3.33}$$

One finds that the 1-line reducible parts are subleading.

3.3 Cosmology: The decay of the false vacuum

In preceding sections we have determined the probability for a ‘false vacuum’ of a quantum field theory to decay through barrier penetration. While the calculation has direct applications for large order behaviour (see chapter 7) and issues in statistical physics, it has also been speculated that such a phenomenon could be linked to the dynamics of the early universe [12].

When the universe started to cool down, some symmetries started to be spontaneously broken. Some region might have been trapped in the wrong phase. The false vacuum must eventually decay in the true vacuum, but if the process is slow enough, it might have occurred at a much later time when the universe was already cool. This is the kind of physical speculation that we here have in mind.

According to the previous discussion, if the universe is in the wrong vacuum, there is some probability at each point in space for some bubble of true vacuum to be created, and if the bubble is large enough, it becomes favourable for it to expand, absorbing eventually the whole space. To discuss what happens once a bubble has been created, it is useful to consider first the analogous problem in ordinary quantum mechanics.

Quantum mechanics. In the language of particle physics, a semi-classical description of the decay process would be the following: a particle is sitting in the well of the potential corresponding to the unstable minimum. At a given time, it makes a quantum jump and reappears outside of the barrier, at the point where the potential has the same value as in the bottom of the well, with zero velocity (by energy conservation). Then its further trajectory can be entirely described by classical mechanics.

Field theory. We apply the same ideas to the field theoretical model we discuss in this chapter. At time zero the system makes quantum jump. According to the previous discussion, the value of the field at time zero is then (with the choice $x_{0\mu} = 0$)

$$\phi(t = 0, \mathbf{x}) = \phi_c(x_d = 0, \mathbf{x}), \qquad (\mathbf{x} = x_1, \ldots, x_{d-1})\,, \tag{3.34}$$

and its time derivative vanishes,

$$\partial_t \phi(t = 0, \mathbf{x}) = 0\,. \tag{3.35}$$

At a later time $\phi(t, \mathbf{x})$ then obeys the *real-time* field equation,

$$\left[\nabla_i^2 - \partial_t^2\right] \phi(t, \mathbf{x}) = \frac{1}{\sqrt{g}} V'(\sqrt{g}\phi). \tag{3.36}$$

The first equation (3.34) tells us that the same function describes the form of the instanton in Euclidean space, and its shape in ordinary $(d-1)$ space when it materializes. We now consider the continuation in real time of the solution of the Euclidean field equation $\phi_c[(\mathbf{x}^2 - t^2)^{1/2}]$ (since $\phi_c(r)$ is an even function, the sign in front of the square root is irrelevant). It satisfies the conditions (3.34,3.35) and obviously obeys the field equation (3.36). It is, therefore, the solution of our problem for positive times.

Since the size of the bubble is given by microphysics, the interior of the bubble corresponds to small values of r on a macroscopic scale,

$$0 \le \mathbf{x}^2 - t^2 = r^2 \ll 1\,.$$

Therefore, after a short time the bubble starts expanding at almost the speed of light.

3.4 The ϕ^4 field theory for negative coupling

We now consider the concrete example of the ϕ^4 field theory which, in the tree approximation, corresponds to the action

$$\mathcal{S}(\phi) = \int \mathrm{d}^d x \left[\frac{1}{2}\left(\partial_\mu \phi(x)\right)^2 + \frac{1}{2} m^2 \phi^2(x) + \frac{1}{4!} g m^{4-d} \phi^4(x)\right], \tag{3.37}$$

m being the mass and g the dimensionless coupling constant (the power of m which appears in front of the interaction term ϕ^4 takes care of the dimension).

The complete n-point correlation function has the functional representation (3.4). We normalize all field integrals with respect to the vacuum amplitude at $g = 0$, to avoid introducing a non-trivial g-dependence through the normalization. Thus, $\mathcal{Z}(g = 0) = 1$.

Instantons. As functions of g, correlation functions are analytic functions with a cut on the real negative axis. We assume that we start from positive values of g and proceed by analytic continuation to define the field integral for g negative. The imaginary part of correlation functions is given by the difference between the continuations above and below the negative g-axis. For g small, only non-trivial saddle points contribute to the imaginary part. Therefore, we look for non-trivial finite action solutions of the Euclidean field equations, that is, instanton configurations, and then calculate the corresponding contributions.

3.4.1 Instantons: Classical solutions and classical action

The instanton solutions. The field equation corresponding to the action (3.37) is

$$\left(-\nabla^2 + m^2\right) \phi_c(x) + \tfrac{1}{6} g m^{4-d} \phi_c^3(x) = 0 \,. \tag{3.38}$$

We set (g is negative),

$$\phi_c(x) = (-6/g)^{1/2} m^{d/2-1} f(mx) \,. \tag{3.39}$$

In terms of f, the classical action (3.37) reads

$$\mathcal{S}(f) = -\frac{6}{g} \int \mathrm{d}^d x \left[\tfrac{1}{2}\left(\partial_\mu f\right)^2 + \tfrac{1}{2} f^2 - \tfrac{1}{4} f^4\right]. \tag{3.40}$$

The function $f(x)$ then satisfies the parameter-free equation

$$\left(-\nabla^2 + 1\right) f(x) - f^3(x) = 0 \,. \tag{3.41}$$

It can be shown that the solution with the smallest action is spherically symmetric. Therefore, we choose an arbitrary origin x_0 and set

$$r = |x - x_0| \,. \tag{3.42}$$

A function $f(x)$ that depends only on the radial variable r satisfies the differential equation,

$$\left[-\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2 - \frac{d-1}{r}\frac{\mathrm{d}}{\mathrm{d}r} + 1\right] f(r) - f^3(r) = 0\,. \tag{3.43}$$

The equation describes the motion of a particle in a potential $-V(f)$:

$$V(f) = \tfrac{1}{2}f^2 - \tfrac{1}{4}f^4, \tag{3.44}$$

submitted in addition to a viscous damping force (for $d > 1$).

Since we look for finite action solutions we impose the boundary condition

$$f(r) \to 0 \quad \text{for} \quad r \to \infty\,. \tag{3.45}$$

Equation (3.43) shows that if $f(r)$ goes to zero at infinity it goes exponentially. The equation has solutions even in r, which are thus determined by the value of f at the origin. For a generic value of $f(0)$, the corresponding solution tends at infinity toward one of the minima $f = \pm 1$ of the potential $-V(f)$. The condition (3.45) is satisfied only for a discrete set of initial values of $f(0)$. Moreover, it can be shown that the minimal action solution corresponds to the function for which $|f(0)|$ is minimal in the set, and which vanishes only at infinity.

One then finds a double family of d-parameter solutions obtained from a particular one by $\pm f(|x - x_0|)$.

Solutions and classical action. Since g is dimensionless, the corresponding classical action has the form

$$\mathcal{S}(\phi_c) \equiv \mathcal{S}(f) = -A/g\,, \tag{3.46}$$

in which A is a pure number. Scaling arguments lead to the relations

$$A = \frac{6}{d}\int [\partial_\mu f(x)]^2\, \mathrm{d}^d x = \frac{3}{2}\int f^4(x)\mathrm{d}^d x = \frac{6}{4-d}\int f^2(x)\mathrm{d}^d x\,, \tag{3.47}$$

which show that A is positive. We also note that these relations can be true only for $d < 4$ and thus the dimension 4 is singular (see chapter 5).

The relevant solutions of equation (3.43) are analytic even functions with singularities closest to the origin poles on the imaginary axis with residues $\pm i\sqrt{2}$. For $r \to \infty$, they converge exponentially toward solutions of the linear equation obtained by omitting the f^3 term. They are determined by the value at the origin. We give here the numerical results for $d = 1, 2, 3$ [15]:

$$d = 1: \; f(0) = \sqrt{2} = 1.4142135623\ldots, \qquad A = 8\,. \tag{3.48}$$

$$d = 2: \; f(0) = 2.20620086465074607(1), \qquad A = 35.10268957367896(1). \tag{3.49}$$

$$d = 3: \; f(0) = 4.3373876799769943(1), \qquad A = 113.38350781527714(1). \tag{3.50}$$

Asymptotically for $r \to \infty$,

$$f(r) = F\sqrt{\frac{2}{\pi}} r^{1-d/2} K_{d/2-1}(r) + o(\mathrm{e}^{-3r})$$

where K_ν is a modified Bessel function of the second kind normalized such that

$$K_\nu(r) \underset{r\to\infty}{\sim} \sqrt{\frac{\pi}{2r}}\,\mathrm{e}^{-r}\,.$$

More precisely, the relative error is proportional to $-f^2/8$.

One finds

$$\begin{cases} \text{for } d=1\,, & F = 2\sqrt{2} = 2.8284271246\ldots\,, \\ \text{for } d=2\,, & F = 3.518062198024(1)\,, \\ \text{for } d=3\,, & F = 2.712808360940(1)\,. \end{cases}$$

For what follows, it is convenient to introduce the notation

$$I_n = \int_0^\infty r^{d-1} f^n(r)\mathrm{d}r\,. \tag{3.51}$$

Then,

$$I_2 = \frac{4-d}{4} I_4\,,\ \int_0^\infty r^{d-1} f'^2(r)\mathrm{d}r = \frac{d}{4} I_4\,,\ A = \frac{3}{2} S_d I_4\,, \tag{3.52}$$

where S_d is given in equation (3.13).

For $d=1$, this yields

$$I_2 = 2\,,\quad I_4 = \tfrac{8}{3} = 2.666666\ldots\,,\quad I_6 = \tfrac{64}{15} = 4.266666\ldots\,. \tag{3.53}$$

For $d=2$,

$$I_2 = 1.862255520490447(1),\ I_4 = 3.724511040980895(1),$$
$$I_6 = 11.3127606567358398(1)\,.$$

For $d=3$,

$$I_2 = 1.5037954778249919(1),\ I_4 = 6.0151819112999679(1),$$
$$I_6 = 52.5106549691091922(1).$$

3.4.2 The result at leading order

The result at leading order involves the operators

$$\begin{aligned} M(x,x') &= \left[-\nabla_x^2 + m^2 + \tfrac{1}{2} g m^{4-d} \phi_c^2(x)\right] \delta^{(d)}(x-x'), \\ &= \left[-\nabla_x^2 + m^2 - 3m^2 f^2(mr)\right] \delta^{(d)}(x-x') \end{aligned} \tag{3.54}$$

and

$$\mathbf{M}_0(x,x') = \left(-\nabla_x^2 + m^2\right) \delta^{(d)}(x-x').$$

Adapting the results of section 3.1.4 to the ϕ^4 example, one then finds

$$\operatorname{Im} Z^{(n)}(x_1,\dots,x_n) = \frac{1}{2i}\left(\frac{A}{2\pi}\right)^{d/2} (\Omega)^{-1/2} \frac{\mathrm{e}^{A/g}}{(-g)^{(d+n)/2}} F_n(x_1,\dots,x_n), \tag{3.55}$$

with

$$F_n(x_1,\dots,x_n) = m^{d+n(d-2)/2} 6^{n/2} \int \mathrm{d}^d x_0 \prod_{i=1}^{n} f\big(m(x_i - x_0)\big), \tag{3.56}$$

and

$$\Omega = \left(\det{}' \mathbf{M}\mathbf{M}_0^{-1}\right)\Big|_{m=1} = \lim_{\varepsilon\to 0_+} \varepsilon^{-d} \det\left[(\mathbf{M}+\varepsilon)(\mathbf{M}_0+\varepsilon)^{-1}\right]\Big|_{m=1}. \tag{3.57}$$

Wave function arguments of the kind used for the Schrödinger equation show directly that $\partial_\mu \phi_c$ is not the ground state of $\mathbf{M}$. One state exists with a negative eigenvalue so that the final result is real as expected.

Discussion. A few comments concerning expression (3.22) are here in order. We have obtained a result for the complete correlation functions, improperly normalized, for convenience, with respect to the free field theory. We notice, however, that, because $\phi_c(x)$ is proportional to $1/\sqrt{-g}$, the imaginary part of the n-point function increases with n for g small. It follows then from the discussion of section 3.2 that at leading order the correlation functions normalized with respect to the partition function corresponding to the complete action (3.37) have the same behaviour as those renormalized with respect to the free field theory.

Moreover, for the same reason, in the complete n-point function, the imaginary part coming from disconnected parts is subleading by at least a power of g. For the connected n-point correlation function, one thus finds at leading order

$$\operatorname{Im} W^{(n)} \sim \operatorname{Im} Z^{(n)},$$

a result that is consistent with the observation that the explicit expression (3.22) is indeed connected. To pass from connected correlation functions to 1PI functions, one has first to subtract the reducible contributions which involve functions with a smaller number of arguments and which are, therefore, negligible at leading order, and then to amputate the remaining part. Again for the same reason only the perturbative part of the propagator matters; therefore, to amputate expression (3.22) one has to simply multiply it by the product of the inverse free propagators corresponding to each external line. Introducing the Fourier transform of f,

$$\tilde{f}(p) = \int \mathrm{d}^d x \; \mathrm{e}^{-ipx} f(r),$$

and writing the n-point 1PI function $\tilde{\Gamma}^{(n)}$ in momentum space representation, one obtains

$$\operatorname{Im}\tilde{\Gamma}^{(n)}(p_1,\ldots,p_n) \sim -\frac{1}{2i}\left(\frac{A}{2\pi}\right)^{d/2}(\Omega)^{-1/2}\frac{\mathrm{e}^{A/g}}{(-g)^{(d+n)/2}}m^{d-n(d/2+1)} \times 6^{n/2}\prod_{i=1}^{n}\tilde{f}(p_i/m)\left(p_i^2+m^2\right). \tag{3.58}$$

At leading order, the structure of the imaginary part of the n-point function is particularly simple in momentum representation; in particular it depends only on the square of the momenta and not of their scalar products.

3.4.3 The determinant

We specialize the expressions of section 3.1.3 to the ϕ^4 theory and $m = 1$. We have to calculate the determinant (3.57) that we can rewrite as

$$\Omega = \lim_{\varepsilon\to 0_+}\varepsilon^{-d}\det\left[\mathbf{1}-\mathbf{\Xi}(\varepsilon)\right]$$

with

$$\mathbf{\Xi}(\varepsilon) = 3(-\nabla_x^2+1+\varepsilon)^{-1}f^2.$$

The operator $\mathbf{\Xi}$ is equivalent to a positive Hermitian operator since f^2 is positive.

To renormalize, we choose a counter-term such that the inverse two-point function in the Fourier representation satisfies

$$\tilde{\Gamma}^{(2)}(p=0) = m^2.$$

The one-loop counter-term is then

$$\delta\mathcal{S}_1 = -\tfrac{1}{4}G_2(0)gm^{4-d}\int \mathrm{d}^d x\,\phi^2(x). \tag{3.59}$$

It has the effect of cancelling $\operatorname{tr}\mathbf{\Xi}$. We can then directly use the expression (3.25):

$$\Omega_{\text{ren.}} = R^d\exp\left[d-\sum_{k=2}\frac{1}{k}\left(\operatorname{tr}\mathbf{\Xi}^k(0)-d\right)\right],$$

where one must still separate the eigenvalues of $\mathbf{\Xi}$ such that $|1-\xi|\geq 1$. For example, here the first contributing trace is

$$\operatorname{tr}\mathbf{\Xi}^2 = \sum_{n=0}\xi_n^2 = 9\int \mathrm{d}^d x\,\mathrm{d}^d x'\,f^2(r)G_2^2(x-x')f^2(r').$$

The spectral equation then reads

$$\mathbf{\Xi}\psi = \xi\psi \;\Leftrightarrow\; \left(-\nabla_x^2+1-3f^2(x)/\xi\right)\psi(x) = 0\,. \tag{3.60}$$

The largest eigenvalue is $\xi_0 = 3$ which corresponds to $\psi(x) = f(r)$. The next eigenvalue $\xi_1 = 1$ is d times degenerate and corresponds to the zero-modes $\psi_\mu(x) = x_\mu f'(r)/r$. All other eigenvalues $n > 1$ satisfy $0 < \xi_n < 1$ and, thus, $|1-\xi| < 1$. It is thus necessary to factorize only the contribution of the first eigenvalue and expand in modified traces

$$\mathrm{tr}'\, \boldsymbol{\Xi}^k = \mathrm{tr}\, \boldsymbol{\Xi}^k - 3^k - d\,. \tag{3.61}$$

Zero-mode sector. In the zero-mode sector, $\xi - 1$ is of order ε and can be considered as inducing a perturbation to the initial potential. Thus, the energy shift can be calculated by first order perturbation theory:

$$\varepsilon \int r^{d-1} f'^2(r)\mathrm{d}r = 3(1-\xi_1) \int r^{d-1} f^2(x) f'^2(x)\mathrm{d}r\,.$$

After an integration by parts, one obtains

$$R \equiv \lim_{\varepsilon\to 0} \frac{1-\xi_1}{\varepsilon} = \frac{dI_4}{4(I_6 - I_4)}\,. \tag{3.62}$$

Then,

$$\Omega_{\text{ren.}} = -2R^d \exp\left(d + 3 - \sum_{k=2} \frac{1}{k}\,\mathrm{tr}'\, \boldsymbol{\Xi}^k\right). \tag{3.63}$$

Dimension 1. For $d = 1$, where no one-loop renormalization is required, one finds

$$R = (1-\xi_1)/\varepsilon = \tfrac{5}{12} \tag{3.64}$$

and

$$\Omega = \lim_{\varepsilon\to 0_+} \varepsilon^{-1} \det\left[\mathbf{1} - \boldsymbol{\Xi}(\varepsilon)\right] = -\tfrac{1}{12}\,.$$

Chapter 4

Metastable Vacua: The O(N) Generalization

We now generalize the study of section 3.4 to the situation where $\boldsymbol{\phi}$ is an N-component field and the action is $O(N)$ invariant. We work out in some detail the example of the $(\boldsymbol{\phi}^2(x))^2$ field theory corresponding to the tree level action

$$\mathcal{S}(\boldsymbol{\phi}) = \int \mathrm{d}^d x \left[\frac{1}{2}\left(\partial_\mu \boldsymbol{\phi}(x)\right)^2 + \frac{1}{2} m^2 \boldsymbol{\phi}^2(x) + \frac{1}{4!} g m^{4-d} \left(\boldsymbol{\phi}^2(x)\right)^2\right], \qquad (4.1)$$

generalizing the action (3.37), but part of the discussion applies to more general scalar field theories. In particular, we calculate the exact form of the Jacobian when the instanton solution breaks both d dimensional space translations and the $O(N)$ internal symmetry.

4.1 Instantons and determinant

The corresponding field equations are

$$\left(-\nabla^2 + m^2\right) \phi_\alpha(x) + \tfrac{1}{6} g m^{4-d} \boldsymbol{\phi}^2(x) \phi_\alpha(x) = 0\,. \qquad (4.2)$$

Using the Sobolev inequalities, one can show that the minimal action solution is

$$\boldsymbol{\phi}_c(x) = \mathbf{u} \phi_c(r), \quad \phi_c(r) = (-6/g)^{1/2} m^{d/2-1} f(mr), \qquad (4.3)$$

where the vector $\mathbf{u}$ of components u_α is a constant unit vector, $\mathbf{u}^2 = 1$, and f the solution of equation (3.43).

The second derivative of the action is then

$$M_{\alpha\beta}(x, x') = \left[\left(-\nabla_x^2 + m^2 - m^2 f^2(mr)\right) \delta_{\alpha\beta} - 2m^2 f^2(mr) u_\alpha u_\beta\right] \delta^{(d)}(x - x'). \qquad (4.4)$$

At x, x' fixed, the matrix $M_{\alpha\beta}$ has two operator eigenvalues, one corresponding to the eigenvector u_α:

$$M_{\mathrm{L}}(x, x') = \left(-\nabla_x^2 + m^2 - 3m^2 f^2(mr)\right) \delta^{(d)}(x - x'), \qquad (4.5)$$

which is the operator for $N = 1$ and the second one, corresponding to the vector space orthogonal to $\mathbf{u}$, thus $(N-1)$ times degenerate:

$$M_{\mathrm{T}}(x,x') = \left(-\nabla_x^2 + m^2 - m^2 f^2(mr)\right)\delta^{(d)}(x-x'). \tag{4.6}$$

This second operator has $f(mr)$ for eigenvector with eigenvalue zero, corresponding to the breaking of the $O(N)$ symmetry. This implies the introduction of $(N-1)$ collective coordinates related to the coset space $SO(N)/SO(N-1)$, which is isomorphic to the sphere S_{N-1}.

4.2 The Jacobian at leading order

We parametrize the field in the form

$$\boldsymbol{\phi}(x) = \phi_{\mathrm{L}}(x+x_0)\mathbf{u} + \boldsymbol{\phi}_{\mathrm{T}}(x+x_0),$$

where

$$\mathbf{u}\cdot\boldsymbol{\phi}_{\mathrm{T}}(x) = 0\,.$$

We then introduce the quantity

$$\mathbf{J}(\boldsymbol{\phi}) = \det g_{ij}\left(\int \mathrm{d}^d x\,\phi_c(x)\phi_{\mathrm{L}}(x)\right)^{N-d-1}\det I_{\mu\nu}$$

with

$$\begin{aligned} I_{\mu\nu}(\boldsymbol{\phi}) = \int \mathrm{d}^d x\,\mathrm{d}^d x'\,[&\partial_\mu\boldsymbol{\phi}_c(x)\cdot\partial_\nu\boldsymbol{\phi}(x)\phi_c(x')\phi_{\mathrm{L}}(x') \\ &-\partial_\mu\phi_c(x)\partial_\nu\phi_c(x')\boldsymbol{\phi}_{\mathrm{T}}(x)\cdot\boldsymbol{\phi}_{\mathrm{T}}(x')]\,. \end{aligned} \tag{4.7}$$

The Jacobian is then (the derivation is postponed to section 4.6):

$$\mathcal{J} = \mathbf{J}(\boldsymbol{\phi})/\mathbf{J}^{1/2}(\boldsymbol{\phi}_c).$$

Leading order calculation. At leading order, $\phi_{\mathrm{L}} = \phi_c$ and $\phi_{\mathrm{T}} = 0$ and the Jacobian factorizes:

$$\mathcal{J} = \mathbf{J}^{1/2}(\boldsymbol{\phi}_c) = J_{\mathrm{tr.}}J_{\mathrm{rot}},$$

where

$$J_{\mathrm{tr.}} = \det{}^{1/2}\int \mathrm{d}^d x\,\partial_\mu\boldsymbol{\phi}_c(x)\cdot\partial_\nu\boldsymbol{\phi}_c(x) \tag{4.8a}$$

$$J_{\mathrm{rot}} = \det{}^{1/2}\mathbf{g}\left[\int \mathrm{d}^d x\,\boldsymbol{\phi}_c^2(x)\right]^{(N-1)/2}, \tag{4.8b}$$

where the matrix $\mathbf{g}$ represents the metric tensor g_{ij} on the sphere. Denoting by θ_i a set of $N-1$ parameters parametrizing the sphere, then

$$g_{ij} = \frac{\partial\mathbf{u}}{\partial\theta_i}\cdot\frac{\partial\mathbf{u}}{\partial\theta_j}$$

and $\int \prod_i \mathrm{d}\theta_i \det^{1/2} \mathbf{g}$ is the covariant surface element of S_{N-1}.

Since $\boldsymbol{\phi}_c(x)$ depends only on the radial coordinate r, the matrix

$$J^{\mu\nu}_{\text{tr.}} \equiv \int \mathrm{d}^d x\, \partial_\mu \boldsymbol{\phi}_c(x) \cdot \partial_\nu \boldsymbol{\phi}_c(x) = \frac{1}{d}\delta_{\mu\nu} \int \mathrm{d}^d x \left(\partial_\mu \boldsymbol{\phi}_c(x)\right)^2, \tag{4.9}$$

and thus

$$J_{\text{tr.}} = \det{}^{1/2} J^{\mu\nu}_{\text{tr.}} = \left[\frac{1}{d}\int \mathrm{d}^d x \left(\partial_\mu \boldsymbol{\phi}_c(x)\right)^2\right]^{d/2} = \left(\frac{A}{g}\right)^{d/2}.$$

Finally, for J_{rot} one needs

$$\int \mathrm{d}^d x\, \boldsymbol{\phi}_c^2(x) = -\frac{6}{m^2 g}\int \mathrm{d}^d x\, f^2(x) = -\frac{6}{m^2 g} S_d I_2 = \frac{d-4}{gm^2} A\,. \tag{4.10}$$

Thus,

$$J_{\text{rot}} = \det{}^{1/2}\mathbf{g} \left(\frac{(d-4)A}{m^2 g}\right)^{(N-1)/2}.$$

Moreover, one must again divide by a factor $\sqrt{2\pi}$ for each collective coordinate, coming from the corresponding Gaussian integrations in the normalization integral. At leading order, this yields the factor

$$\det{}^{1/2}\mathbf{g}\, m^{1-N}(d-4)^{(N-1)/2}\left(\frac{A}{2\pi g}\right)^{(d+N-1)/2}.$$

4.3 The instanton contribution at leading order

To $M_{\text{L}}(x,x')$ is associated $\mathbf{K}_{\text{L}}$, whose spectrum has already been discussed and to $M_{\text{T}}(x,x')$ for $m=1$

$$\mathbf{K}_{\text{T}} = \mathbf{1} - \boldsymbol{\Xi}_{\text{T}}$$

with

$$\boldsymbol{\Xi}_{\text{T}} = (-\nabla_x^2 + 1 + \varepsilon)^{-1} f^2 = \boldsymbol{\Xi}_{\text{L}}/3\,.$$

The leading eigenvalue of $\boldsymbol{\Xi}_{\text{T}}$ is 1 and corresponds to the zero-mode.

Finally, the relevant determinant is

$$\Omega_{\text{T}} = \lim_{\varepsilon\to 0_+} \frac{1}{\varepsilon} \det\left[(\mathbf{M}_0+\varepsilon)^{-1}(\mathbf{M}_{\text{T}}+\varepsilon)\right]\Big|_{m=1}.$$

In the zero-mode sector, the relation between the eigenvalue $\xi_{\text{T}\,0}$ and ε is again given by first order perturbation theory:

$$R_{\text{T}} \equiv \lim_{\varepsilon\to 0}\frac{1-\xi_{\text{T}\,0}}{\varepsilon} = \frac{I_2}{I_4}\,. \tag{4.11}$$

Thus, before renormalization,

$$\Omega_{\mathrm{T}} = R_{\mathrm{T}} \exp\left[-\sum_{k=1} \frac{1}{k}\left(\operatorname{tr} \boldsymbol{\Xi}_{\mathrm{L}}^{k}/3^{k} - 1\right)\right].$$

The determinant has to be renormalized. We choose a counter-term such that the inverse two-point function satisfies

$$\tilde{\Gamma}^{(2)}(p=0) = m^2 .$$

The counter-term is then

$$\delta\mathcal{S}_1 = -\tfrac{1}{12}(N+2)G_2(0)gm^{4-d}\int \mathrm{d}^d x\, \phi^2(x). \tag{4.12}$$

It has the effect of cancelling $\operatorname{tr}\boldsymbol{\Xi}$ and this leads to the cancellation of $\operatorname{tr}\boldsymbol{\Xi}_{\mathrm{T}}$. Thus,

$$[\Omega_{\mathrm{T}}]_{\mathrm{ren.}} = R_{\mathrm{T}} \exp\left[1-\sum_{k=2} \frac{1}{k}\left(\operatorname{tr} \boldsymbol{\Xi}_{\mathrm{L}}^{k}/3^{k} - 1\right)\right]. \tag{4.13}$$

The leading order result is then multiplied by the factor $[\Omega_{\mathrm{T}}]_{\mathrm{ren.}}^{-(N-1)/2}$.

The integration over the sphere S_{N-1}. In the case of the partition function, the integration over collective coordinates yields the product of the surface of the S_{N-1} sphere, $2\pi^{N/2}/\Gamma(N/2)$, and the space volume. Collecting all factors, one obtains

$$\frac{2\pi^{N/2}}{\Gamma(N/2)}\left(\frac{(d-4)A}{2\pi g\, [\Omega_{\mathrm{T}}]_{\mathrm{ren.}}}\right)^{(N-1)/2} . \tag{4.14}$$

In the case of correlation functions, the integration over the sphere has the effect of averaging the product $(\phi_c)_{\alpha_1}\ldots(\phi_c)_{\alpha_n}$ and thus the factor $u_{\alpha_1}u_{\alpha_2}\ldots u_{\alpha_n}$. Setting

$$T_{\alpha_1\alpha_2\ldots\alpha_n} = \left\langle u_{\alpha_1}u_{\alpha_2}\ldots u_{\alpha_n}\right\rangle_{S_{N-1}}, \tag{4.15}$$

one finds for the two-point function, for example,

$$T_{\alpha\beta} = \frac{1}{N}\delta_{\alpha\beta}\,. \tag{4.16}$$

Similarly, for the four-point function

$$T_{\alpha\beta\gamma\delta} = \frac{1}{N(N+2)}\left(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\gamma\beta}\right). \tag{4.17}$$

By convention

$$T = \langle 1\rangle_{S_{N-1}} = 1\,.$$

Dimension 1. The case $d=1$ corresponds to the $O(N)$ symmetric anharmonic oscillator with the Hamiltonian

$$H = \tfrac{1}{2}\mathbf{p}^2 + \tfrac{1}{2}m^2\mathbf{q}^2 + \tfrac{1}{4!}g(\mathbf{q}^2)^2. \tag{4.18}$$

Then, $J=-24/g$,

$$\det{}'(\mathbf{1}-\boldsymbol{\Xi}_{\mathrm{T}}) = \tfrac{1}{3}\,,$$

and (equation (3.53))

$$R_{\mathrm{T}} = \tfrac{3}{4} \;\Rightarrow\; \Omega_{\mathrm{T}} = \tfrac{1}{4}\,.$$

4.4 Jacobian and continuous symmetries: Ordinary integrals

We now justify the form of the Jacobian used in chapter 4. We begin the analysis with ordinary integrals, the generalization to path and field integrals being then simple.

4.4.1 Ordinary integrals

We want to evaluate the integral

$$\mathcal{I} = \int_{\mathbb{R}^N} \mathrm{d}^N x \; \mathrm{e}^{-S(\mathbf{x})/g}, \tag{4.19}$$

in the limit $g \to 0_+$, where the function S is analytic and symmetric under the transformations of a continuous Lie group G, subgroup of $O(N)$, acting on $\mathbf{x}$. We assume that, in this limit, the function S is minimum at non G-symmetric saddle points $\mathbf{x}_c$ that are left invariant by the transformations of a subgroup H of G. The solution $\mathbf{x}_c$ then depends on p parameters τ^i parametrizing the coset (homogeneous) space G/H. The second derivative of S thus has a multiple zero eigenvalue corresponding to the p eigenvectors $\partial\mathbf{x}_c/\partial\tau^i$ (zero modes). To apply the steepest descent method, one must take the parameters τ^i as collective coordinates and restrict the steepest descent calculation to the remaining $N-p$ variables. The problem is then to calculate the Jacobian of the corresponding change of variables.

Collective coordinates and Jacobian. We introduce an orthonormal basis $\mathbf{e}_\alpha$, $\alpha = 1, \ldots, N$, such that the vectors $\mathbf{e}_\alpha$ with $\alpha > p$ span the subspace orthogonal to all vectors $\partial\mathbf{x}_c/\partial\tau^i$:

$$\mathbf{e}_\alpha \cdot \frac{\partial \mathbf{x}_c}{\partial \tau^i} = 0 \;\forall \alpha > p\,. \tag{4.20}$$

We then change variables $\mathbf{x} \mapsto \{\tau^i, r^a\}$, setting

$$\mathbf{x} = \mathbf{x}_c(\boldsymbol{\tau}) + \sum_{a>p} r^a \mathbf{e}_a(\boldsymbol{\tau}). \tag{4.21}$$

The corresponding Jacobian is

$$J = \det\left(\frac{\partial \mathbf{x}}{\partial \tau^i}, \frac{\partial \mathbf{x}}{\partial r^a}\right) = \det\left(\frac{\partial \mathbf{x}}{\partial \tau^i}, \mathbf{e}_a(\boldsymbol{\tau})\right), \; a > p\,,$$

where $\mathbf{x}(\boldsymbol{\tau})$ is a substitute for the expansion (4.21). We then expand the vectors $\partial\mathbf{x}/\partial\tau^i$ on the basis $\{\mathbf{e}_\alpha\}$:

$$\frac{\partial \mathbf{x}}{\partial \tau^i} = \sum_\alpha \mathbf{e}_\alpha(\boldsymbol{\tau}) \, \frac{\partial \mathbf{x}(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_\alpha(\boldsymbol{\tau})\,. \tag{4.22}$$

Inside the determinant, the components with $\alpha > p$ can be omitted and the Jacobian becomes ($a > p$)

$$J = \det\left(\sum_{j \le p} \mathbf{e}_j \, \frac{\partial \mathbf{x}(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_j \,, \mathbf{e}_a\right) = \det \frac{\partial \mathbf{x}(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_j\,, \tag{4.23}$$

because the basis is orthonormal.

The expansion (4.22) can be also applied to $\mathbf{x}_c$, where it reduces to

$$\frac{\partial \mathbf{x}_c}{\partial \tau^i} = \sum_{j \le p} \mathbf{e}_j(\boldsymbol{\tau})\, \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_j(\boldsymbol{\tau})$$

and, introducing the $p \times p$ matrix

$$R_{ij}(\boldsymbol{\tau}) = \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_j(\boldsymbol{\tau}),$$

conversely,

$$\mathbf{e}_i(\boldsymbol{\tau}) = \sum_j R^{-1}_{ij}(\boldsymbol{\tau}) \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^j}.$$

It follows that

$$J = \det \frac{\partial \mathbf{x}(\boldsymbol{\tau})}{\partial \tau^i} \cdot \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^j} \det \mathbf{R}^{-1}(\boldsymbol{\tau}) = \det \frac{\partial \mathbf{x}(\boldsymbol{\tau})}{\partial \tau^i} \cdot \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^j} \Big/ \det \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_j \,.$$

Finally,

$$\begin{aligned} \det{}^2 \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_j &= \det \left(\sum_k \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_k \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^j} \cdot \mathbf{e}_k \right) \\ &= \det \left(\frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^j} \right), \end{aligned}$$

because the projector

$$\Pi_{\alpha\beta} = \sum_{i \le p} e_i^\alpha e_i^\beta \,, \tag{4.24}$$

is the identity in the subspace spanned by the vectors $\partial x_c^\alpha / \partial \tau^i$.

It is convenient to introduce the metric tensor on the manifold G/H, which can be written as

$$g_{ij} = \frac{\partial \mathbf{x}_c}{\partial \tau^i} \cdot \frac{\partial \mathbf{x}_c}{\partial \tau^j}. \tag{4.25}$$

One can then rewrite the integration measure Jacobian as [9]

$$J \, \mathrm{d}^N \mathbf{x} \, \delta^{(p)}(\mathbf{x}_\mathrm{T}) \prod_i \mathrm{d}\tau^i \tag{4.26}$$

with

$$J = (\det g_{ij})^{-1/2} \det \left(\frac{\partial \mathbf{x}}{\partial \tau^i} \cdot \frac{\partial \mathbf{x}_c}{\partial \tau^j} \right), \tag{4.27}$$

where $\mathbf{x}_\mathrm{T}$ is the projection of $\mathbf{x} - \mathbf{x}_c$ on the basis $\mathbf{e}_{i \le p}$. The form (4.26, 4.27) is the easiest to generalize to functional integrals.

The Faddeev–Popov method. An alternative method is to impose the conditions

$$C_i(\boldsymbol{\tau}) \equiv \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \big(\mathbf{x} - \mathbf{x}_c(\boldsymbol{\tau})\big) = 0\,,$$

which determine $\boldsymbol{\tau}$ as a function of $\mathbf{x}$. This can be achieved by introducing inside the integral (4.19) the identity

$$\int \prod_i \mathrm{d}\tau^i\, \delta\big(C_i(\boldsymbol{\tau})\big) \det\left(\frac{\partial C_j}{\partial \tau^k}\right) = 1\,.$$

Inside the integral we can then solve for $\mathbf{x}$ in terms of $\boldsymbol{\tau}$ by parametrizing $\mathbf{x}$ as in expression (4.21). We note that $(a > p)$

$$\mathbf{e}_a(\boldsymbol{\tau}) \cdot \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} = 0 \;\Rightarrow\; \frac{\partial \mathbf{e}_a(\boldsymbol{\tau})}{\partial \tau^j} \cdot \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} + \mathbf{e}_a(\boldsymbol{\tau}) \cdot \frac{\partial^2 \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i \partial \tau^j} = 0\,.$$

Thus,

$$\frac{\partial C_i}{\partial \tau^j} = -\frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \frac{\partial \mathbf{x}(\boldsymbol{\tau})}{\partial \tau^j}.$$

Finally,

$$\prod_i \delta\big(C_i(\boldsymbol{\tau})\big) = \delta^{(p)}(\mathbf{x}_{\mathrm{T}}) \det{}^{-1} \frac{\partial \mathbf{x}_c(\boldsymbol{\tau})}{\partial \tau^i} \cdot \mathbf{e}_j$$

and the preceding result in the form (4.26) is recovered.

Note that nowhere the explicit group structure has been used. Assuming $\boldsymbol{\tau} = 0$ belongs to the manifold G/H, there exists, therefore, elements $\mathbf{g}$ of G such that

$$\mathbf{x}_c(\boldsymbol{\tau}) = \mathbf{g}\mathbf{x}_c(0). \tag{4.28}$$

which leads to additional simplifications since the explicit dependence in $\boldsymbol{\tau}$ can then be eliminated.

Application to the $O(N)$ Jacobian. We consider the special example of a function S that depends only on $\mathbf{x}^2$. We assume that S has non-trivial saddle points of the form

$$\mathbf{x}_c = \mathbf{u}|\mathbf{x}_c| \text{ with } \mathbf{u}^2 = 1\,.$$

The groups G and H are thus $O(N)$ and $O(N-1)$, respectively. The coset space $O(N)/O(N-1)$ is isomorphic to the sphere S_{N-1}.

Then,

$$\frac{\partial \mathbf{x}_c}{\partial \tau^i} = |\mathbf{x}_c| \frac{\partial \mathbf{u}}{\partial \tau^i}$$

and $\mathbf{x}$ can be written as

$$\mathbf{x} = \mathbf{x}_c(\boldsymbol{\tau}) + r\mathbf{u}\,,$$

since $\mathbf{u}$ is the only vector orthogonal to all vectors $\partial \mathbf{x}_c/\partial \tau^i$. The projector (4.24) then becomes

$$\Pi_{\alpha\beta} = \delta_{\alpha\beta} - u^\alpha u^\beta, \tag{4.29}$$

and g_{ij} (defined in equation (4.25)) is the metric on the sphere S_{N-1} in the τ^i parametrization. The expression (4.27) reduces to

$$J = \det\left[(|\mathbf{x}_c| + r)\left(\frac{\partial \mathbf{u}}{\partial \tau^i} \cdot \frac{\partial \mathbf{u}}{\partial \tau^j}\right)\right] = \det\left[g_{ij}\left(|\mathbf{x}_c| + r\right)\right] = \left(|\mathbf{x}_c| + r\right)^{N-1} \det g_{ij}.$$

Thus the Jacobian of the change of variables $\mathbf{x} \mapsto \{\tau^i, r\}$ becomes

$$J = \left(|\mathbf{x}_c| + r\right)^{N-1} \det{}^{1/2} g_{ij}(\boldsymbol{\tau}).$$

We use invariance under rotation of the $\mathbf{x}$ integral to rotate the $\mathbf{e}_i$ basis to a fixed basis with $\mathbf{u} \mapsto (1, 0...)$ in terms of an orthonormal basis containing $\mathbf{u}$, calling x_1 the component on $\mathbf{u}$. We can then integrate over $\mathbf{u}$ and obtain the surface σ_N of the S_{N-1} sphere. We call x_1 the sum $|\mathbf{x}_c| + r$ and find

$$\mathcal{I} = \sigma_N \int \mathrm{d}^N x \, x_1^{N-1} \, \delta^{(N-1)}(\mathbf{x}_\mathrm{T}) \, \mathrm{e}^{-S(\mathbf{x})/g} = \sigma_N \int_0^\infty \mathrm{d}x_1 \, x_1^{N-1} \, \mathrm{e}^{-S(x_1)/g},$$

which is the result that one obtains by introducing immediately radial and angular variables.

4.5 Jacobian with $O(N)$ symmetry: Path integrals

The generalization of expressions (4.26, 4.27) is simple (in particular, because no specific group properties have been used). We denote by $\mathbf{q}(t)$, $t \in \mathbb{R}$, the N-component path over which one integrates. Scalar products of vectors are then replaced by space integrals and sums. The Jacobian can be written as [9]

$$\mathcal{J} = \det \mathbf{J}(\mathbf{q}) / \det{}^{1/2} \mathbf{J}(\mathbf{q}_c)\,, \tag{4.30}$$

where $\mathbf{q}_c$ is the instanton solution and $\mathbf{J}(\mathbf{q})$ the matrix with elements

$$J_{ij}(\mathbf{q}) = \int \mathrm{d}t \, \frac{\partial \mathbf{q}}{\partial \tau^i} \cdot \frac{\partial \mathbf{q}_c}{\partial \tau^j}. \tag{4.31}$$

4.5.1 Space translations

We first assume that $q(t)$ has one component and the instanton solution breaks only the symmetry of the action under space translations. Then, the function $J(q)$ in (4.31) reduces to the expression

$$J(q) = \int \mathrm{d}t \, \dot{q}(t) \dot{q}_c(t),$$

derived directly (equation (1.29)). Moreover, one integrates over all paths $q(t)$ with the constraint

$$\int \mathrm{d}t \big(q(t) - q_c(t)\big) \dot{q}_c(t) = 0\,.$$

Setting

$$q(t) = q_c(t) + r(t),$$

after an integration by parts one obtains (assuming the boundary terms cancel)

$$J(q) = J(q_c)\left[1 - \frac{1}{J(q_c)} \int \mathrm{d}t \, \ddot{q}_c(t) r(t)\right].$$

4.5.2 Path integrals: Space translations and $O(N)$ internal rotations

We now consider a path integral where the integrand is both invariant under space translations and internal $O(N)$ group transformations. Under rather general conditions, one can show that the instanton solution with minimal action can be factorized in the form

$$\mathbf{q}_c(t) = \mathbf{u}\, q_c(t + t_0), \tag{4.32}$$

where $\mathbf{u}$ is a time-independent unit vector: $\mathbf{u}^2 = 1$, a form that breaks both time translation and $O(N)$ invariance. The subgroup that leaves the vector $\mathbf{u}$ invariant is $O(N-1)$. As a variant with the notation of section 4.4.1, we denote by t_0 the collective coordinate corresponding to time translations and we restrict the notation $\boldsymbol{\tau} \equiv \{\tau^i\}$, $1 \le i \le N-1$, to the collective coordinates parametrizing the sphere $O(N)/O(N-1) \equiv S_{N-1}$. We further assume that $\mathbf{q}_c(t) \to 0$ when $|t| \to \infty$.

We then set

$$\mathbf{q}(t) = q_{\mathrm{L}}(t + t_0)\mathbf{u}(\boldsymbol{\tau}) + \mathbf{q}_{\mathrm{T}}(t + t_0), \tag{4.33}$$

where

$$\mathbf{u} \cdot \mathbf{q}_{\mathrm{T}}(t) = 0\,. \tag{4.34}$$

We now express the conditions that the zero-modes should be omitted. Translation invariance yields

$$\int \mathrm{d}t\, \dot{q}_c(t)\bigl(q_{\mathrm{L}}(t) - q_c(t)\bigr) = \int \mathrm{d}t\, \dot{q}_c(t) q_{\mathrm{L}}(t) = 0\,. \tag{4.35}$$

The second condition coming from $O(N)$ transformations reads

$$\int \mathrm{d}t\, q_c(t) \frac{\partial \mathbf{u}}{\partial \tau^i} \cdot \mathbf{q}_{\mathrm{T}}(t) = 0\,.$$

The $(N-1)$ vectors $\partial \mathbf{u}/\partial \tau_i$ span the space orthogonal to $\mathbf{u}$ and, thus, the latter condition is equivalent to

$$\int \mathrm{d}t\, q_c(t) \mathbf{q}_{\mathrm{T}}(t) = 0\,. \tag{4.36}$$

More explicit form of the Jacobian. The matrix $\mathbf{J}(\mathbf{q})$ introduced in equation (4.30) can now be written as

$$\mathbf{J}(\mathbf{q}) = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}, \tag{4.37}$$

where $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ are submatrices with elements

$$A_{ij} = \int \mathrm{d}t\, \frac{\partial \mathbf{q}(t)}{\partial \tau^i} \cdot \frac{\partial \mathbf{q}_c(t)}{\partial \tau^j}\,, \quad B_j = \int \mathrm{d}t\, \frac{\partial \mathbf{q}(t)}{\partial t_0} \cdot \frac{\partial \mathbf{q}_c(t)}{\partial \tau^j}\,,$$
$$C_i = \int \mathrm{d}t\, \frac{\partial \mathbf{q}(t)}{\partial \tau^i} \cdot \frac{\partial \mathbf{q}_c(t)}{\partial t_0}\,, \qquad D = \int \mathrm{d}t\, \frac{\partial \mathbf{q}(t)}{\partial t_0} \cdot \frac{\partial \mathbf{q}_c(t)}{\partial t_0},$$

where the derivatives with respect to t_0 and τ^i refer to the parametrization (4.33).

Introducing the parametrization (4.33), we obtain

$$\frac{\partial \mathbf{q}}{\partial t_0} = \dot{\mathbf{q}}(t) = \dot{q}_{\mathrm{L}}(t+t_0)\mathbf{u} + \dot{\mathbf{q}}_{\mathrm{T}}(t+t_0), \quad \frac{\partial \mathbf{q}}{\partial \tau^i} = q_{\mathrm{L}}(t+t_0)\frac{\partial \mathbf{u}}{\partial \tau^i} + \frac{\partial \mathbf{q}_{\mathrm{T}}(t+t_0)}{\partial \tau^i},$$

as well as

$$\frac{\partial \mathbf{q}_c}{\partial t_0} = \dot{\mathbf{q}}_c(t) = \mathbf{u}\dot{q}_c(t+t_0), \quad \frac{\partial \mathbf{q}_c}{\partial \tau^i} = \frac{\partial \mathbf{u}}{\partial \tau^i} q_c(t+t_0).$$

We now calculate the various contributions relevant for expression (4.37). First,

$$D = \int \mathrm{d}t\, \dot{\mathbf{q}}(t) \cdot \dot{\mathbf{q}}_c(t) = \int \mathrm{d}t\, \dot{q}_{\mathrm{L}}(t)\dot{q}_c(t).$$

Also,

$$B_i = \int \mathrm{d}t\, \dot{\mathbf{q}}(t) \cdot \frac{\partial \mathbf{q}_c(t)}{\partial \tau^i} = \frac{\partial \mathbf{u}}{\partial \tau^i} \cdot \int \mathrm{d}t\, \dot{\mathbf{q}}_{\mathrm{T}}(t) q_c(t),$$
$$C_i = \int \mathrm{d}t\, \dot{\mathbf{q}}_c(t) \cdot \frac{\partial \mathbf{q}(t)}{\partial \tau^i} = \mathbf{u} \cdot \int \mathrm{d}t\, \dot{q}_c(t) \frac{\partial \mathbf{q}_{\mathrm{T}}(t)}{\partial \tau^i}.$$

Integrating by parts, we obtain

$$B_i = -\frac{\partial \mathbf{u}}{\partial \tau^i} \cdot \int \mathrm{d}t\, \mathbf{q}_{\mathrm{T}}(t)\dot{q}_c(t).$$

From equation (4.34), we derive

$$\mathbf{u} \cdot \frac{\partial \mathbf{q}_{\mathrm{T}}(t)}{\partial \tau^i} + \frac{\partial \mathbf{u}}{\partial \tau^i} \cdot \mathbf{q}_{\mathrm{T}}(t) = 0\,.$$

Thus,

$$C_i = -\frac{\partial \mathbf{u}}{\partial \tau^i} \cdot \int \mathrm{d}t\, \dot{q}_c(t)\mathbf{q}_{\mathrm{T}}(t).$$

Finally,

$$\begin{aligned} A_{ij} &= \int \mathrm{d}t\, \frac{\partial \mathbf{q}(t)}{\partial \tau^i} \cdot \frac{\partial \mathbf{q}_c(t)}{\partial \tau^j} = \frac{\partial \mathbf{u}}{\mathrm{d}\tau^j} \cdot \int \mathrm{d}t\, q_c(t) \left(\frac{\partial \mathbf{u}}{\mathrm{d}\tau^i} q_{\mathrm{L}}(t) + \frac{\partial \mathbf{q}_{\mathrm{T}}}{\partial \tau^i} \right) \\ &= g_{ij} \int \mathrm{d}t\, q_{\mathrm{L}}(t) q_c(t) + \frac{\partial \mathbf{u}}{\mathrm{d}\tau^j} \cdot \int \mathrm{d}t\, q_c(t) \frac{\partial \mathbf{q}_{\mathrm{T}}}{\partial \tau^i}, \end{aligned} \tag{4.38}$$

where we have introduced the metric (4.25) on S_{N-1}:

$$g_{ij} = \frac{\partial \mathbf{u}}{\mathrm{d}\tau^i} \cdot \frac{\partial \mathbf{u}}{\mathrm{d}\tau^j}\,.$$

Then, differentiating the condition (4.36) with respect to τ_i, we find that the second term in (4.38) vanishes. The matrix $\mathbf{A}$ reduces to

$$A_{ij} = g_{ij} \int \mathrm{d}t\, q_{\mathrm{L}}(t) q_c(t).$$

We use the general identity

$$\det \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} = \det \mathbf{A} \det \left(\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B}\right), \tag{4.39}$$

valid for all submatrices. We introduce the inverse g^{ij} of the metric tensor: $\sum_k g_{ik} g^{kj} = \delta_i^j$. We need

$$\begin{aligned} \mathbf{C}\mathbf{A}^{-1}\mathbf{B} = {} & \left(\int \mathrm{d}t\, q_{\mathrm{L}}(t) q_c(t)\right)^{-1} \\ & \times \int \mathrm{d}t\, \mathrm{d}t' \sum_{i,j} \frac{\partial \mathbf{u}}{\partial \tau^i} \cdot \mathbf{q}_{\mathrm{T}}(t) \dot{q}_c(t) g^{ij} \frac{\partial \mathbf{u}}{\partial \tau^j} \cdot \mathbf{q}_{\mathrm{T}}(t') \dot{q}_c(t'). \end{aligned}$$

The expression involves the symmetric matrix

$$\Pi_{\alpha\beta} = \sum_{i,j} \frac{\partial u_\alpha}{\partial \tau^i} g^{ij} \frac{\partial u_\beta}{\partial \tau^j},$$

which is given by equation (4.29):

$$\Pi_{\alpha\beta} = \delta_{\alpha\beta} - u_\alpha u_\beta\,.$$

It follows

$$\mathbf{C}\mathbf{A}^{-1}\mathbf{B} = \left(\int \mathrm{d}t\, q_{\mathrm{L}}(t) q_c(t)\right)^{-1} \int \mathrm{d}t\, \mathrm{d}t'\, q_c(t) q_c(t') \dot{\mathbf{q}}_{\mathrm{T}}(t) \cdot \dot{\mathbf{q}}_{\mathrm{T}}(t').$$

Also

$$\det \mathbf{A} = \det g_{ij} \left[\int \mathrm{d}t\, q_{\mathrm{L}}(t) q_c(t)\right]^{N-1}.$$

We conclude

$$\begin{aligned} \det \mathbf{J}(\mathbf{q}) = \det g_{ij} & \left[\int \mathrm{d}t\, \mathbf{q}(t) \cdot \mathbf{q}_c(t)\right]^{N-2} \int \mathrm{d}t\, \mathrm{d}t' \, [\dot{\mathbf{q}}(t) \cdot \dot{\mathbf{q}}_c(t) \mathbf{q}(t') \cdot \mathbf{q}_c(t') \\ & - \dot{q}_c(t) \dot{q}_c(t') \mathbf{q}_{\mathrm{T}}(t) \cdot \mathbf{q}_{\mathrm{T}}(t')]\,. \end{aligned} \tag{4.40}$$

The complete Jacobian then is

$$\begin{aligned} \mathcal{J} = (\det g_{ij})^{1/2} & \left[\int \mathrm{d}t\, \mathbf{q}_c^2(t)\right]^{(1-N)/2} \left[\int \mathrm{d}t\, \dot{\mathbf{q}}_c^2(t)\right]^{-1/2} \left[\int \mathrm{d}t\, \mathbf{q}(t) \cdot \mathbf{q}_c(t)\right]^{N-2} \\ & \times \int \mathrm{d}t\, \mathrm{d}t' \, [\dot{\mathbf{q}}(t) \cdot \dot{\mathbf{q}}_c(t) \mathbf{q}(t') \cdot \mathbf{q}_c(t') - \dot{q}_c(t) \dot{q}_c(t') \mathbf{q}_{\mathrm{T}}(t) \cdot \mathbf{q}_{\mathrm{T}}(t')]\,. \end{aligned} \tag{4.41}$$

Using the first condition (4.35), one can also rewrite this expression as [9]

$$\mathcal{J} = (\det g_{ij})^{1/2} \left[\int \mathrm{d}t\, \mathbf{q}_c^2(t)\right]^{(1-N)/2} \left[\int \mathrm{d}t\, \dot{\mathbf{q}}_c^2(t)\right]^{-1/2} \left[\int \mathrm{d}t\, \mathbf{q}(t)\cdot\mathbf{q}_c(t)\right]^{N-2}$$
$$\times \int \mathrm{d}t\, \mathrm{d}t' \left[\dot{\mathbf{q}}(t)\cdot\dot{\mathbf{q}}_c(t)\mathbf{q}(t')\cdot\mathbf{q}_c(t') + \dot{\mathbf{q}}_c(t)\cdot\mathbf{q}_c(t')\mathbf{q}(t)\cdot\dot{\mathbf{q}}(t')\right]. \qquad (4.42)$$

In the case of the partition function, we can integrate explicitly over t_0 and τ^i after a translation and an $O(N)$ rotation and find a factor $\beta\sigma_N$, where β is the time interval and σ_N the surface of S_{N-1}.

Note that this expression factorizes into a Jacobian for translations and a Jacobian for $O(N)$ rotations only at leading order.

4.6 Jacobian with $O(N)$ symmetry: Field integrals

We denote by $\boldsymbol{\phi}(x)$, $x \in \mathbb{R}^d$, $d > 1$, the N-component field over which one integrates. Scalar products of vectors are then replaced by space integrals and sums. The Jacobian then reads [10]

$$\mathcal{J} = \det \mathbf{J}(\boldsymbol{\phi}) / \left(\det \mathbf{J}(\boldsymbol{\phi}_c)\right)^{1/2}, \qquad (4.43)$$

where $\mathbf{J}(\boldsymbol{\phi})$ is the matrix with elements

$$J_{ij}(\boldsymbol{\phi}) = \int \mathrm{d}^d x \frac{\partial \boldsymbol{\phi}}{\partial \tau^i}\cdot\frac{\partial \boldsymbol{\phi}_c}{\partial \tau^j}.$$

Space translations. If the scalar field $\phi(x)$ has only one component, the instanton solution only breaks the space translation symmetry of the action and vanishes at large distance. Then, the Jacobian (4.43) involves the determinant of a $d \times d$ matrix $\mathbf{J}$ with elements

$$J_{\mu\nu}(\phi) = \int \mathrm{d}^d x\, \partial_\mu \phi_c(x) \partial_\nu \phi(x). \qquad (4.44)$$

Space translations and $O(N)$ rotations. We now assume that we integrate over an N-component field $\boldsymbol{\phi}(x)$, $x \in \mathbb{R}^d$ with an integrand that has both space-translation and $O(N)$ rotation invariance. We also assume that the solution breaks both symmetries of the action and can be written as

$$\boldsymbol{\phi}_c(x) = \mathbf{u}\, \phi_c(x + x_0),$$

where the unit vector $\mathbf{u}$ and $\mathbf{x}_0$ are constants (this is in general the case for the minimal action solution). We choose as collective coordinates the unit vector $\mathbf{u}$, in some parametrization τ^i, $1 \le i < N$, and the d-component vector $\mathbf{x}_0$. The calculation follows the same lines as in the path integral example.

We parametrize the field in the form

$$\boldsymbol{\phi}(x) = \phi_{\mathrm{L}}(x+x_0)\mathbf{u} + \boldsymbol{\phi}_{\mathrm{T}}(x+x_0),$$

where

$$\mathbf{u}\cdot\boldsymbol{\phi}_{\mathrm{T}}(x) = 0$$

and (zero-mode conditions)

$$\int \mathrm{d}^d x\,\partial_\mu \phi_c(x)\,[\phi_{\mathrm{L}}(x)-\phi_c(x)] = 0\,, \qquad (4.45a)$$

$$\int \mathrm{d}^d x\,\phi_c(x)\boldsymbol{\phi}_{\mathrm{T}}(x) = 0\,. \qquad (4.45b)$$

The calculation of the determinant involves the $d\times d$ matrix $\mathbf{D}$ (immediate generalization of expression (4.44)) with elements

$$D_{\mu\nu}(\boldsymbol{\phi}) = \int \mathrm{d}^d x\,\partial_\mu \boldsymbol{\phi}_c(x)\cdot\partial_\nu\boldsymbol{\phi}(x) = \int \mathrm{d}^d x\,\partial_\mu\phi_c(x)\partial_\nu\phi_{\mathrm{L}}(x). \qquad (4.46)$$

Then,

$$\partial_\mu\boldsymbol{\phi}_c(x) = \mathbf{u}\,\partial_\mu\phi_c(x), \qquad \frac{\partial\boldsymbol{\phi}_c(x)}{\partial\tau^i} = \frac{\partial\mathbf{u}}{\partial\tau^i}\phi_c(x).$$

We infer

$$\begin{aligned}
B_{i\mu} &= \int \mathrm{d}^d x\,\partial_\mu\boldsymbol{\phi}(x)\cdot\frac{\partial\boldsymbol{\phi}_c(x)}{\partial\tau^i} = \frac{\partial\mathbf{u}}{\partial\tau^i}\cdot\int \mathrm{d}^d x\,\phi_c(x)\partial_\mu\boldsymbol{\phi}_{\mathrm{T}}(x)\\
&= -\frac{\partial\mathbf{u}}{\partial\tau^i}\cdot\int \mathrm{d}^d x\,\partial_\mu\phi_c(x)\boldsymbol{\phi}_{\mathrm{T}}(x)\\
C_{\mu i} &= \int \mathrm{d}^d x\,\partial_\mu\boldsymbol{\phi}_c(x)\cdot\frac{\partial\boldsymbol{\phi}(x)}{\partial\tau^i} = \mathbf{u}\cdot\int \mathrm{d}^d x\,\partial_\mu\phi_c(x)\frac{\partial\boldsymbol{\phi}_{\mathrm{T}}(x)}{\partial\tau^i}\\
&= -\frac{\partial\mathbf{u}}{\partial\tau^i}\cdot\int \mathrm{d}^d x\,\partial_\mu\phi_c(x)\boldsymbol{\phi}_{\mathrm{T}}(x).
\end{aligned}$$

Finally, as in the path integral example,

$$A_{ij} = \int \mathrm{d}^d x\,\frac{\partial\boldsymbol{\phi}_c(x)}{\partial\tau^i}\cdot\frac{\partial\boldsymbol{\phi}(x)}{\partial\tau^j} = g_{ij}\int \mathrm{d}^d x\,\phi_c(x)\phi_{\mathrm{L}}(x),$$

where the derivative of the condition (4.45b) has been used.

As before, we use the rule (4.39) of expanding determinant by blocks, identifying one block with g_{ij}. We need the $d\times d$ matrix

$$\begin{aligned}
E_{\mu\nu} &= \left(\mathbf{C}\mathbf{A}^{-1}\mathbf{B}\right)_{\mu\nu}\\
&= \left(\int \mathrm{d}^d x\,\phi_c(x)\phi_{\mathrm{L}}(x)\right)^{-1}\int \mathrm{d}^d x\,\mathrm{d}^d x'\,\partial_\mu\phi_c(x)\partial_\nu\phi_c(x')\boldsymbol{\phi}_{\mathrm{T}}(x)\cdot\boldsymbol{\phi}_{\mathrm{T}}(x').
\end{aligned}$$

We finally obtain [10]

$$\mathbf{J}(\boldsymbol{\phi}) = \det g_{ij} \left(\int \mathrm{d}^d x \, \phi_c(x) \phi_{\mathrm{L}}(x) \right)^{N-d-1} \det I_{\mu\nu}$$

with

$$\begin{aligned} I_{\mu\nu}(\boldsymbol{\phi}) = \int \mathrm{d}^d x \, \mathrm{d}^d x' \, [&\partial_\mu \boldsymbol{\phi}_c(x) \cdot \partial_\nu \boldsymbol{\phi}(x) \phi_c(x') \phi_{\mathrm{L}}(x') \\ &- \partial_\mu \phi_c(x) \partial_\nu \phi_c(x') \boldsymbol{\phi}_{\mathrm{T}}(x) \cdot \boldsymbol{\phi}_{\mathrm{T}}(x')] \, . \end{aligned} \qquad (4.47)$$

The Jacobian follows:

$$\mathcal{J} = \mathbf{J}(\boldsymbol{\phi}) / \mathbf{J}^{1/2}(\boldsymbol{\phi}_c).$$

In the case of the partition function, the integration over collective coordinates yields the product of the surface of the S_{N-1} sphere and the space (or space-time) volume.

Chapter 5

The ϕ^4 Field Theory in Dimension 4

For the ϕ^4 field theory four dimensions is special because the theory is just renormalizable. Moreover, one discovers that only the massless field equations have instanton solutions. This leads to a set of new problems which we now examine. We first consider the massless theory which is simpler, although it has some subtle IR problems. A technical advantage is that the classical theory is conformal invariant and the instanton solution can be found explicitly. Note that the barrier penetration is somewhat peculiar since it is not generated by the potential but only by the kinetic term of the action.

We explain the leading order calculation of instanton contribution for the one-component ϕ^4 theory, but the extension to the $O(N)$ symmetric model is simple, and explicit expressions can be found in the literature [16],[17].

The Euclidean action of the massless theory ϕ^4 theory in the tree approximation can be written as

$$\mathcal{S}(\phi) = \int \mathrm{d}^4 x \left[\tfrac{1}{2}\left(\nabla_x \phi(x)\right)^2 + \tfrac{1}{4} g \phi^4(x)\right], \tag{5.1}$$

and the corresponding field equation reads:

$$-\nabla^2 \phi(x) + g\phi^3(x) = 0\,. \tag{5.2}$$

Note the unconventional normalization of the coupling constant. To return to the usual convention one has to substitute $g \mapsto g/6$.

We know that the solution of minimal action is spherically symmetric, thus we set (g is negative)

$$\phi(x) = \frac{1}{\sqrt{-g}} f(r) \tag{5.3}$$

with

$$r = |x - x_0|\,. \tag{5.4}$$

We then obtain the non-linear differential equation

$$-\left[\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2 + \frac{3}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right] f(r) = f^3(r). \tag{5.5}$$

We now use the scale invariance of the classical theory (the theory is actually conformal invariant). If $\phi(x)$ is the solution to the equation, then $\psi(x)$ is also a solution with

$$\phi(x) = \lambda\psi(\lambda x). \tag{5.6}$$

This suggests the changes

$$f(r) = \mathrm{e}^{-t}\, h(t), \qquad r = \mathrm{e}^{t}\,, \tag{5.7}$$

which transform equation (5.5) into

$$\ddot{h}(t) = h(t) - h^3(t). \tag{5.8}$$

We recognize the equation of motion of the anharmonic oscillator that we have solved in chapter 1:

$$h_c(t) = \pm\frac{\sqrt{2}}{\cosh(t - t_0)}. \tag{5.9}$$

The solution $\phi_c(x)$ of equation (5.2) then is

$$f(r) = \pm\frac{2\sqrt{2}\lambda}{1 + \lambda^2 r^2}, \tag{5.10a}$$

$$\Rightarrow \phi_c(x) = \pm\frac{1}{\sqrt{-g}}\frac{2\sqrt{2}\lambda}{1 + \lambda^2\,(x - x_0)^2}, \tag{5.10b}$$

where we have defined $\lambda = \mathrm{e}^{-t_0}$. The value of corresponding classical action is

$$\mathcal{S}(\phi_c) = -A/g\,, \qquad A = 8\pi^2/3\,. \tag{5.11}$$

With the standard normalization of g one finds $A = 16\pi^2$.

Because the classical theory is scale invariant, the instanton solution now depends on a scale parameter λ, in addition to the four translation parameters $x_{0\mu}$. Therefore, to calculate the instanton contribution we must introduce a fifth collective coordinates.

5.1 Instanton contributions at leading order

The general strategy. The second derivative $M(x,x')$ of the action at the saddle point is

$$M(x,x') = \frac{\delta^2\mathcal{S}}{\delta\phi_c(x)\delta\phi_c(x')} = \left[-\nabla^2 - \frac{24\lambda^2}{(1+\lambda^2 x^2)^2}\right]\delta^{(4)}(x - x'). \tag{5.12}$$

To find the eigenvalues the operator of $\mathbf{M}$, one has to solve a 4-dimensional Schrödinger equation with a spherically symmetric potential. We immediately note at this stage two serious problems. The operator $\mathbf{M}$ has, as expected, five eigenvectors, $\partial_\mu \phi_c(x)$ and $(\mathrm{d}/\mathrm{d}\lambda)\phi_c(x)$, with eigenvalue zero, but the last of these eigenvectors is not normalizable with the natural measure of the problem,

$$\int \left[\frac{\mathrm{d}}{\mathrm{d}\lambda}\phi_c(x)\right]^2 \mathrm{d}^4 x = \infty\,. \tag{5.13}$$

This is an IR problem which arises because the theory is massless.

Another difficulty comes from the mass counter-term which has to be added to the action. It has the form:

$$\tfrac{1}{2}\delta m_0^2 \int \mathrm{d}^4 x\, \phi_c^2(x) = \infty\,. \tag{5.14}$$

The integral of $\phi_c^2(x)$ is also IR divergent, and this IR divergence is expected to cancel with an IR divergence of $\det \mathbf{M}$. Thus we need in general some kind of IR regularization. In the particular case of the dimensional regularization, this problem is postponed to two-loop order.

These problems will be solved in several steps. First we realize that we do not need the eigenvalues of $\mathbf{M}$ but only the determinant $\det' \mathbf{M}\mathbf{M}_0^{-1}$ (equations (3.57)). We can multiply $\mathbf{M}$ and $\mathbf{M_0}$ by the same operator. A specific choice that makes full use of the scale invariance of the classical theory, then transforms $\mathbf{M}$ into an operator whose eigenvalues can be calculated analytically. Because the calculations are somewhat tedious, we indicate here only the various steps, without giving all details.

The transformation. We extend the transformation (5.7) to arbitrary fields, setting:

$$\phi(x) = \mathrm{e}^{-t}\, h(t,\hat{n}) \qquad \text{with} \quad t = \ln|x|, \qquad \hat{n}_n = \frac{x^\mu}{|x|}\,. \tag{5.15}$$

The classical action then becomes

$$\mathcal{S}(\phi) = \tilde{\mathcal{S}}(h) = \int \mathrm{d}t\, \mathrm{d}\Omega \left[\frac{1}{2}\left(\dot{h} - h\right)^2 + h\mathbf{L}^2 h + \frac{1}{4} g h^4\right]. \tag{5.16}$$

The symbol $\int \mathrm{d}\Omega$ means integration over the angular variables $\hat{n}$, and $\mathbf{L}^2$ is the square of the angular momentum operator with eigenvalues $l(l+2)$ and degeneracy $(l+1)^2$. The expression (5.16) can be rewritten

$$\tilde{\mathcal{S}}(h) = \int \mathrm{d}t\, \mathrm{d}\Omega \left\{\frac{1}{2}\left[\dot{h}^2 + h\left(\mathbf{L}^2 + 1\right)h\right] + \frac{1}{4} g h^4\right\}. \tag{5.17}$$

The integral of $\dot{h}h$ vanishes due to boundary conditions.

With the parametrization

$$\lambda = \mathrm{e}^{-t_0}, \qquad \mathbf{x}_0 = \mathrm{e}^{t_0}\,\mathbf{v}\,,$$

the classical solution (5.10*b*) transforms into $h_c(t)$:

$$\sqrt{-g}\,h_c(t) = \frac{\pm 2\sqrt{2}}{\mathrm{e}^{(t-t_0)} - 2\mathbf{v}\cdot\mathbf{n} + \mathrm{e}^{-(t-t_0)}(\mathbf{v}^2+1)}\,. \tag{5.18}$$

We note that in these new variables translations take a complicated form, unlike dilatation which simply corresponds to a translation of the variable t.

The second derivative of the classical action at the saddle point now takes the form (for $t_0 = x_{0\mu} = 0$)

$$\mathbf{M} = \frac{\delta^2 \mathcal{S}}{\delta h_c \delta h_c} = -\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + \mathbf{L}^2 + 1 - \frac{6}{\cosh^2 t}. \tag{5.19}$$

The natural measure associated to this Hamiltonian problem is

$$\int \mathrm{d}t \, \mathrm{d}\Omega \,,$$

which in the original language means

$$\int \frac{\mathrm{d}^4 x}{\mathbf{x}^2}.$$

This measure is not translation invariant, and thus the Jacobian resulting from the introduction of collective coordinates, and the determinant depend individually on $x_{0\mu}$. However, the product of the corresponding contributions to the final result should not, thus we perform the calculation for $x_{0\mu} = 0$.

5.1.1 The Jacobian

With the new measure $\mathrm{d}\phi_c / \mathrm{d}\lambda$ is normalizable:

$$J_1 = \left[\int \frac{\mathrm{d}^4 x}{\mathbf{x}^2} \left(\frac{\mathrm{d}}{\mathrm{d}\lambda}\phi_c(x)\right)^2\right]^{1/2}, \tag{5.20}$$

$$= \left[\frac{16\pi^2}{(-g)} \int_0^\infty r \mathrm{d}r \frac{\left(1-\lambda^2 r^2\right)^2}{(1+\lambda^2 r^2)^4}\right]^{1/2}. \tag{5.21}$$

This leads to a first Jacobian factor:

$$J_1 = \frac{1}{\lambda}\sqrt{\frac{8}{3}} \frac{\pi}{\sqrt{-g}}\,. \tag{5.22}$$

The second Jacobian J_2 comes from the collective coordinates $x_{0\mu}$:

$$J_2 = \left[\frac{1}{4} \int \frac{\mathrm{d}^4 x}{\mathbf{x}^2} \sum_{\mu=1}^{4} \left(\partial_\mu \phi_c\right)^2\right]^2, \tag{5.23}$$

$$= \frac{1}{g^2}\left[16\pi^2 \int_0^\infty \frac{r^3 \mathrm{d}r \lambda^6}{\left(1+\lambda^2 r^2\right)^4}\right]^2 = \frac{\lambda^4}{g^2} \times \frac{16}{9}\pi^4. \tag{5.24}$$

The complete Jacobian J is thus

$$J = J_1 J_2 = \frac{\lambda^3}{(-g)^{5/2}} \pi^5 \times \frac{32\sqrt{2}}{9\sqrt{3}}\,. \tag{5.25}$$

5.1.2 The determinant

For each value l of the angular momentum, the operator $\mathbf{M}$ is the form of a Hamiltonian corresponding to a Bargman potential:

$$M_l = -\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + (1+l)^2 - \frac{6}{\cosh^2 t} \tag{5.26}$$

and the determinant can be calculated explicitly. One finds

$$\det\left(M_l+\varepsilon\right)\left(M_{0l}+\varepsilon\right)^{-1} = \frac{\sqrt{\varepsilon+(l+1)^2}-1}{\sqrt{\varepsilon+(l+1)^2}+2}\,\frac{\sqrt{\varepsilon+(l+1)^2}-2}{\sqrt{\varepsilon+(l+1)^2}+1]}, \tag{5.27}$$

in which M_{0l} is the operator of the corresponding free theory. As we know, this determinant is UV divergent and we have to renormalize it. However, let us first calculate formally the unrenormalized determinant:

$$l \ge 2: \qquad \det M_l M_{0l}^{-1} = \frac{l(l-1)}{(l+2)(l+3)}, \tag{5.28}$$

$$l = 1: \qquad \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\det\left(M_1+\varepsilon\right)\left(M_{01}+\varepsilon\right)^{-1} = \frac{1}{48}, \tag{5.29}$$

$$l = 0: \qquad \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\det\left(M_{l=0}+\varepsilon\right)\left(M_{0l=0}+\varepsilon\right)^{-1} = -\frac{1}{12}. \tag{5.30}$$

As expected the determinant is negative and we obtain the formal expression

$$\det{}' \mathbf{M}\mathbf{M}_0^{-1} = -\frac{1}{12}\times\left(\frac{1}{48}\right)^4 \times \prod_{l=2}^{\infty}\left[\frac{l(l-1)}{(l+2)(l+3)}\right]^{(l+1)^2}. \tag{5.31}$$

Renormalization. In these variables, the UV divergences appear as divergences of the infinite product on l. We thus use in an intermediate step a maximum value L of l as a cut-off. From the general analysis one knows the UV divergent part of $\ln\det\mathbf{M}$ is completely contained in the two first terms of the expansion in powers of ϕ_c^2. Therefore, one can proceed in the following way: the determinant of the operator $\mathbf{M}(s)$,

$$\mathbf{M}(s) = -\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 - \frac{s(s+1)}{\cosh^2 t}\,, \tag{5.32}$$

is exactly known

$$\det\left[\mathbf{M}(s)+z\right]\left[\mathbf{M}_0+z\right]^{-1} = \frac{\Gamma(1+\sqrt{z})\Gamma(\sqrt{z})}{\Gamma(1+s+\sqrt{z})\Gamma(\sqrt{z}-s)}. \tag{5.33}$$

Setting:

$$s(s+1) = 6\gamma\,, \tag{5.34}$$

one expands $\ln\det \mathbf{M}(s)$ in powers of γ. One deduces from this expansion, the expansion up to second order of $\ln\det\mathbf{M}$ in powers of the potential $-6/\cosh^2 t$ in the representation (5.27). One then subtracts these two terms from $\ln\det\mathbf{M}$ as obtained from the representation (5.31). One then verifies that indeed the large L limit of the subtracted quantity:

$$\left\{\det{}' \mathbf{M}\mathbf{M}_0^{-1}\right\}_{\text{ren}}^{-1/2} = \lim_{L\to+\infty} i2\sqrt{3}\times(48)^2 \prod_{l=2}^{L}\left[\frac{(l+2)(l+3)}{(l-1)}\right]^{(l+1)^2/2} \prod_{l=0}^{L} \mathrm{e}^{-3(l+1)} \times \prod_{l=0}^{L} \mathrm{e}^{-18(l+1)^2}\left[\sum_{k=l+1}^{\infty}\frac{1}{k^2}-\frac{1}{l+1}-\frac{1}{2(l+1)^2}\right], \tag{5.35}$$

is finite. We set:

$$\left\{\det{}' \mathbf{M}\mathbf{M}_0^{-1}\right\}_{\text{ren}}^{-1/2} = iC_1\,. \tag{5.36}$$

Taking into account the Jacobians, the factor $(2\pi)^{-1/2}$ for each collective mode, the factor $(2i)^{-1}$ and a factor two for the two saddle points, we get a first factor C_2 of the form

$$C_2 = \frac{\lambda^3}{(-g)^{5/2}}\times\pi^5\times\frac{32\sqrt{2}}{9\sqrt{3}}\times\frac{C_1}{(2\pi)^{5/2}}, \tag{5.37}$$

which we write as

$$C_2 = C_3\lambda^3/(-g)^{5/2}\,. \tag{5.38}$$

We then have to add to the classical action the two terms we have subtracted above from $\ln\det\mathbf{M}$. However, we can now write them in the normal space representation, regularized as we have regularized the perturbative correlation functions, and take into account the one-loop counter-terms. The first term in the expansion in powers of ϕ_c^2 is exactly cancelled by the mass counter-term, as we have already discussed. The second term in the expansion, which is the one-loop contribution to the four-point function, is logarithmically divergent. In the next section we calculate explicitly the finite difference between this term and the coupling constant counter-term which cancels the divergence.

5.2 Coupling constant renormalization

The terms we want to calculate involve the renormalized four-point function. We have to choose a renormalization scheme: we assume, therefore, that we have renormalized the field theory by minimal subtraction after dimensional regularization. The renormalization constants can be easily calculated. Notice the different normalization of the coupling constant. The contribution $\delta\mathcal{S}_2$ which we have to add to the action, coming from the subtraction of $\ln\det\mathbf{M}$ and the one-loop coupling renormalization constant, is

$$\delta\mathcal{S}_2 = \frac{9}{4}\frac{N_d}{\varepsilon}g^2\int\phi_c^4(x)\mathrm{d}^4x - \frac{9}{4}g^2\,\mathrm{tr}\left[\phi_c^2\left(-\nabla^2\right)^{-1}\phi_c^2\left(-\nabla^2\right)^{-1}\right], \tag{5.39}$$

in which N_d is the usual loop factor,

$$N_d = 2(4\pi)^{-d/2}/\Gamma(d/2)\,. \tag{5.40}$$

and $d = 4 - \varepsilon$. The expression can be rewritten as

$$\begin{aligned}\delta\mathcal{S}_2 = -\frac{9}{4}g^2 \int \mathrm{d}^4x\,\mathrm{d}^4y\,\frac{\mathrm{d}^4p}{(2\pi)^4}\,\mathrm{e}^{ip(x-y)}\,\phi_c^2(x)\phi_c^2(y) \\ \times \lim_{d\to 4}\left(\int \frac{\mathrm{d}^dq}{(2\pi)^d}\frac{\mu^\varepsilon}{q^2(p-q)^2} - \frac{N_d}{\varepsilon}\right),\end{aligned} \tag{5.41}$$

in which μ is the renormalization scale. The integral over $\mathbf{q}$ yields

$$\int \frac{\mathrm{d}^dq}{(2\pi)^d}\frac{1}{q^2(p-q)^2} - \frac{N_d}{\varepsilon} = \frac{1}{8\pi^2}\left(\frac{1}{2} - \ln p\right) + O(\varepsilon)\,. \tag{5.42}$$

We also introduce the Fourier transform of the function $f^2(r)$ ($f(r)$ is given by equation (5.10a)):

$$v(p) = \frac{1}{(2\pi)^4}\int \mathrm{d}^4x\frac{8\,\mathrm{e}^{ipx}}{(1+x^2)^2}. \tag{5.43}$$

The solution $\phi_c(x)$ depends on the scale λ. Rescaling the variables x, y, and p, we can then write the total expression more explicitly:

$$\delta\mathcal{S}_2 = -\frac{9\pi^2}{2}\int \mathrm{d}^4p\,v^2(p)\left[\tfrac{1}{2} - \ln(\lambda p/\mu)\right]. \tag{5.44}$$

From the definition of $v(p)$ we deduce after a short calculation:

$$\int \mathrm{d}^4p\,v^2(p) = \frac{2}{(3\pi^2)}, \tag{5.45}$$

$$\int \mathrm{d}^4p\,\ln p\,v^2(p) = \frac{2}{3\pi^2}\left(\ln 2 + \gamma + \frac{1}{6}\right), \tag{5.46}$$

in which γ is Euler's constant: $\gamma = -\psi(1) = 0.577215\ldots$. We then obtain

$$\delta\mathcal{S}_2 = 3\ln\lambda/\mu - \ln C_4 \tag{5.47}$$

with

$$\ln C_4 = 1 - 3\ln 2 - 3\gamma\,. \tag{5.48}$$

We note that the right hand side of equation (5.47) now depends on the scale parameter λ. The interpretation of this result is the following: the coupling constant renormalization breaks the scale invariance of the classical theory, and, therefore, the scale parameter λ remains in the expression. Moreover, the term proportional to $\ln\lambda$ together with the contribution from the classical action can be rewritten as

$$\frac{8\pi^2}{3g} - 3\ln\lambda/\mu = \frac{8\pi^2}{3g(\lambda)} + O(g)\,, \tag{5.49}$$

in which $g(\lambda)$ is the effective coupling at the scale λ, solution of the renormalization group equation,

$$\frac{\mathrm{d}g(\lambda)}{\mathrm{d}\ln\lambda} = \beta\left[g(\lambda)\right], \tag{5.50}$$

with

$$\beta(g) = \frac{9}{8\pi^2}g^2 + O\left(g^3\right). \tag{5.51}$$

This property is expected. The renormalization of the perturbative expansion renders the instanton contribution, before integration over dilatation, finite. Consequently this contribution should satisfy a renormalization group equation, and the coupling constant g can be present only in the combination $g(\lambda)$, since λ fixes the scale in the calculation.

5.3 The imaginary part of the n-point function

We can now write the complete contribution to the imaginary part of the n-point function,

$$\begin{aligned} &\operatorname{Im} Z^{(n)}(x_1,\ldots,x_n) \\ &\underset{g\to 0_-}{\sim} C_5 \int \mathrm{d}^4 x_0 \int_0^\infty \frac{\mathrm{d}\lambda}{\lambda}\lambda^4 \prod_{i=1}^n \frac{2\sqrt{2}\lambda}{1+\lambda^2\left(x_i-x_0\right)^2} \frac{\mathrm{e}^{8\pi^2/3g(\lambda)}}{(-g)^{(n+5)/2}}, \end{aligned} \tag{5.52}$$

where we have set:

$$C_5 = C_3 C_4 \,.$$

To calculate the Fourier transform of the expression (5.52), we introduce

$$u(p) = 2\sqrt{2}\int \mathrm{e}^{ipx}\,\frac{\mathrm{d}^4 x}{1+x^2}. \tag{5.53}$$

Then, after factorizing the δ-function of momentum conservation,

$$\operatorname{Im}\tilde{Z}^{(n)}(p_1,\ldots,p_n) \sim \frac{C_5}{(-g)^{(n+5)/2}}\int_0^\infty \mathrm{d}\lambda\,\lambda^{3-3n}\,\mathrm{e}^{8\pi^2/3g(\lambda)}\prod_{i=1}^n u(p_i/\lambda). \tag{5.54}$$

We can express the result in terms of 1PI correlation functions $\tilde{\Gamma}^{(n)}t(p_1,\ldots,p_n)$:

$$\operatorname{Im}\tilde{\Gamma}^{(n)}(p_1,\ldots,p_n) \sim \frac{C_5}{(-g)^{(n+5)/2}}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda}\lambda^{4-n}\,\mathrm{e}^{8\pi^2/3g(\lambda)}\prod_{i=1}^n (p_i^2/\lambda^2)\,u\,(p_i/\lambda). \tag{5.55}$$

One verifies that $p^2 u(p)$ goes to a constant for $|p|$ small.

In contrast to the super-renormalizable case, because the theory is only renormalizable the final result is not totally explicit, but involves instead a final integration over dilatations whose convergence is not obvious. Let us now discuss this point.

The small instanton contribution. Small instantons correspond to λ large. For λ large, the integral behaves like

$$\int^{\infty} \mathrm{d}\lambda\, \lambda^{3-n}\, \mathrm{e}^{8\pi^2/3g(\lambda)}, \tag{5.56}$$

and, therefore, we have to examine the behaviour of $g(\lambda)$ for λ large. From equation (5.51) we see that the theory is UV asymptotically free because for g negative, that is, $g(\lambda)$ goes to zero for λ large. Thus perturbation theory is applicable and we can use the approximation (5.49). The argument remains true even if we take g slightly complex. Thus the integral has the form

$$\int^{\infty} \mathrm{d}\lambda\, \lambda^{-n}. \tag{5.57}$$

We see that the power behaviour in λ depends explicitly on the coefficient of the g^2 term of the $\beta(g)$-function. Without the contribution coming from $g(\lambda)$, the integral (5.57) would have a UV divergence similar to the one found in the corresponding perturbative expansion. Due to the additional power of λ coming from $g(\lambda)$, only the vacuum amplitude is divergent.

The convergence of the dilatation integral is thus better than expected: indeed the renormalization constants are now themselves given by divergent series and are complex for g negative. Their imaginary part contributes directly to the imaginary part of $\tilde{\Gamma}^{(n)}(p_1,\ldots,p_n)$ for $n \le 4$. In the ϕ^6 field theory in dimension 3, for example, these contributions cancel the divergences coming from the integral over λ. By contrast, here the integrals over λ are finite at this order. This implies in particular that in the minimal subtraction scheme the imaginary parts of the renormalization constants vanish at leading order. In another renormalization scheme (fixed momentum subtraction for example) these imaginary parts are finite at leading order.

The large instanton contribution. We now examine the convergence of the λ integral for λ small. The behaviour of $g(\lambda)$ is totally unknown. On the other hand, it is easy to verify that the factors $u(p_i/\lambda)$ decrease exponentially for λ small. Thus, if the behaviour of $g(\lambda)$ is not too dramatic, the integrals will converge and it will be justified to replace $g(\lambda)$ by the expansion (5.49). For the vacuum amplitude, this argument does not apply, and so the result is unknown.

This analysis shows that, although this calculation seems to be a simple formal extension of the calculation for lower dimensions, coupling constant renormalization introduces a set of new problems which are not all completely under control. The fact that the theory is massless only makes matters worse. Consideration of the massive theory improves the situation in this respect, but the instanton calculation becomes more complicated.

5.4 The massive theory

It can be shown that massive field equations have no instanton solutions and that the minimum of the action is obtained from the massless theory. To study the massive theory, we thus start from the instanton solution of the massless theory, with its scale parameter λ. However, we notice a difficulty: as explained in section 5.1 the integral of ϕ_c^2 is IR divergent. We have thus to modify the field configuration at large distances, by connecting it smoothly to the solution of the massive free equation with mass m. Qualitatively speaking we consider a configuration $\phi_c(x,m)$ that up to a distance R, $\lambda R \gg 1$, $mR \ll 1$, is $\lambda\phi_c(\lambda x)$ and for $|x| > R$, is proportional to the free massive solution. An analogous problem is met in the case of multi-instanton configuration. Although the theory is no longer scale invariant, λ has to be kept as a collective coordinate. The mass term then acts as an IR cut-off, and restrict the domain of integration in λ to values large with respect to m. The corresponding classical action has the form

$$\mathcal{S}_m(\phi_c) = -\frac{1}{g}\left(\frac{8\pi^2}{3} + 8\pi^2\frac{m^2}{\lambda^2}\ln\frac{\lambda}{m}\right) \quad \text{for} \quad \lambda \gg m\,, \tag{5.58}$$

where the $\ln m$ term is directly related to the initial IR divergence of the ϕ^2 integral.

The remaining part of the calculation closely follows the calculation for the massless case and the reader is referred to the literature for details.

In the massless theory, the instanton contribution to the vacuum energy could not be evaluated without some knowledge of the non-perturbative IR behaviour of the RG β-function. In the massive theory the problem is solved because the λ integral is cut at a scale $m/\sqrt{-g}$. For correlation functions the integral will be cut by the largest between momenta and $m/\sqrt{-g}$. This implies that the limits $m \to 0$ and $g \to 0$ do not commute.

Chapter 6

Quantum Field Theory: Degenerate Classical Minima

In this chapter, we consider a generalization to field theory of a situation that we have discussed in chapter 1 in which instantons play a role: classical actions with degenerate isolated minima.

In quantum (or statistical) field theory the problem is more subtle because phase transitions are possible and the quantum ground state or vacuum can be degenerate. There again, the presence of instantons confirms that the classical minima are connected and that the symmetry between them is not spontaneously broken.

Examples of instantons of this type are provided in two dimensions by the $CP(N-1)$ models and in four dimensions by $SU(2)$ gauge theories. In both examples, the classical vacua have a periodic structure, reminiscent of the periodic cosine potential discussed in section 1.5 and the classification of instanton solution and the determination of their contributions involve topological considerations.

6.1 Instantons in stable boson field theories: General remarks

We first briefly discuss the possible existence of instantons in stable boson field theories, connecting for example degenerate classical minima. Unfortunately, the physically most interesting examples correspond to scale invariant classical theories and the evaluation of the instanton contributions at leading order, which formally follows the lines presented in chapter 3, leads to difficulties due both to UV and IR divergences. Some of them have been examined in chapter 5. Since for the two examples we consider in sections 6.2, 6.3, they have not been satisfactorily solved yet, we restrict ourselves here to classical considerations.

6.1.1 Scalar field theories

We first assume that the action has the general form

$$\mathcal{S}(\phi) = \int \left[\tfrac{1}{2} g_{ij}(\boldsymbol{\phi}) \partial_\mu \phi^i \partial_\mu \phi^j + V(\boldsymbol{\phi})\right] \mathrm{d}^d x\,, \tag{6.1}$$

in which ϕ^i is a multicomponent scalar boson field, $g_{ij}(\phi)$ a positive matrix (positive definite almost everywhere) and $V(\phi)$ an analytic potential that vanishes at its minima:

$$\min_{\{\boldsymbol{\phi}\}} V(\boldsymbol{\phi}) = 0\,. \tag{6.2}$$

We denote by $\boldsymbol{\phi}_c$ an instanton solution. In the action $\mathcal{S}(\boldsymbol{\phi}_c)$, we substitute $\boldsymbol{\phi}_c(x) \mapsto \boldsymbol{\phi}_c(\lambda x)$, then change variables $\lambda x \mapsto x$ and express the stationarity of the action for $\lambda = 1$. We obtain a simple generalization of equation (3.14): [3]

$$(2-d)\int \tfrac{1}{2}\left(g_{ij}(\phi)\partial_\mu \phi_c^i \partial_\mu \phi_c^j\right) \mathrm{d}^d x = d \int V(\boldsymbol{\phi}_c) \mathrm{d}^d x\,.$$

We see that this equation has no solution for $d > 2$. For $d = 2$, it has solutions only if

$$V\big(\boldsymbol{\phi}_c(x)\big) = 0\,. \tag{6.3}$$

The condition (6.2) then implies that $\boldsymbol{\phi}_c(x)$ is for all x a minimum of the potential:

$$\frac{\partial V(\boldsymbol{\phi}_c)}{\partial \phi^i} = 0\,,$$

and, therefore, $\boldsymbol{\phi}_c(x)$ is a solution of the field equations:

$$\frac{\delta}{\partial \phi^k(y)} \int \frac{1}{2} g_{ij}(\boldsymbol{\phi}) \partial_\mu \phi^i \partial_\mu \phi^j \, \mathrm{d}^2 x = 0\,.$$

These two equations are in general incompatible, except if $V(\boldsymbol{\phi})$ vanishes identically. In the latter case the action (6.1) corresponds to two-dimensional models based on Riemannian manifolds with g_{ij} as a metric tensor. Of particular interest are models based on homogeneous spaces, which have a group structure and, even more specifically, on symmetric spaces because they have a unique metric. Among them, the $CP(N-1)$ models are known to admit instanton solutions and we describe them in section 6.2.

Finally, note that the classical field theory is then scale invariant in the sense that the action is invariant under the dilatation $\phi(x) \mapsto \phi(\lambda x)$.

Gauge theories. We now consider a gauge invariant field theory, in which gauge fields A^a_μ interact with scalar fields, the gauge invariant action taking the form

$$\mathcal{S}(\boldsymbol{\phi}, \mathbf{A}_\mu) = \int \mathrm{d}^d x \left[\tfrac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu} + \tfrac{1}{2}\left(\mathrm{D}_\mu \phi_i\right)^2 + V(\boldsymbol{\phi})\right]. \tag{6.4}$$

Again we assume the existence of a finite action solution $\{\boldsymbol{\phi}^c,\ \mathbf{A}^c_\mu\}$ (in which $\mathbf{A}^c_\mu$ is not a pure gauge), and calculate the action for $\lambda \mathbf{A}^c_\mu(\lambda x)$ and $\boldsymbol{\phi}^c(\lambda x)$. After the change of variables $\lambda x \mapsto x$, we obtain [3]

$$\mathcal{S}(\boldsymbol{\phi}^c, \mathbf{A}^c_\mu; \lambda) = \lambda^{4-d} \int \frac{1}{4}\left(\mathbf{F}_{\mu\nu}\right)^2 \mathrm{d}^d x + \lambda^{2-d} \int \frac{1}{2}\left(\mathrm{D}_\mu \boldsymbol{\phi}\right)^2 \mathrm{d}^d x + \lambda^{-d} \int V(\boldsymbol{\phi}) \mathrm{d}^d x\,. \tag{6.5}$$

Stationarity at $\lambda = 1$ implies

$$(4-d)\int \frac{1}{4}\left(\mathbf{F}_{\mu\nu}\right)^2 \mathrm{d}^d x + (2-d)\int \frac{1}{2}\left(\mathrm{D}_\mu \boldsymbol{\phi}\right)^2 \mathrm{d}^d x - d\int V(\boldsymbol{\phi})\mathrm{d}^d x = 0\,. \quad (6.6)$$

We see that no solution can exist for $d > 4$, since a sum of negative terms cannot vanish.

For $d = 4$ we find two conditions:

$$V(\boldsymbol{\phi}) = 0\,, \quad (6.7a)$$

$$\mathrm{D}_\mu \boldsymbol{\phi} = 0\,. \quad (6.7b)$$

From the field equations, we then conclude that $\mathbf{A}^c_\mu$ is the solution of the pure gauge field equations. As we show in section 6.3, instantons can indeed be found in pure non-Abelian gauge theories. Equation (6.7*b*), which now is an equation for $\boldsymbol{\phi}^c$, then leads to the integrability conditions:

$$[\mathrm{D}_\mu, \mathrm{D}_\nu] = F_{\mu\nu} \Longrightarrow \left(F^a_{\mu\nu}\right)^c t^a_{ij} \phi^c_j = 0\,, \quad (6.8)$$

in which the matrices t^a are the generators of the Lie algebra. The conditions (6.8) together with the equation (6.7*a*) show that in general the system has only the trivial solution $\boldsymbol{\phi}^c = 0$.

Then, following the same argument, one verifies that the pure gauge theory is scale invariant.

6.2 Instantons in $CP(N-1)$ models

The preceding considerations can be illustrated by the two-dimensional $CP(N-1)$ models [19]. We mainly describe the nature of the instanton solutions and refer the reader to the literature for a more detailed analysis.

The $CP(N-1)$ manifold. The $CP(N-1)$ manifold (for $(N-1)$-dimensional Complex Projective) is isomorphic to the $U(N)/U(1)/U(N-1)$ symmetric (coset) space, a complex Grassmannian manifold. It can be parametrized by an N-component complex unit vector $\boldsymbol{\varphi}$ with the equivalence relation

$$\boldsymbol{\varphi} \sim \boldsymbol{\varphi}' \;\Leftrightarrow\; \boldsymbol{\varphi}' = \mathrm{e}^{i\Lambda}\,\boldsymbol{\varphi}\,,\ \Lambda \in \mathbb{R}\,.$$

A symmetric space admits a unique metric.

The $CP(N-1)$ field theory. We consider an N-component complex scalar field $\boldsymbol{\varphi}$ belonging to $CP(N-1)$, that is, subject to the condition

$$\bar{\boldsymbol{\varphi}}(x)\cdot\boldsymbol{\varphi}(x) = 1\,, \quad (6.9)$$

with an equivalence relation that now takes a form of an Abelian $U(1)$ gauge transformation:

$$\boldsymbol{\varphi}(x) \sim \boldsymbol{\varphi}'(x) \;\Leftrightarrow\; \boldsymbol{\varphi}'(x) = \mathrm{e}^{i\Lambda(x)}\,\boldsymbol{\varphi}(x)\,,\ \Lambda \in \mathbb{R}\,. \quad (6.10)$$

There exists a unique classical action with only two derivatives, up to a multiplicative constant, which can be written as

$$\mathcal{S}(\boldsymbol{\varphi}, A_\mu) = \frac{1}{g} \int \mathrm{d}^2 x \, \overline{\mathrm{D}_\mu \boldsymbol{\varphi}} \cdot \mathrm{D}_\mu \boldsymbol{\varphi} \,, \tag{6.11}$$

(g plays the role of $\hbar$) in which the field A_μ is a gauge field that implements the equivalence (6.10) and D_μ is the associated covariant derivative,

$$\mathrm{D}_\mu = \partial_\mu + i A_\mu \,. \tag{6.12}$$

Since the action is a quadratic form in A_μ that contains no kinetic term, A_μ is an auxiliary field that can be integrated out. The integration results in replacing A_μ by the solution of the A_μ field equation:

$$A_\mu(x) = \tfrac{1}{2} i \left[\bar{\boldsymbol{\varphi}}(x) \cdot \partial_\mu \boldsymbol{\varphi}(x) - \partial_\mu \bar{\boldsymbol{\varphi}}(x) \cdot \boldsymbol{\varphi}(x) \right] = i \bar{\boldsymbol{\varphi}}(x) \cdot \partial_\mu \boldsymbol{\varphi}(x), \tag{6.13}$$

where the relation (6.9) has been used. After this substitution, $\bar{\boldsymbol{\varphi}}(x) \cdot \partial_\mu \boldsymbol{\varphi}(x)$ can be considered as a composite gauge field. However, below we work mainly with the initial representation (6.11).

Instantons and topology. To prove the existence of locally stable non-trivial minima of the action, the following Bogomolny inequality [18] can be used:

$$\int \mathrm{d}^2 x \left| \mathrm{D}_\mu \boldsymbol{\varphi} \mp i \epsilon_{\mu\nu} \mathrm{D}_\nu \boldsymbol{\varphi} \right|^2 \geq 0 \,, \tag{6.14}$$

($\epsilon_{\mu\nu}$ being the antisymmetric tensor, $\epsilon_{12} = 1$). After expansion, the inequality can be cast into the form

$$\mathcal{S}(\boldsymbol{\varphi}) \geq 2\pi |Q(\boldsymbol{\varphi})| / g \tag{6.15}$$

with

$$Q(\boldsymbol{\varphi}) = -\frac{i}{2\pi} \epsilon_{\mu\nu} \int \mathrm{d}^2 x \, \mathrm{D}_\mu \boldsymbol{\varphi} \cdot \overline{\mathrm{D}_\nu \boldsymbol{\varphi}} = \frac{i}{2\pi} \int \mathrm{d}^2 x \, \epsilon_{\mu\nu} \bar{\boldsymbol{\varphi}} \cdot \mathrm{D}_\nu \mathrm{D}_\mu \boldsymbol{\varphi} \,. \tag{6.16}$$

Then,

$$i \epsilon_{\mu\nu} \mathrm{D}_\nu \mathrm{D}_\mu = \tfrac{1}{2} i \epsilon_{\mu\nu} [\mathrm{D}_\nu, \mathrm{D}_\mu] = \tfrac{1}{2} F_{\mu\nu} \,, \tag{6.17}$$

where $F_{\mu\nu}$ is the curvature:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \,.$$

Therefore, using (6.9),

$$Q(\boldsymbol{\varphi}) = \frac{1}{4\pi} \int \mathrm{d}^2 x \, \epsilon_{\mu\nu} F_{\mu\nu} \,. \tag{6.18}$$

The integrand is a total divergence since

$$\tfrac{1}{2}\epsilon_{\mu\nu}F_{\mu\nu}=\partial_\mu\epsilon_{\mu\nu}A_\nu\,,$$

proportional to the two-dimensional Abelian chiral anomaly. Substituting this form into equation (6.18) and integrating over a large disc of radius R, one obtains

$$Q(\boldsymbol{\varphi})=\frac{1}{2\pi}\lim_{R\to\infty}\oint_{|x|=R}\mathrm{d}x_\mu\,A_\mu(x). \tag{6.19}$$

$Q(\boldsymbol{\varphi})$ thus depends only on the behaviour of the classical solution for $|x|$ large and is a topological charge. Finiteness of the action demands that at large distances $\mathrm{D}_\mu\boldsymbol{\varphi}$ vanishes and, therefore,

$$\mathrm{D}_\mu\boldsymbol{\varphi}=0\ \Rightarrow\ [\mathrm{D}_\mu,\mathrm{D}_\nu]\boldsymbol{\varphi}=F_{\mu\nu}\boldsymbol{\varphi}=0\,.$$

Since $\boldsymbol{\varphi}\neq 0$, this equation implies that $F_{\mu\nu}$ vanishes and, thus, that A_μ is a pure gauge and $\boldsymbol{\varphi}$ a gauge transform of a constant vector:

$$A_\mu(x)=\partial_\mu\Lambda(x),\quad \boldsymbol{\varphi}(x)=\mathrm{e}^{-i\Lambda(x)}\,\mathbf{v}\text{ with }\bar{\mathbf{v}}\cdot\mathbf{v}=1\,.$$

Thus,

$$Q(\boldsymbol{\varphi})=\frac{1}{2\pi}\lim_{R\to\infty}\oint_{|x|=R}\mathrm{d}x_\mu\partial_\mu\Lambda(x)\,. \tag{6.20}$$

The topological charge measures the variation of the angle $\Lambda(x)$ on a large circle, which is a multiple of 2π because $\boldsymbol{\varphi}$ is regular. One is thus led to the consideration of the homotopy classes of continuous mappings from $U(1)$, that is, S_1 to S_1, which are characterized by an integer n, the winding number. This is equivalent to the statement that the homotopy group $\pi_1(S_1)$ is isomorphic to the additive group of integers $\mathbb{Z}$.

Then,

$$Q(\boldsymbol{\varphi})=n\ \Rightarrow \mathcal{S}(\boldsymbol{\varphi})\geq 2\pi|n|/g\,. \tag{6.21}$$

Instanton solutions. The equality $\mathcal{S}(\boldsymbol{\varphi})=2\pi|n|/g$ corresponds to a local minimum of the action. Field configurations that satisfy this condition, satisfy the field equations but also the first order partial differential (self-duality) equations

$$\mathrm{D}_\mu\boldsymbol{\varphi}=\pm i\epsilon_{\mu\nu}\mathrm{D}_\nu\boldsymbol{\varphi}\,. \tag{6.22}$$

For each sign, there is really only one equation, for instance $\mu=1,\nu=2$. It is simple to verify that both equations imply the φ-field equations, and combined with the constraint (6.9), the A-field equation (6.13). In complex coordinates $z=x_1+ix_2$, $\bar z=x_1-ix_2$ and, thus,

$$\partial_z=\tfrac{1}{2}\left(\partial_{x_1}-i\partial_{x_2}\right),\quad \partial_{\bar z}=\tfrac{1}{2}\left(\partial_{x_1}+i\partial_{x_2}\right),$$

they can be written as

$$\partial_{\bar z}\varphi_\alpha(z,\bar z)=-iA_{\bar z}(z,\bar z)\varphi_\alpha(z,\bar z), \tag{6.23a}$$

$$\partial_{z}\varphi_\alpha(z,\bar z)=-iA_{z}(z,\bar z)\varphi_\alpha(z,\bar z), \tag{6.23b}$$

where

$$A_z = \tfrac{1}{2}(A_1 - iA_2), \quad A_{\bar z} = \tfrac{1}{2}(A_1 + iA_2).$$

If $\boldsymbol{\varphi}$ satisfies equation (6.23*a*), $\bar{\boldsymbol{\varphi}}$ satisfies equation (6.23*b*). Thus, exchanging the two equations just amounts to exchanging $\boldsymbol{\varphi}$ and $\bar{\boldsymbol{\varphi}}$. Therefore, we solve only the equation (6.23*a*). The general solution can be written as

$$\varphi_\alpha(z,\bar z) = \kappa(z,\bar z) P_\alpha(z),$$

where $\kappa(z,\bar z)$ is a particular solution of

$$\partial_{\bar z}\kappa(z,\bar z) = -iA_{\bar z}(z,\bar z)\kappa(z,\bar z).$$

Vector solutions of equations (6.22) are thus proportional to holomorphic or anti-holomorphic (depending on the sign in equation (6.22)) vectors (this reflects the underlying conformal invariance of the classical field theory). The phase of the function $\kappa(z,\bar z)$ can be cancelled by a gauge transformation (6.10). The function $\kappa(z,\bar z)$ can thus be chosen real (this corresponds to the $\partial_\mu A_\mu = 0$ gauge), then is constrained by the condition (6.9):

$$\kappa^2(z,\bar z)\, P\cdot \bar P = 1\,.$$

The asymptotic conditions constrain the functions $P_\alpha(z)$ to be polynomials. Common roots to all P_α would correspond to non-integrable singularities for φ_α and, therefore, are excluded by the condition of finiteness of the action. Finally, if the polynomials have maximal degree n, asymptotically

$$P_\alpha(z) \sim c_\alpha z^n \ \Rightarrow\ \varphi_\alpha \sim \frac{c_\alpha}{\sqrt{\mathbf{c}\cdot\bar{\mathbf{c}}}}(z/\bar z)^{n/2}.$$

When the phase of z varies by 2π, the phase of φ_α varies by $2n\pi$, showing that the corresponding winding number is n.

The structure of the semi-classical vacuum. In contrast to our analysis of periodic potentials in quantum mechanics, here we have discussed the existence of instantons without reference to the structure of the classical vacuum. To find an interpretation of instantons in gauge theories, it is useful to express the results in the temporal gauge $A_2 = 0$. Then, the action is still invariant under space-dependent gauge transformations. The minima of the classical φ potential correspond to fields $\boldsymbol{\varphi}(x_1)$, where x_1 is the space variable, gauge transforms of a constant vector:

$$\boldsymbol{\varphi}(x_1) = \mathrm{e}^{i\Lambda(x_1)}\,\mathbf{v}\,, \quad \bar{\mathbf{v}}\cdot\mathbf{v} = 1\,.$$

Moreover, if the vacuum state is invariant under space reflection, $\boldsymbol{\varphi}(+\infty) = \boldsymbol{\varphi}(-\infty)$ and, thus,

$$\Lambda(+\infty) - \Lambda(-\infty) = 2\nu\pi \quad \nu\in\mathbb{Z}\,.$$

Again ν is a topological number that classifies degenerate classical minima, and the semi-classical vacuum has a periodic structure. This analysis is consistent with Gauss's law, which implies only that states are invariant under infinitesimal gauge transformations and, thus, under gauge transformations of the class $\nu = 0$ that are continuously connected to the identity and do not change the topological number.

We now consider a large rectangle with extension R in the space direction and T in the Euclidean time direction and by a smooth gauge transformation continue the instanton solution to the temporal gauge. Then, the variation of the pure gauge comes entirely from the sides at fixed time. For $R \to \infty$, one finds

$$\Lambda(+\infty, 0) - \Lambda(-\infty, 0) - [\Lambda(+\infty, T) - \Lambda(-\infty, T)] = 2n\pi\,.$$

Therefore, instantons interpolate between different classical minima. Like in the example of the cosine potential and in analogy with the expression (1.54), to project onto a proper quantum eigenstate, the 'θ-vacuum' corresponding to an angle θ, one can add a topological term to the classical action. Here,

$$\mathcal{S}(\boldsymbol{\varphi}) \mapsto \mathcal{S}(\boldsymbol{\varphi}) + i\frac{\theta}{4\pi}\int \mathrm{d}^2 x\, \epsilon_{\mu\nu} F_{\mu\nu}. \tag{6.24}$$

Remark. Replacing in the topological charge Q the gauge field by the explicit expression (6.13), one finds

$$Q(\varphi) = \frac{i}{2\pi}\int \mathrm{d}^2 x\, \epsilon_{\mu\nu}\partial_\mu \bar{\boldsymbol{\varphi}} \cdot \partial_\nu \boldsymbol{\varphi} = \frac{i}{2\pi}\int \mathrm{d}\bar{\varphi}_\alpha \wedge \mathrm{d}\varphi_\alpha\,,$$

where the notation of exterior differential calculus has been used. We recognize the integral of a two-form, a symplectic form, and $4\pi Q$ is the area of a 2-surface embedded in $CP(N-1)$. A symplectic form is always closed. Here it is also exact, so that Q is the integral of a one-form (*cf.* equation (6.19)):

$$Q(\varphi) = \frac{i}{2\pi}\int \bar{\varphi}_\alpha \mathrm{d}\varphi_\alpha = \frac{i}{4\pi}\int (\bar{\varphi}_\alpha \mathrm{d}\varphi_\alpha - \varphi_\alpha \mathrm{d}\bar{\varphi}_\alpha)\,.$$

The $O(3)$ non-linear σ-model. The $CP(1)$ model is locally isomorphic to the $O(3)$ non-linear σ-model, with the identification

$$\phi^i(x) = \bar{\varphi}_\alpha(x)\sigma^i_{\alpha\beta}\varphi_\beta(x)\,, \tag{6.25}$$

where $\boldsymbol{\sigma}^i$ are the three Pauli matrices.

Using, for example, an explicit representation of Pauli matrices, one indeed verifies

$$\phi^i(x)\phi^i(x) = 1\,, \quad \partial_\mu\phi^i(x)\partial_\mu\phi^i(x) = 4\,\overline{\mathrm{D}_\mu\boldsymbol{\varphi}} \cdot \mathrm{D}_\mu\boldsymbol{\varphi}\,.$$

Therefore, the field theory can be expressed in terms of the field ϕ^i and takes the form of the non-linear σ-model. The fields ϕ are gauge invariant and the whole physical picture is a picture of confinement of the charged scalar 'quarks'

$\varphi_\alpha(x)$ and the propagation of neutral bound states corresponding to the fields ϕ^i.

Instantons in the ϕ description take the form of ϕ configurations with uniform limit for $|x| \to \infty$. Thus, they define a continuous mapping from the compactified plane topologically equivalent to S_2 to the sphere S_2 (the ϕ^i configurations). Since $\pi_2(S_2) = \mathbb{Z}$, the φ and ϕ pictures are consistent.

In the example of $CP(1)$, a solution of winding number 1 is

$$\varphi_1 = \frac{1}{\sqrt{1+z\bar{z}}}\,, \quad \varphi_2 = \frac{z}{\sqrt{1+z\bar{z}}}\,.$$

Translating the $CP(1)$ minimal solution into the $O(3)$ σ-model language, one finds

$$\phi_1 = \frac{z+\bar{z}}{1+\bar{z}z}\,, \quad \phi_2 = \frac{1}{i}\frac{z-\bar{z}}{1+\bar{z}z}\,, \quad \phi_3 = \frac{1-\bar{z}z}{1+\bar{z}z}\,.$$

This defines a stereographic mapping of the plane onto the sphere S_2, as one verifies by setting $z = \tan(\eta/2)\,\mathrm{e}^{i\theta}$, $\eta \in [0, \pi]$.

In the $O(3)$ representation

$$Q = \frac{i}{2\pi}\int \mathrm{d}\bar{\varphi}_\alpha \wedge \mathrm{d}\varphi_\alpha = \frac{1}{8\pi}\epsilon_{ijk}\int \phi_i \mathrm{d}\phi_j \wedge \phi_k \equiv \frac{1}{8\pi}\epsilon_{\mu\nu}\epsilon_{ijk}\int \mathrm{d}^2x\, \phi_i\partial_\mu\phi_j\partial_\nu\phi_k\,.$$

The topological charge $4\pi Q$ has the interpretation of the area of the sphere S_2, multiply covered, and embedded in $\mathbb{R}^3$. Its value is a multiple of the area of S_2, which in this interpretation explains the quantization.

6.3 Instantons in the $SU(2)$ gauge theory

We now give an example of instantons in four dimensions [20], directly relevant to particle physics. According to the analysis of section 6.1, we can consider only pure gauge theories. Actually it is sufficient to consider the gauge group $SU(2)$ since a general theorem states that for a Lie group containing $SU(2)$ as a subgroup the instantons are those of the $SU(2)$ subgroup.

In the absence of matter fields it is convenient to use a $SO(3)$ notation. The gauge field $\mathbf{A}_\mu$ is a $SO(3)$ vector that is related to the corresponding element $\mathfrak{A}_\mu$ of the Lie algebra by

$$\mathfrak{A}_\mu = -\tfrac{1}{2}i\mathbf{A}_\mu^a\boldsymbol{\sigma}^a\,, \tag{6.26}$$

where $\boldsymbol{\sigma}^a$ are the three Pauli matrices. The gauge action then reads

$$\mathcal{S}(\mathbf{A}_\mu) = \frac{1}{4g^2}\int \left[\mathbf{F}_{\mu\nu}(x)\right]^2 \mathrm{d}^4x\,, \tag{6.27}$$

(g is the gauge coupling constant) where the curvature

$$\mathbf{F}_{\mu\nu} = \partial_\mu\mathbf{A}_\nu - \partial_\nu\mathbf{A}_\mu + \mathbf{A}_\mu \times \mathbf{A}_\nu, \tag{6.28}$$

is also an $SO(3)$ vector.

The corresponding classical field equations are

$$\mathbf{D}_\nu \mathbf{F}_{\nu\mu} = \partial_\nu \mathbf{F}_{\nu\mu} + \mathbf{A}_\nu \times \mathbf{F}_{\nu\mu} = 0\,, \tag{6.29}$$

where $\mathbf{D}_\mu$ is the gauge covariant derivative.

The existence and some properties of instantons in this theory follow from considerations analogous to those presented for the $CP(N-1)$ models.

Instantons and topology. We define the dual of the tensor $\mathbf{F}_{\mu\nu}$ by

$$\tilde{\mathbf{F}}_{\mu\nu} = \tfrac{1}{2}\epsilon_{\mu\nu\rho\sigma}\mathbf{F}_{\rho\sigma}\,. \tag{6.30}$$

Then, the Bogomolny inequality

$$\int \mathrm{d}^4x \left[\mathbf{F}_{\mu\nu}(x) \pm \tilde{\mathbf{F}}_{\mu\nu}(x)\right]^2 \geq 0 \tag{6.31}$$

implies

$$\mathcal{S}(\mathbf{A}_\mu) \geq 8\pi^2 |Q(\mathbf{A}_\mu)|/g^2 \tag{6.32}$$

with

$$Q(\mathbf{A}_\mu) = \frac{1}{32\pi^2}\int \mathrm{d}^4x\, \mathbf{F}_{\mu\nu}(x)\cdot\tilde{\mathbf{F}}_{\mu\nu}(x). \tag{6.33}$$

The expression $Q(\mathbf{A}_\mu)$ is proportional to the integral of the chiral anomaly (*cf.*, equation (6.50)), here written in $SO(3)$ notation.

One verifies that the quantity $\mathbf{F}_{\mu\nu}\cdot\tilde{\mathbf{F}}_{\mu\nu}$ is a pure divergence:

$$\mathbf{F}_{\mu\nu}\cdot\tilde{\mathbf{F}}_{\mu\nu} = \partial_\mu V_\mu$$

with

$$V_\mu = -4\,\epsilon_{\mu\nu\rho\sigma}\,\mathrm{tr}\left(\mathfrak{A}_\nu\partial_\rho\mathfrak{A}_\sigma + \tfrac{2}{3}\mathfrak{A}_\nu\mathfrak{A}_\rho\mathfrak{A}_\sigma\right) \tag{6.34a}$$

$$= 2\epsilon_{\mu\nu\rho\sigma}\left[\mathbf{A}_\nu\cdot\partial_\rho\mathbf{A}_\sigma + \tfrac{1}{3}\mathbf{A}_\nu\cdot(\mathbf{A}_\rho\times\mathbf{A}_\sigma)\right]. \tag{6.34b}$$

The integral thus depends only on the behaviour of the gauge field at large distances. Here again, as in the $CP(N-1)$ model, the bound involves a topological charge: $Q(\mathbf{A}_\mu)$.

Stokes theorem implies

$$\int_{\mathcal{D}} \mathrm{d}^4x\,\partial_\mu V_\mu = \int_{\partial\mathcal{D}} \mathrm{d}S\;\hat{n}_\mu V_\mu\,,$$

where $\mathrm{d}S$ is the measure on the boundary $\partial\mathcal{D}$ of the four-volume $\mathcal{D}$ and $\hat{n}_\mu$ the unit vector normal to $\partial\mathcal{D}$. We then take for $\mathcal{D}$ a sphere of large radius R and find for the topological charge

$$Q(\mathbf{A}_\mu) = \frac{1}{32\pi^2}\int \mathrm{d}^4x\;\mathrm{tr}\,\mathbf{F}_{\mu\nu}(x)\cdot\tilde{\mathbf{F}}_{\mu\nu}(x) = \frac{1}{32\pi^2}R^3\int_{r=R}\mathrm{d}\Omega\;\hat{n}_\mu V_\mu\,, \tag{6.35}$$

where we have set $\mathrm{d}S = R^3 \mathrm{d}\Omega$.

The finiteness of the action implies that the classical solution must asymptotically become a pure gauge, that is, with our conventions,

$$\mathfrak{A}_\mu = -\tfrac{1}{2} i \mathbf{A}_\mu \cdot \boldsymbol{\sigma} = \mathbf{g}(x)\partial_\mu \mathbf{g}^{-1}(x) + O\left(|x|^{-2}\right) \quad |x| \to \infty \,. \tag{6.36}$$

The element $\mathbf{g}$ of the $SU(2)$ group can be parametrized in terms of Pauli matrices:

$$\mathbf{g} = u_4 \mathbf{1} + i\mathbf{u} \cdot \boldsymbol{\sigma} \,, \tag{6.37}$$

where the four-component real vector $(u_4, \mathbf{u})$ satisfies

$$u_4^2 + \mathbf{u}^2 = 1 \,,$$

and thus belongs to the unit sphere S_3. Since $SU(2)$ is topologically equivalent to the sphere S_3, the pure gauge configurations on a sphere of large radius $|x| = R$ define a continuous mapping from S_3 to S_3. Such mappings belong to different homotopy classes that are characterized by an integer $n \in \mathbb{Z}$ called the *winding number*. Here, we identify the homotopy group $\pi_3(S_3)$, which again is isomorphic to the additive group of integers $\mathbb{Z}$.

The $n = 1$ example. The simplest one to one mapping corresponds to an element of the form

$$\mathbf{g}(x) = \frac{x_4 \mathbf{1} + i\mathbf{x} \cdot \boldsymbol{\sigma}}{r}, \quad r = (x_4^2 + \mathbf{x}^2)^{1/2} \tag{6.38}$$

and thus

$$A_m^i \underset{r\to\infty}{\sim} 2\left(x_4 \delta_{im} + \epsilon_{imk} x_k\right) r^{-2}, \quad A_4^i = -2x_i r^{-2}. \tag{6.39}$$

Note that the transformation

$$\mathbf{g}(x) \mapsto \mathbf{U}_1 \mathbf{g}(x) \mathbf{U}_2^\dagger = \mathbf{g}(\mathbf{R}x),$$

where $\mathbf{U}_1$ and $\mathbf{U}_2$ are two constant $SU(2)$ matrices, induces a $SO(4)$ rotation of matrix $\mathbf{R}$ of the vector x_μ. Then,

$$\mathbf{U}_2 \partial_\mu \mathbf{g}^\dagger(x) \mathbf{U}_1^\dagger = R_{\mu\nu} \partial_\nu \mathbf{g}^\dagger(\mathbf{R}x), \quad \mathbf{U}_1 \mathbf{g}(x) \partial_\mu \mathbf{g}^\dagger(x) \mathbf{U}_1^\dagger = \mathbf{g}(\mathbf{R}x) R_{\mu\nu} \partial_\nu \mathbf{g}^\dagger(\mathbf{R}x)$$

and, therefore,

$$\mathbf{U}_1 \mathfrak{A}_\mu(x) \mathbf{U}_1^\dagger = R_{\mu\nu} \mathfrak{A}_\nu(\mathbf{R}x).$$

Introducing this relation into the definition (6.34a) of V_μ, one verifies that the dependence on the matrix $\mathbf{U}_1$ cancels in the trace and, thus, V_μ transforms like a 4-vector. Since only one vector is available, and taking into account dimensional analysis, one concludes that

$$V_\mu \propto x_\mu / r^4 \,.$$

We still have to calculate the coefficient. For $r \to \infty$, $\mathbf{A}_\mu$ approaches a pure gauge (equation (6.36)) and, therefore, V_μ can be transformed into

$$V_\mu \underset{r\to\infty}{\sim} -\tfrac{1}{3}\epsilon_{\mu\nu\rho\sigma}\mathbf{A}_\nu \cdot (\mathbf{A}_\rho \times \mathbf{A}_\sigma).$$

It is sufficient to calculate V_1. We choose $\rho = 3, \sigma = 4$ and multiply by a factor six to take into account all other choices. Then,

$$V_1 \underset{r\to\infty}{\sim} 16\epsilon_{ijk}(x_4\delta_{2i} + \epsilon_{i2l}x_l)(x_4\delta_{3j} + \epsilon_{j3m}x_m)x_k/r^6 = 16x_1/r^4$$

and, thus, the proportionality coefficient is determined:

$$V_\mu \sim 16x_\mu/r^4 = 16\hat{n}_\mu/R^3\,. \tag{6.40}$$

The powers of R in equation (6.35) cancel and since $\int \mathrm{d}\Omega = 2\pi^2$, the value of the topological charge is simply

$$Q(\mathbf{A}_\mu) = 1\,. \tag{6.41}$$

General situation. As in the case of the $CP(N-1)$ model, the second expression in equation (6.35), in which V_μ is replaced by its general asymptotic form, has a geometric interpretation. Quite generally, in the parametrization (6.37) one finds

$$V_\mu \underset{r\to\infty}{\sim} \tfrac{8}{3}\epsilon_{\mu\nu\rho\sigma}\epsilon_{\alpha\beta\gamma\delta}u_\alpha\partial_\nu u_\beta\partial_\rho u_\gamma\partial_\sigma u_\delta\,.$$

A few algebraic manipulations starting from (again in the notation of exterior differential calculus)

$$\int_{S_3} R^3\mathrm{d}\Omega\ \hat{n}_\mu V_\mu = \tfrac{1}{6}\epsilon_{\mu\nu\rho\sigma}\int V_\mu \mathrm{d}x_\nu \wedge \mathrm{d}x_\rho \wedge \mathrm{d}x_\sigma\,,$$

then yield

$$Q = \frac{1}{12\pi^2}\epsilon_{\alpha\beta\gamma\delta}\int u_\alpha \mathrm{d}u_\beta \wedge \mathrm{d}u_\gamma \wedge \mathrm{d}u_\delta\,, \tag{6.42}$$

has been used. The expression is proportional to the area Σ_4 of the sphere S_3, which in the same notation can be written as

$$\Sigma_4 = \frac{1}{3!}\epsilon_{\alpha\beta\gamma\delta}\int u_\alpha \mathrm{d}u_\beta \wedge \mathrm{d}u_\gamma \wedge \mathrm{d}u_\delta = 2\pi^2\,,$$

when the vector u_μ describes the sphere S_3 only once. Because in general u_μ describes S_3 n times when x_μ describes S_3 only once, a factor n is generated.

The inequality (6.33) then implies

$$\mathcal{S}(\mathbf{A}_\mu) \ge 8\pi^2|n|/g^2\,. \tag{6.43}$$

On the other hand, without any explicit calculation, it is known from the study of the index of the gauge covariant Dirac operator $\not{\mathbf{D}} = \gamma_\mu \mathbf{D}_\mu$, that the topological charge is an integer. In $SO(3)$ notation,

$$Q(\mathbf{A}_\mu) = \frac{1}{32\pi^2} \int \mathrm{d}^4x \, \mathbf{F}_{\mu\nu} \cdot \tilde{\mathbf{F}}_{\mu\nu} = n_+ - n_- \, , \tag{6.44}$$

where $n_\pm$ is the number of eigenvectors with eigenvalue zero and with chirality $\pm$.

Instanton solutions. The equality is obtained for fields satisfying the *self-duality equations*

$$\mathbf{F}_{\mu\nu} = \pm \tilde{\mathbf{F}}_{\mu\nu} \, . \tag{6.45}$$

Because the inequality corresponds to a local minimum of the action, the solutions satisfy also the general classical field equations (6.29) but the equations (6.45) are first order partial differential equations and, thus, easier to solve. The one-instanton solution, which depends on an arbitrary scale parameter λ, can be written as

$$A^i_m = \frac{2}{r^2 + \lambda^2} \left(x_4 \delta_{im} + \epsilon_{imk} x_k \right) , \quad m = 1, 2, 3 \, , \quad A^i_4 = -\frac{2x_i}{r^2 + \lambda^2}. \tag{6.46}$$

The semi-classical vacuum. We now proceed in analogy with the analysis of the $CP(N-1)$ model. In the temporal gauge $\mathbf{A}_4 = 0$, the classical minima of the potential correspond to gauge field components $\mathbf{A}_i$, $i = 1, 2, 3$, which are pure gauge functions of the three space variables x_i:

$$\mathfrak{A}_m = -\tfrac{1}{2} i \mathbf{A}_m \cdot \boldsymbol{\sigma} = \mathbf{g}(x_i) \partial_m \mathbf{g}^{-1}(x_i) \, . \tag{6.47}$$

The structure of the classical minima is related to the homotopy classes of mappings of the group elements $\mathbf{g}$ into compactified $\mathbb{R}^3$ (because $\mathbf{g}(x)$ goes to a constant for $|x| \to \infty$), that is, again of S_3 into S_3 and thus the semi-classical vacuum, as in the $CP(N-1)$ model, has a periodic structure. One verifies that the instanton solution (6.46), transported into the temporal gauge by a gauge transformation, connects minima with different winding numbers. Therefore, as in the case of the $CP(N-1)$ model (equation (6.24)), to project onto a θ-vacuum, one adds a term to the classical action of gauge theories:

$$\mathcal{S}_\theta(\mathbf{A}_\mu) = \mathcal{S}(\mathbf{A}_\mu) + \frac{i\theta}{32\pi^2} \int d^4x \, \mathbf{F}_{\mu\nu}(x) \cdot \tilde{\mathbf{F}}_{\mu\nu}(x), \tag{6.48}$$

and then integrates over all fields $\mathbf{A}_\mu$ without restriction. At least in the semi-classical approximation, the gauge theory thus depends on one additional parameter, the angle θ.

The strong CP violation problem. For non-vanishing values of θ, due to instanton contributions the additional term violates CP (charge conjugation times space reflection) conservation in strong interactions and is at the origin of the *strong CP violation problem*: Except if θ vanishes for some as yet unknown reason then, according to experimental data, it can only be unnaturally small. Indeed, limits on the neutron electric dipole moment imply $|\theta| < 10^{-10}$.

6.3.1 Fermions in an instanton background

In QCD gauge fields are coupled to quarks $\mathbf{Q}$, $\bar{\mathbf{Q}}$ with an action of the form (now in $SU(3)$ notation and gauge fields and curvature tensor being matrices in the Lie algebra):

$$\mathcal{S}(\mathbf{A}_\mu, \bar{\mathbf{Q}}, \mathbf{Q}) = -\int \mathrm{d}^4x \left[\frac{1}{4g^2} \operatorname{tr} \mathbf{F}^2_{\mu\nu} + \sum_{f=1}^{N_F} \bar{\mathbf{Q}}_f \left(\not{\mathbf{D}} + m_f \right) \mathbf{Q}_f \right],$$

N_F being the number of flavours.

The strong CP violation problem. Instantons contribute to the θ-term in (6.48) and this leads to the strong CP violation problem. However, if at least one fermion field is massless, the determinant resulting from the fermion integration vanishes. Indeed, in presence of instantons the Dirac operator has at least one vanishing eigenvalue because the index $n_+ - n_-$ of the Dirac operator does not vanish, being related to the chiral anomaly by (equation (6.24)) [25]

$$-\frac{1}{16\pi^2} \int \mathrm{d}^4x \ \operatorname{tr} \mathbf{F}_{\mu\nu}(x) \tilde{\mathbf{F}}_{\mu\nu}(x) = n_+ - n_- \,, \tag{6.49}$$

$n_\pm$ being the number of eigenvectors with eigenvalue zero and with chirality $\pm$. Then, the instantons do not contribute to the functional integral and the strong CP violation problem is solved.

However, such an hypothesis seems to be inconsistent with experimental data and an indirect determination of quark masses, the lightest $\mathbf{u}$ quark mass being found in the range $1.5\text{MeV} < m_{\mathbf{u}} < 3.5\text{MeV}$. Another scheme is based on a scalar field, the *axion*, which unfortunately has remained, up to now, experimentally invisible [21].

The $U(1)$ problem. Experimentally it is observed that the masses of a number of pseudo-scalar mesons are smaller or even much smaller (in the case of pions) than the masses of the corresponding scalar mesons. This strongly suggests that pseudo-scalar mesons are almost Goldstone bosons associated with an approximate chiral symmetry realized in a phase of spontaneous symmetry breaking. (When a continuous (non gauge) symmetry is spontaneously broken, the spectrum of the theory exhibits massless scalar particles called Goldstone bosons.) This picture is confirmed by its many other phenomenological implications.

In the Standard Model, this approximate symmetry is viewed as the consequence of the very small masses of the $\mathbf{u}$ and $\mathbf{d}$ quarks and the moderate value of the strange $\mathbf{s}$ quark mass.

Indeed, in a theory in which the quarks are massless, the action has a chiral $U(N_\mathrm{F}) \times U(N_\mathrm{F})$ symmetry, in which N_F is the number of flavours. The spontaneous breaking of chiral symmetry to its diagonal subgroup $U(N_\mathrm{F})$ leads to expect N_F^2 Goldstone bosons associated with all axial currents (corresponding to the generators of $U(N) \times U(N)$ that do not belong to the remaining $U(N)$ symmetry group). In the physically relevant theory, the masses of quarks are non-vanishing but small, and one expects this picture to survive approximately with, instead of Goldstone bosons, light pseudo-scalar mesons.

However, the experimental mass pattern is consistent only with a slightly broken $SU(2) \times SU(2)$ and more badly violated $SU(3) \times SU(3)$ symmetries.

The solution of the problem is related to the axial anomaly: due to the anomaly, the divergence of the axial current J^5_λ corresponding to the $U(1)$ Abelian subgroup does not vanish and is given by

$$\left\langle \partial_\lambda J^5_\lambda(x) \right\rangle = -\frac{i}{8\pi^2} \operatorname{tr} \mathbf{F}_{\mu\nu}(x) \tilde{\mathbf{F}}_{\mu\nu}(x). \tag{6.50}$$

The WT identities, which imply the existence of Goldstone bosons, correspond to constant (global or space-independent) group transformations and, thus, involve only the space integral of the divergence of the current. Since the anomaly is a total derivative, one might have expected the integral to vanish. However, non-Abelian gauge theories have configurations that give non-vanishing values of the form (6.44) to the space integral of the anomaly (6.50). For small couplings, these configurations are in the neighbourhood of instanton solutions (as discussed in section 6.3). This indicates (though no satisfactory calculation of the instanton contribution has been performed yet) that for small, but non-vanishing, quark masses the $U(1)$ axial current is far from being conserved and, therefore, no corresponding light almost Goldstone boson is generated [22].

Instanton contributions to the anomaly thus resolve a long standing experimental puzzle.

For additional speculations and a review see, for example, [23,24].

6.3.2 The Gaussian integration

Both in $CP(N-1)$ models and non-Abelian gauge theories the classical theory is scale invariant. Therefore, solutions depend on a scale parameter that is an additional collective coordinate over which one has to integrate. This leads to a number of difficulties as the analysis of the massless ϕ^4_4 field theory reveals (see chapter 5). Both theories are asymptotically free and the main problems come from the infrared region, that is, from instantons of large size for which the semi-classical approximation is no longer legitimate because the interaction increases with distance.

The role of instantons thus is not fully understood, a complete calculation being possible only with an IR cut-off, provided, for example, by a finite volume. Moreover, singularities not of semi-classical nature may also be expected.

Chapter 7

Perturbation Series at Large Orders. Summation Methods

In section 2.3, we have determined the analytic structure of the ground state energy $E(g)$ of the quartic anharmonic oscillator. We have shown that $E(g)$ is analytic in a cut-plane, and calculated by instanton methods its imaginary part on the cut for g small and negative. On the other hand, perturbation theory yields $E(g)$ for g small as a power series in g:

$$E(g) = \sum_{k=0}^{\infty} E_k g^k . \tag{7.1}$$

In this chapter, we estimate the behaviour of the coefficients E_k when the order k becomes large by relating it to the behaviour of $\operatorname{Im} E(g)$ for $g \to 0_-$. We then generalize the method to the class of potentials for which we have calculated instanton contributions. The same method can be readily applied to boson field theories [16, 17, 3] using the results of chapter 3, while the extension to field theories involving fermions requires, as we show, solving some additional problems [26].

We already know that the expansion (7.1) is divergent for all values of g. This implies that, even for g small, the series does not determine the function $E(g)$ uniquely. We thus examine the implications of the large order behaviour for the problem of the summation of the series. Finally, we describe a few practical methods commonly used to sum divergent series of the type met in quantum mechanics and quantum field theory. Some of these methods have been successfully applied to the $(\phi^2)^2$ field theory in two and three dimensions and have led to precise predictions of critical exponents, universal quantities relevant to the theory of continuous phase transitions.

7.1 Quantum mechanics

We first consider two situations where we have already found instantons, both related to quantum metastability. We then argue that for other analytic potentials complex solutions to the Euclidean equation of motion are also relevant.

7.1.1 Metastable states: Real instantons

The quartic anharmonic oscillator. We first consider the ground state energy $E(g)$ of the quartic anharmonic oscillator introduced in section 2.3. Since $E(g)$ is analytic in the cut-plane and behaves like $g^{1/3}$ for g large, it has a Cauchy representation of the form

$$E(g) = \frac{1}{2} + \frac{g}{\pi} \int_{-\infty}^{0} \frac{\operatorname{Im} E(g')\,\mathrm{d}g'}{g'(g'-g)}. \tag{7.2}$$

Expanding the integrand in powers of g, one obtains an integral representation for the coefficients E_k:

$$E_k = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\operatorname{Im} E(g)\,\mathrm{d}g}{g^{k+1}} \quad \text{for } k > 0\,. \tag{7.3}$$

When k, the order in the expansion, becomes large, due to the factor g^{-k} the dispersion integral (7.3) is dominated by the small negative g values. In section 2.3, we have calculated $\operatorname{Im} E(g)$ for g small and negative. We can here use this result to estimate the large k behaviour of E_k:

$$E_k \underset{k\to\infty}{\sim} \frac{1}{\pi} \int^{0-} \left(\frac{8}{\pi}\right)^{1/2} \frac{1}{\sqrt{-g}} \frac{\mathrm{e}^{4/3g}}{g^{k+1}} \left[1 + O(g)\right] \mathrm{d}g\,. \tag{7.4}$$

The explicit integration yields

$$E_k = (-1)^{k+1} \left(\frac{6}{\pi^3}\right)^{1/2} \left(\frac{3}{4}\right)^{k} \Gamma(k+1/2) \left[1 + O\left(1/k\right)\right]. \tag{7.5}$$

The factor $\Gamma(k+1/2)$ is thus responsible for the divergence of the series.

Successive corrections to the semi-classical result yield a series in powers of g which, integrated, generates a systematic expansion in powers of $1/k$.

Remark. We note that for $g > 0$, the stable situation, the series is alternating due to sign factor, while in the metastable situation $g < 0$ all terms have the same sign.

General potentials. The same argument is applicable to the generic situation described in section 2.1. We can calculate the energy of the metastable state in power series of the coupling constant g by making a systematic expansion around the relative minimum of the potential. On the other hand we can, as above, derive from the knowledge of the imaginary part of the energy level for small coupling, an estimate of the behaviour of the perturbative coefficients at large order. Let us consider the action

$$\mathcal{S}(q) = \int \mathrm{d}t \left[\tfrac{1}{2}\dot{q}^2(t) + g^{-1} V(q\sqrt{g})\right], \tag{7.6}$$

where here g plays the role of $\hbar$.

The analogue of the dispersion integral (7.3) is

$$E_k \sim \frac{1}{\pi}\int_0^{\infty} \frac{\operatorname{Im} E(g)}{g^{k+1}} \mathrm{d}g\,.$$

The behaviour of $\operatorname{Im} E(g)$ for g small is given by expression (2.13) with the changes $m = 1$, $E_0 \mapsto E_0/\hbar$ and $\hbar \mapsto g$:

$$\operatorname{Im} E_0 \sim \frac{1}{2i}\left[\det{}'(MM_0^{-1})\right]^{-1/2} \sqrt{\frac{A}{2\pi g}}\, \mathrm{e}^{-A/g}\,. \tag{7.7}$$

Integrating near $g = 0$, one obtains

$$E_k \sim \frac{1}{i(2\pi)^{3/2}}\left[\det{}'(MM_0^{-1})\right]^{-1/2} A^{-k}\Gamma(k+1/2), \tag{7.8}$$

where A is the classical action

$$A = 2\int_0^{q_0} \sqrt{2V(q)}\,\mathrm{d}q > 0\,. \tag{7.9}$$

We now see generic features emerge: at large orders, the perturbative coefficients E_k behave like

$$E_k \underset{k\to\infty}{\sim} Ck^{b-1}k!\,A^{-k}. \tag{7.10}$$

The factor $k!$ is universal and characteristic of the semi-classical or loop expansion. It shows that the perturbation series is a divergent series. The factor A^{-k} depends only on the action, since it is the action of the classical solution; in particular, it also characterizes the behaviour at large orders of the excited energy levels or of correlation functions. The power k^b comes from the power of g in front of the result. It depends, in particular, on the number of continuous symmetries broken by the classical solution, but it would also change if we considered an excited state rather than the ground state. This can be verified by explicitly calculating the imaginary parts of the energy of the excited levels. The parameter b is in general a half integer. Finally, there is a constant multiplicative factor C which depends in a more complicated way of the expanded quantity.

Discussion. In both examples, we have calculated the large order behaviour of perturbation series from the decay rate, due to barrier penetration, of a metastable minimum of the potential. In particular, we have found that in the metastable case, all terms of the series at larger order have the same sign since either A is positive or g is negative.

By contrast, for g positive, in which case perturbation series has been expanded around the stable minimum of the potential, we observe that the perturbative coefficients oscillate in sign. Moreover, we note that for $g > 0$, the instanton solution becomes purely imaginary. This helps to understand how the large behaviour in the generic stable situation can be determined.

7.1.2 Complex instantons

Up to now, we have characterized the large order behaviour of perturbation theory in two cases, in the generic case in which we expand around a relative minimum of the potential, and in one special case in which we were expanding around an absolute minimum of the potential, but which by analytic continuation in the coupling constant could become a relative one.

We now consider actions of the form (7.6), in which the potential $V(q)$ is an entire function of q. We assume that perturbation theory is expanded around $q = 0$, the absolute minimum of the potential.

Then, clearly no real instanton solution can be found. Following the example of the anharmonic oscillator, we thus assume that we can introduce parameters in the potential that allow an analytic continuation to a metastable situation. We then obtain the large order behaviour from the expression (7.8). We then invert the analytic continuation to return to the initial situation. We expect that the large behaviour of the initial expansion will be given by the analytic continuation of the expression (7.8).

We can now formulate the rules of the large order behaviour calculation directly in the initial theory: to the complex zeros (at finite or infinite distance) of the potential $V(q)$ are associated complex instanton solutions, with, in general, complex (or exceptionally negative) action. These instantons are candidates to contribute to the large order behaviour. In the expression (7.8), we see that the action(s) with the smallest modulus (when the action is complex, there will be at least two complex conjugate actions) gives the dominant contribution to the large order behaviour. Note that the instanton solutions always start from a minimum of the potential and return to the same minimum.

Let us stress, here, that the difference we have found between the anharmonic oscillator and the metastable case is generic. In the stable case, the classical action is non-real positive, and the perturbative coefficients at large order have an order-dependent phase factor. This property has direct implications for the summability of divergent series (see section 7.6).

7.1.3 Potentials with degenerate minima

The preceding discussion does not immediately apply to the case of potentials with degenerate minima because no solution can be found that starts from a minimum and return to the same minimum. However, let us consider such a potential as the limit of a potential which has two minima at which the values of the potential are very close and assume that we have expanded around the relative minimum. From the explicit form of the action, we see that the classical action has a limit that is twice the action (1.19) of the instanton that connects the two minima of the potential:

$$A = 2\int_{-\infty}^{+\infty} \mathrm{d}t\, \dot{q}_c^2(t) = 2\int_{-q_0}^{+q_0} \mathrm{d}q\, \sqrt{2V(q)}\,.$$

Alternatively, one can verify that the same result is obtained when one starts from the absolute minimum of the potential. The asymptotic configuration has converges to the succession of an instanton and its time reversed, often called anti-instanton.

As a consequence, even though we consider here a stable situation, the action of the instanton is positive like in the metastable situation, a problem that requires a deeper analysis. This is the source of serious difficulties when one tries to sum the perturbation series. The solution requires a multi-instanton analysis [27, 5, 6].

Gaussian integration. One verifies that the amplitude in front of the expression (7.8) diverges the degenerate limit. This result can be easily understood. When the values at the two minima approach each other, the time spent close to the second minimum of the potential by the classical trajectory corresponding to the instanton solution diverges: the instanton decomposes in the sequel of an instanton and an anti-instanton, each with its own collective coordinate: therefore, fluctuations which tend to change this time leave the action almost stationary. Correspondingly one eigenvalue of the operator $\delta^2 S(q_c)/\delta q \delta q$ goes to zero, and this explains the divergence of expression (7.8) in this case. To obtain the correct answer, one must introduce a second time collective coordinate to integrate over these fluctuations.

Non-Abelian gauge theories. [28] We discuss in the coming sections the application of these methods to quantum field theory. However, anticipating this discussion, let us point out that in non-Abelian gauge theories the classical vacuum has a periodic structure (section 6.3) and the degeneracy is lifted by instantons. In the same way as for the periodic cosine potential, the semi-classical contributions to the large order behaviour are governed by instanton-anti-instanton configurations.

7.2 Scalar field theory

In chapter 3, we have shown how to evaluate the contributions of instantons to the decay rate of metastable states. These results can be applied to large order behaviour estimates. In a general scalar boson field theory, if instanton solutions can be found, the same arguments lead to

$$\left\{ Z^{(n)}(x_1, \ldots, x_n) \right\}_k \underset{k \to \infty}{\sim} \sum_{\substack{\text{dominant} \\ \text{saddle points}}} C_n(x_1, \ldots, x_n) k^{b-1} A^{-k} k! \,, \qquad (7.11)$$

in which

(i) A is the instanton action, which is in general complex;

(ii) $b = \frac{1}{2}(n + \delta)$ and δ is the number of symmetries broken by the classical solution;

(iii) $C_n(x_1, \ldots, x_n)$, which does not depend on k, contains the whole dependence in the external arguments.

In the case of the ϕ^4 field theory, the discontinuity across the cut of the n-point function reads (equation (3.22), note the change in notation $A \mapsto -A$)

$$\text{disc.}\, Z^{(n)}(x_1, \ldots, x_n) \underset{g \to 0_-}{\sim} \left(\frac{A}{2\pi} \right)^{d/2} \Omega \frac{e^{A/g}}{(-g)^{(d+n)/2}} F_n(x_1, \ldots, x_n) \qquad (7.12)$$

Table 7.1

The coefficients β_k of the coupling constant RG function $\beta(g)$ divided by the large order estimate for the $O(N)$ symmetric $(\boldsymbol{\phi}^2)^2_3$ field theory.

k	2	3	4	5	6	7
$N=0$	3.53	1.55	1.185	1.022	0.967	0.951
$N=1$	3.98	1.75	1.32	1.120	1.050	1.023
$N=2$	4.82	2.09	1.53	1.29	1.20	1.15
$N=3$	6.14	2.58	1.86	1.55	1.41	1.35

with

$$\Omega = \left(\det M' M_0^{-1}\right)^{-1/2}_{\text{ren}}$$

and

$$F_n(x_1,\ldots,x_n) = m^{d+n(d-2)/2} 6^{n/2} \int \mathrm{d}^d x_0 \prod_{i=1}^{n} f\bigl(m(x_i - x_0)\bigr). \tag{7.13}$$

Using previous arguments, we can immediately translate this result into a large order behaviour estimate for correlation functions

$$\left\{Z^{(n)}(x_1,\ldots,x_n)\right\}_k = \frac{1}{2i\pi}\int_{-\infty}^{0} \frac{\mathrm{d}g}{g^{k+1}} \operatorname{disc} Z^{(n)}(x_1,\ldots,x_n)$$

and, therefore,

$$\left\{Z^{(n)}(x_1,\ldots,x_n)\right\}_k \underset{k\to\infty}{\sim} \frac{1}{2i\pi}\frac{\Omega}{(2\pi)^{d/2}} F_n(x_1,\ldots,x_n) \frac{\Gamma\bigl(k+(d+n)/2\bigr)}{A^{n/2+k}}. \tag{7.14}$$

Example: the renormalization group β-function in the $(\boldsymbol{\phi}^2)^2$ field theory in dimension 3. The large order behaviour has been determined by solving the field equations numerically to determine the classical action A [15] and then by evaluating the determinant [31]. The predictions of the asymptotic formulae have been compared with the terms of the series which have been calculated. The agreement is quite reasonable and gives us confidence that the large order behaviour estimates are indeed correct (see table 7.1).

7.3 The ϕ^4 field theory in four dimensions

As a by-product of the calculation of the instanton contribution in sections 5–5.3, we can evaluate the semi-classical contribution to the large order behaviour in the ϕ^4 field theory in four dimensions [16, 17]. However, because the theory is exactly renormalizable, it has been found out that, as a consequence of their large momenta properties, individual diagrams at order k grow themselves like $k!$, introducing some new complications in the large order behaviour analysis [29]. Moreover, IR singularities in the massless theory also yield contributions of order $k!$, but with a different sign [30].

7.3.1 Semi-classical contribution

The instanton contribution to the large order behaviour is given by

$$\left\{\Gamma^{(n)}(p_1,\ldots,p_n)\right\}_k = \frac{1}{\pi}\int_{-\infty}^{0} \frac{\operatorname{Im}\Gamma^{(n)}(p_1,\ldots,p_n)}{g^{k+1}}\mathrm{d}g\,. \qquad (7.15)$$

This yields a result of the form

$$\left\{\Gamma^{(n)}(p_1,\ldots,p_n)\right\}_k \underset{k\to\infty}{\sim} C_n(p_1,\ldots,p_n)\int^{0-} \frac{\mathrm{e}^{8\pi^2/3g}}{(-g)^{n+5/2}}\frac{\mathrm{d}g}{g^{k+1}}\,. \qquad (7.16)$$

After integration, one obtains

$$\left\{\Gamma^{(n)}(p_1,\ldots,p_n)\right\}_k \sim C_n(p_1,\ldots,p_n)(-1)^k\left(\frac{3}{8\pi^2}\right)^{n+3+k}\Gamma(k+n/2+5/2). \qquad (7.17)$$

From this expression, it is straightforward to derive the large order behaviour of various RG functions in, for example, the fixed momentum subtraction scheme. A comparison between large order behaviour and explicit calculations can be found in table 7.2, in the case of the RG β-function.

Table 7.2

The coefficients β_k of the RG β-function divided by the asymptotic estimate, in the case of the $O(N)$ symmetric ϕ_4^4 field theory.

k	2	3	4	5
$N=1$	0.10	0.66	1.08	1.57
$N=2$	0.06	0.49	0.87	1.32
$N=3$	0.04	0.33	0.66	1.09

The large order behaviour of Wilson–Fisher's ε-expansion, which is important for the theory of critical phenomena, can instead only be guessed at because the RG functions in the minimal subtraction scheme vanish at leading order. A calculation of the next order would be necessary and this has not yet been done. Since at leading order the fixed point constant $g^*(\varepsilon)$ is

$$6g^*(\varepsilon) \sim 48\pi^2\varepsilon/(N+8)\,,$$

except if for some unknown reason the accident of leading order persists, the ε-expansion is likely to involve a factor $(-3/(N+8))^k k!$ multiplied by an unknown power of k.

Finally, note that in the massive theory the calculation is slightly modified because the integral over the collective dilatation coordinate is cut at a scale of order $m\sqrt{k}$ (see section 5.4).

7.3.2 UV and IR (renormalons) contributions

Implicit in the large order behaviour calculation is the assumption that the singularities of correlation functions come entirely, in the neighbourhood of the origin, from barrier penetration effects. If this assumption is certainly correct in quantum mechanics, if we have convincing evidence that it is valid for super-renormalizable theories, it is much more questionable for renormalizable theories, not to mention massless renormalizable theories. Indeed, individual diagrams can then have a $k!$ behaviour while the $k!$ of the semi-classical analysis comes from the number of Feynman diagrams.

We first explain the large momentum problem [29] and then the IR problem of massless theories [30].

UV singularities: renormalons [29]. If the semi-classical analysis is valid for the regularized field theory, it becomes somewhat formal for the renormalized theory in the infinite cut-off limit. We have already seen in section 5.3 that even in the naive calculation, non-trivial questions arise about the global RG properties of the theory. Direct investigation of the perturbative expansion raises new questions and suggests that UV singularities yield additional contributions to the large order behaviour.

Let us consider the $(\boldsymbol{\phi}^2)^2$ field theory in dimension 4, in which $\boldsymbol{\phi}$ is an N-component vector, and the model has an $O(N)$ symmetry,

$$\mathcal{S}(\boldsymbol{\phi}) = \int \mathrm{d}^4 x \left[\frac{1}{2}\left(\partial_\mu \boldsymbol{\phi}(x)\right)^2 + \frac{m^2}{2}\boldsymbol{\phi}^2(x) + \frac{g}{4}\left(\boldsymbol{\phi}^2(x)\right)^2\right]. \tag{7.18}$$

It can be shown that at order $1/N$ in the large N expansion the renormalized two-point function is given by a divergent integral because the integrand has a pole, corresponding to the Landau ghost. We briefly recall the argument. The $1/N$ contribution to the two-point function in the massive renormalized theory is

$$F_2(p) = \frac{2g}{(2\pi)^4}\int \frac{\mathrm{d}^4 q}{[(p+q)^2+m^2]\,[1+NgB_\mathrm{r}(q)]} - \text{subtractions}\,, \tag{7.19}$$

where the renormalized 'bubble' diagram is given by

$$B_\mathrm{r}(p) = \frac{1}{(2\pi)^4}\int \frac{\mathrm{d}^4 q}{[(p+q)^2+m^2]\,(q^2+m^2)} - \text{subtraction}\,. \tag{7.20}$$

For large momenta, $B_\mathrm{r}(p)$ behaves like

$$B_\mathrm{r}(p) \sim \frac{1}{8\pi^2}\ln(m/p)\,, \quad p \ \to \infty\,. \tag{7.21}$$

Therefore, the sum of the bubble diagrams that appears in expression (7.19) has a singularity for g small (which justifies the large momentum approximation) and positive at momentum

$$|p| \sim m\,\mathrm{e}^{8\pi^2/\mathbf{N}g} \quad \text{for } g \to 0_+\,. \tag{7.22}$$

Since the theory is IR free, and not UV asymptotically free, this singularity occurs for positive values of the coupling constant. Once this sum of bubbles is inserted into expression (7.19), it produces a cut for g small and positive. More precisely, after subtraction, and for q large, the integrand of F_2 at large momenta behaves like

$$\int_{|q|\gg 1} \frac{\mathrm{d}q}{q^3}\left[1+\frac{Ng}{8\pi^2}\ln(m/q)\right]^{-1} + \cdots\ . \tag{7.23}$$

The change of variables $t = \ln(q/m)$ transforms the expression (7.23) into

$$\int^{\infty} \mathrm{d}t\ \mathrm{e}^{-2t}\,\frac{1}{1-Ngt/(8\pi^2)}. \tag{7.24}$$

This yields an imaginary contribution to the correlation functions for g small and positive of the form $\exp(-16\pi^2/Ng)$. Alternatively, by expanding expression (7.19) in powers of g, we obtain the contribution of individual diagrams containing bubble insertions. These diagrams behave like $(N/16\pi^2)^k k!$ at large order k. Therefore, in contrast to super-renormalizable theories in which an individual diagram behaves like a power in k and the $k!$ comes from the number of diagrams, here some individual diagrams give a $k!$ contribution, without the sign oscillations characteristic of the semi-classical result.

Further investigations show that if a non-perturbative contribution exists, it should satisfy the homogeneous RG equations. Let us for simplicity consider the case of a dimensionless ratio of correlation functions $R(p/m, g)$ without anomalous dimensions,

$$\left(m\frac{\partial}{\partial m}+\beta(g)\frac{\partial}{\partial g}\right)R(p/m,g)=0\,. \tag{7.25}$$

The RG equation tells us that the function $R(p/m, g)$ is actually a function of only one variable $s(g)p/m$, in which $s(g)$ then satisfies

$$\beta(g)s'(g) = s(g), \tag{7.26}$$

which after integration yields

$$s(g)\sim\exp\left[\int^{g}\frac{\mathrm{d}g'}{\beta(g')}\right]. \tag{7.27}$$

For g small, $s(g)$ behaves like

$$\beta(g) = \beta_2 g^2 + O\left(g^3\right) \quad \text{with} \quad \beta_2 = \frac{N+8}{8\pi^2}, \tag{7.28}$$

$$s(g) \underset{g\to 0}{\propto} g^{-\beta_3/\beta_2^2}\,\mathrm{e}^{-1/\beta_2 g}\,. \tag{7.29}$$

Since the correlation function depends only on the mass squared, only $s^2(g)$ enters the calculation, and the contribution to the large order behaviour has the form

$$\int_0 \frac{s(g)}{g^{k+1}}\mathrm{d}g \propto (\beta_2/2)^k \Gamma(k+1+2\beta_3/\beta_2^2), \tag{7.30}$$

a result which coincides in the large N limit with the contribution that we obtained from the set of bubble diagrams.

This potential contribution has to be compared with the semi-classical result (7.17).

These problems are in fact related to the question of the existence of the renormalized ϕ^4 field theory in four dimensions. If the theory does not exist, then probably the sum of perturbation theory is complex for g positive, and these singular terms, sometimes called *renormalon* effects, are the small coupling evidence of this situation. More generally, the existence of renormalons shows that the perturbation series is not Borel summable and does not define unique correlation functions.

Finally, we note that, at leading order in the $1/N$ expansion, for the Wilson–Fisher ε-expansion, and thus also for suitably defined RG functions, the renormalon singularities cancel. We conjecture on this basis and on the basis of the numerical evidence that the ε-expansion is free of renormalon singularities.

Massless renormalizable theories [30]. We again illustrate the problem with the $(\boldsymbol{\phi}^2)^2$ field theory in the large N limit. We now work in a massless theory with fixed cut-off Λ. We evaluate the contribution of the small momentum region to the mass renormalization constant. The bubble diagram (7.20) behaves like

$$I(p) \sim \frac{1}{8\pi^2}\ln(\Lambda/p).$$

The sum of bubbles yields a contribution to the mass renormalization proportional to

$$\int^{\Lambda} \frac{\mathrm{d}^4 q}{q^2\bigl(1+NgI(q)\bigr)} = \int \frac{\mathrm{d}^4 q}{q^2\bigl(1+\frac{N}{8\pi^2}g\ln(\Lambda/q)\bigr)}\,.$$

Expanded in powers of g this yields a contribution of order $(-1)^k(N/16\pi^2)^k k!$ for large order k. This contribution has the sign oscillations of the semi-classical term. More generally for finite N one finds $(-\beta_2/2)^k k!$. IR singularities yield an additional Borel summable contribution to the large order behaviour.

For massless, but asymptotically free theories the role of the IR and UV regions are interchanged. UV renormalons are expected yielding additional singularities to the Borel transform on the real negative axis, while IR contributions destroy Borel summability. When these theories have real instantons like QCD or the $CP(N-1)$ models (see sections 6.2, 6.3), the Borel transform has also semi-classical singularities on the real positive axis.

7.4 Field theories with fermions

In the case of boson field theories, we have related the large order behaviour of perturbation theory to the decay of a metastable vacuum for, in general, unphysical values of the coupling constant. We expect some modifications in the case of self-interacting fermions, or of fermions interacting with bosons that themselves have no self-interaction. (The first case can be reduced to the second one by introducing an auxiliary boson field but additional difficulties then arise.) Indeed, the Pauli principle makes the decay of the false vacuum more difficult because several fermions cannot be in the same state to generate a classical field, and this effect is especially strong in low dimensions. Note that if the bosons have self-interactions, these interactions will, in general, drive the decay of the vacuum, and the fermions may no longer play a role.

Seen from the point of view of integrals, the difference between fermions and bosons is also immediately apparent. We have shown that the simple integral counting the number of Feynman diagrams, which is also the ϕ^4 field theory in $d = 0$ dimensions, already has the characteristic $k!$ behaviour at large orders. Let us instead consider a zero-dimensional fermion theory, that is, an integral over a finite number of fermion degrees of freedom:

$$I(\lambda) = \int \prod_{i=1}^{N} \mathrm{d}\bar{\xi}_i \mathrm{d}\xi_i \exp\left[\bar{\xi}_i D_{ij} \xi_j + \lambda C_{ijkl} \bar{\xi}_i \bar{\xi}_j \xi_k \xi_l\right]. \tag{7.31}$$

The quantities ξ_i and $\bar{\xi}_i$ are anticommuting variables and D_{ij} and C_{ijkl} are a set of numbers. Because we assume a finite number of anticommuting variables, the expansion of the exponential yields a polynomial and thus $I(\lambda)$ is a polynomial in λ.

7.4.1 Example of a Yukawa-like field theory

We now consider the vacuum amplitude or partition function of the Yukawa-like theory with Dirac fermions $\bar{\psi}(\mathbf{x})$, $\psi(\mathbf{x})$, and a scalar boson $\phi(\mathbf{x})$ without self-interaction:

$$\mathcal{Z} = \int [\mathrm{d}\phi(\mathbf{x})] \left[\mathrm{d}\bar{\psi}(\mathbf{x})\right] [\mathrm{d}\psi(\mathbf{x})] \exp\left[-\mathcal{S}(\phi, \bar{\psi}, \psi)\right], \tag{7.32}$$

in which the action is

$$\mathcal{S}(\phi, \bar{\psi}, \psi) = \int \mathrm{d}^d x \left[-\bar{\psi}\left(\partial\!\!\!/ + M + \lambda\phi\right)\psi + \tfrac{1}{2}\left(\partial_\mu \phi\right)^2 + \tfrac{1}{2} m^2 \phi^2\right], \tag{7.33}$$

where we choose $\lambda > 0$. In this form, $g = \lambda^2$ is a loop expansion parameter and the partition function a series in g. Since a fermion field has no classical limit, the expression (7.32) is not very well suited to the study of the vacuum decay. In fact, we expect the fermion fields to generate an effective interaction for the boson field $\phi(\mathbf{x})$, and this effective interaction will lead to the decay of the vacuum. This suggests that we should integrate over the ψ and $\bar{\psi}$ variables, and study the instantons of the effective theory for $\phi(\mathbf{x})$. In addition, the zero-dimensional example has shown that the fermion integration gives some hints about the analytic structure of the theory. After the integration over ψ and $\bar\psi$, we obtain

$$\mathcal{Z} = \int [\mathrm{d}\phi(\mathbf{x})] \det\left\{[\not\partial + M + \lambda\phi(\mathbf{x})]\,[\not\partial + M]^{-1}\right\}$$
$$\times \exp\left[-\tfrac{1}{2}\int \mathrm{d}^d x\big((\partial_\mu\phi)^2 + m^2\phi^2\big)\right], \tag{7.34}$$

where we have normalized the integral with respect to the free theory.

We are faced with a new difficulty arising from the integration, the effective action now is no longer local in $\phi(\mathbf{x})$, and leads to non-local field equations. However, because we are concerned only with the determination of the large behaviour, we can simplify the effective action. The determinant generated by the fermion integration is, at least for the class of relevant $\phi(\mathbf{x})$ fields, an entire function of the coupling constant λ. As a consequence, essential singularities can only be generated by the infinite range of the ϕ-integration. It is thus sufficient to calculate the contribution to the functional integral of large fields $\phi(\mathbf{x})$ [37]. This situation has to be contrasted with what would have happened if $\psi(\mathbf{x})$ and $\bar\psi(\mathbf{x})$ would have been commuting variables. The integration then would have generated the inverse of the determinant, a function that has singularities for all zeros in λ of the determinant. These singularities would have yielded essential singularities in the coupling constant after integration. Finally, we note that this difference, determinant versus inverse determinant, is responsible for the minus sign for each fermion loop in perturbation theory, which allows for cancellations.

7.4.2 The determinant

The contribution to the action generated by the fermion integration can be written as

$$\Sigma(\phi) \equiv -\ln\det\left(\mathbf{1} + \lambda\,\boldsymbol{\Xi}\right) \tag{7.35}$$

with

$$\boldsymbol{\Xi} = (\not\partial + M)^{-1}\phi(\mathbf{x}),$$

an expression that, for instanton purpose, we have to evaluate for large (and smooth enough) fields ϕ decaying at infinity.

The perturbative expansion of the expression (7.35) involves the successive traces of $\boldsymbol{\Xi}$. Both $\operatorname{tr}\boldsymbol{\Xi}$ and $\operatorname{tr}\boldsymbol{\Xi}^2$ are divergent for $d \geq 2$ and have to be renormalized:

$$\begin{aligned}
\operatorname{tr}\boldsymbol{\Xi} &= \int \mathrm{d}^d x\, \phi(x)\frac{1}{(2\pi)^d}\operatorname{tr}_\gamma \int \frac{\mathrm{d}^d p}{i\not{p}+M} = \int \mathrm{d}^d x\, \phi(x)\frac{NM}{(2\pi)^d}\int \frac{\mathrm{d}^d p}{p^2+M^2},\\
\operatorname{tr}\boldsymbol{\Xi}^2 &= \int \mathrm{d}^d x\,\mathrm{d}^d y\, \phi(x)\phi(y)\frac{1}{(2\pi)^{2d}}\operatorname{tr}_\gamma \int \mathrm{d}^d p\,\mathrm{d}^d q \frac{\mathrm{e}^{i(x-y)p}}{(i\not{q}+M)(i(\not{p}+\not{q})+M)}\,,\\
&= \int \mathrm{d}^d x\,\mathrm{d}^d y\, \phi(x)\phi(y)\frac{N}{(2\pi)^{2d}}\int \mathrm{d}^d p\,\mathrm{d}^d q \frac{\mathrm{e}^{i(x-y)p}(M^2-q^2-pq)}{(q^2+M^2)((p+q)^2+M^2)}\,,\\
&= -\int \mathrm{d}^d x\, \phi^2(x)\frac{N}{(2\pi)^d}\int \frac{\mathrm{d}^d q}{q^2+M^2}\\
&\quad + \int \mathrm{d}^d x\,\mathrm{d}^d y\, \phi(x)\phi(y)\frac{N}{(2\pi)^{2d}}\int \frac{\mathrm{d}^d p\,\mathrm{d}^d q\ \mathrm{e}^{i(x-y)p}(p^2/2+M^2)}{(q^2+M^2)((p+q)^2+M^2)}\,,
\end{aligned}$$

where tr_γ means trace over Dirac γ-matrices and $N = \operatorname{tr}_\gamma \mathbf{1}$. We can choose the counter-terms such that

$$\begin{aligned}
&\operatorname{tr}\boldsymbol{\Xi}_{\text{ren.}} = 0\,,\\
&\operatorname{tr}\boldsymbol{\Xi}^2_{\text{ren.}} = \int \mathrm{d}^d x\,\mathrm{d}^d y\, \phi(x)\phi(y)\frac{N}{(2\pi)^{2d}}\int \frac{\mathrm{d}^d p\,\mathrm{d}^d q\ \mathrm{e}^{i(x-y)p}(p^2/2+M^2)}{(q^2+M^2)((p+q)^2+M^2)}\,.
\end{aligned}$$

Then, $\operatorname{tr}\boldsymbol{\Xi}^3$ and $\operatorname{tr}\boldsymbol{\Xi}^4$ are only divergent for $d \geq 4$. Since the higher order traces are finite, the operator $\boldsymbol{\Xi}$ has a discrete spectrum. We denote by $\xi_n(\phi)$ the eigenvalues. The eigenvalues accumulate at the origin. Then, for $d < 4$,

$$\Sigma_{\text{ren.}}(\phi) = -\sum_n \left[\ln\bigl(1+\lambda\xi_n(\phi)\bigr) - \lambda\xi_n(\phi) + \tfrac{1}{2}\lambda^2\xi_n^2(\phi)\right] - \tfrac{1}{2}\lambda^2 \operatorname{tr}\boldsymbol{\Xi}^2_{\text{ren.}}$$

This expression shows that the determinant is an entire function of λ.

7.4.3 Evaluation of the fermion determinant for large fields

We now evaluate the large field or large λ contribution [37]. For convenience we set

$$M + \lambda\phi(\mathbf{x}) = \kappa V(\mathbf{x}),$$

and we differentiate Σ with respect to the parameter κ using the identity

$$\mathrm{d}(\ln\det\Omega) = \operatorname{tr}\mathrm{d}\Omega\,\Omega^{-1}.$$

We find

$$\Sigma'(\kappa) = -\operatorname{tr}_\gamma \int \mathrm{d}^d x\, V(\mathbf{x})\,\langle\mathbf{x}|\left[\not{\partial}+\kappa V\right]^{-1}|\mathbf{x}\rangle\,.$$

In the large V (and V smooth enough) or equivalently large κ limit, the operator $\left[\not{\partial}+\kappa V\right]^{-1}$ tends toward a local operator and the operator V can be replaced by its expectation value $V(\mathbf{x})$ in the state $|\mathbf{x}\rangle$. The calculation of the matrix element is then simple:

$$\begin{aligned}\langle \mathbf{x}| \left[\not{\partial} + \kappa V\right]^{-1} |\mathbf{x}\rangle &= \frac{1}{(2\pi)^d}\int \mathrm{d}^d p \, \mathrm{tr}_\gamma (i\not{p} + \kappa V(\mathbf{x}))^{-1} \\ &= \frac{N}{(2\pi)^d}\kappa V(\mathbf{x})\int \frac{\mathrm{d}^d p}{p^2+\kappa^2 V^2(\mathbf{x})} \\ &= \frac{N}{(4\pi)^{d/2}}\Gamma(1-d/2)\kappa^{d-1}V(\mathbf{x})|V(\mathbf{x})|^{d-2}.\end{aligned}$$

We then integrate over κ. Substituting $\kappa V(\mathbf{x}) \mapsto M + \lambda\phi(\mathbf{x})$, neglecting M for $\lambda\phi(\mathbf{x})$ large, we obtain the large field behaviour:

$$\Sigma(\phi) \sim \frac{N}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}\int \mathrm{d}^d x \, |M + \lambda\phi(x)|^d \sim \frac{N}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}\lambda^d \int \mathrm{d}^d x \, |\phi(\mathbf{x})|^d. \tag{7.36}$$

This expression shows that the determinant is an entire function of order d in λ or of order $d/2$ in $g=\lambda^2$.

For d even, the expression diverges and the divergence is cancelled by the counter-terms required to render the one-loop diagrams finite.

We can then examine various dimensions of interest. For $d=2$, the mass counter-term has to be added and on finds

$$\Sigma(\phi) \sim \frac{N\lambda^2}{4\pi}\int \mathrm{d}^2 x \, \phi^2(\mathbf{x}) \ln|\phi(\mathbf{x})|. \tag{7.37}$$

For $d=3$,

$$\Sigma(\phi) \sim \frac{N}{12\pi}\lambda^3 \int \mathrm{d}^3 x \, |\phi(\mathbf{x})|^3 \tag{7.38}$$

and, finally, for $d=4$ a ϕ^4 coupling counter-term is required and the result becomes

$$\Sigma(\phi) \sim -\frac{N}{32\pi^2}\lambda^4 \int \mathrm{d}^4 x \, \phi^4(\mathbf{x}) \ln|\phi(\mathbf{x})|. \tag{7.39}$$

In the latter dimension, the induced term leads to an unstable local theory.

7.4.4 The large order behaviour

We can now study the essential singularity of the theory at $\lambda = 0$ small from the properties of the effective local boson action

$$\mathcal{S}_{\mathrm{eff}}(\phi) = \int \mathrm{d}^d \mathbf{x} \left[\frac{1}{2}\left(\partial_\mu \phi(\mathbf{x})\right)^2 + \frac{1}{2}m^2\phi^2(\mathbf{x}) + \frac{N}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}\lambda^d |\phi(\mathbf{x})|^d\right], \tag{7.40}$$

where the fermion term has to be replaced by its renormalized form for d even. Some care is required in handling this expression since the fermion term is only asymptotic and the exact determinant is an entire function of the coupling λ.

For $d<4$ the additional contribution leads to a stable theory and instantons correspond to complex values of λ while for $d=4$ the additional term renders the theory unstable and instantons exist for $\lambda > 0$. However, in $d = 4$ renormalization requires a ϕ^4 interaction that, generically, dominates the large order behaviour.

Formal derivation. Since the action (7.40) is not a regular function of ϕ and is unrenormalized, the arguments that follow are somewhat formal and the problem has to be analysed more carefully.

We now assume the existence of an instanton solution. We then rescale the field ϕ to factorize the g-dependence in front of the classical action:

$$\phi(\mathbf{x}) \mapsto \phi(\mathbf{x})\lambda^{-d/(d-2)}. \tag{7.41}$$

The classical action calculated for a solution takes thus the form

$$\mathcal{S}(\phi_c) = (A/\lambda^2)^{d/d-2}, \tag{7.42}$$

where A is constant. At this point it is useful to introduce the loop expansion parameter $g = \lambda^2$. Introducing this form into the Cauchy representation, we find

$$\mathcal{Z}_k \underset{k\to\infty}{\sim} \int_0 \frac{\mathrm{e}^{-(A/g)^{d/d-2}}}{g^{k-1}} \mathrm{d}g\,. \tag{7.43}$$

The integration yields the large order estimate

$$\mathcal{Z}_k \sim A^{-k}\Gamma\left[k(d-2)/d\right]. \tag{7.44}$$

We observe that, as expected, this theory is less divergent than a purely boson field theory. The boson result is recovered (in a cut-off field theory) for d large, because the Pauli principle becomes decreasingly effective when the dimension increases.

Dimension $d = 3$. This is a simple situation. The action becomes

$$\mathcal{S}_{\text{eff}}(\phi) = \int \mathrm{d}^3\mathbf{x} \left[\frac{1}{2}\left(\partial_\mu\phi(\mathbf{x})\right)^2 + \frac{1}{2}m^2\phi^2(\mathbf{x}) + \frac{N}{12\pi}\lambda^3|\phi(\mathbf{x})|^3\right].$$

Since the problem of analytic continuation in λ is not simple, we use another method. We expand the partition function in powers of λ and estimate directly

$$\zeta_k = \frac{(-1)^k}{k!}\left(\frac{N}{12\pi}\right)^k \lambda^3 \mathcal{I}_k$$

with

$$\mathcal{I}_k = \int [\mathrm{d}\phi] \left(\int \mathrm{d}^3\mathbf{x}\,|\phi(\mathbf{x})|^3\right)^k \exp\left[-\tfrac{1}{2}\int \mathrm{d}^3\mathbf{x}\left(\left(\partial_\mu\phi(\mathbf{x})\right)^2 + m^2\phi^2(\mathbf{x})\right)\right].$$

We have to look for the minimum of the quantity

$$\Sigma(\phi) = \tfrac{1}{2}\int \mathrm{d}^3\mathbf{x}\left(\left(\partial_\mu\phi(\mathbf{x})\right)^2 + m^2\phi^2(\mathbf{x})\right) - k\ln\int \mathrm{d}^3\mathbf{x}\,|\phi(\mathbf{x})|^3.$$

To extract the k dependence we set $\phi \mapsto k^{1/2}\phi$ and obtain

$$\Sigma(\phi) = \tfrac{1}{2}k \int \mathrm{d}^3\mathbf{x} \left((\partial_\mu \phi(\mathbf{x}))^2 + m^2\phi^2(\mathbf{x}) \right) - k \ln \int \mathrm{d}^3\mathbf{x}\, |\phi(\mathbf{x})|^3 - \tfrac{3}{2}k \ln k \,.$$

The corresponding field equation is

$$(-\nabla_x^2 + m^2)\phi(\mathbf{x}) - \frac{3}{I_3}\,\mathrm{sgn}(\phi(\mathbf{x}))\phi^2(\mathbf{x}) = 0\,,$$

where we have defined

$$I_3 = \int \mathrm{d}^3\mathbf{x}\, |\phi(\mathbf{x})|^3. \tag{7.45}$$

This equation has instanton solutions ϕ_c. Note that the constraint (7.45) changes the determinant. Then, integrating the field equation, we conclude that

$$\tfrac{1}{2}k \int \mathrm{d}^3\mathbf{x} \left((\partial_\mu \phi_c(\mathbf{x}))^2 + m^2\phi_c^2(\mathbf{x}) \right) = \tfrac{3}{2}k\,.$$

We conclude

$$\mathcal{I}_k \propto [I_3(\phi_c)]^k\, \mathrm{e}^{3k/2 \ln k - 3k/2}$$

and, thus,

$$\zeta_k \propto (-1)^k \left(\frac{N I_3 \sqrt{2}}{12\pi} \right)^k \Gamma(k/2)\lambda^{3k}.$$

The large order behaviour of the coefficient of g^k is then

$$\mathcal{Z}_k \propto \left(\frac{N I_3 \sqrt{2}}{12\pi} \right)^{2k/3} \Gamma(k/3),$$

a result consistent, but more explicit than the result (7.44).

The method can be generalized to generic values of d.

Dimension $d = 2$ and $d = 4$. For $d = 2$, the expression (7.44) becomes

$$\mathcal{Z}_k \propto A^{-k}(\ln k)^k, \tag{7.46}$$

in agreement with rigorous bounds that yield

$$|\mathcal{Z}_k| < (k!\,)^{\varepsilon} \quad \text{for all } \varepsilon > 0\,. \tag{7.47}$$

For $d = 4$, the expression (7.44) is also modified by the same kind of logarithmic factor

$$\mathcal{Z}_k \propto A^{-k}(\ln k)^k \Gamma(k/2). \tag{7.48}$$

However, in $d = 4$ for renormalization purpose a ϕ^4 interaction has to be added to the action (7.33), as the expression (7.40) shows. Then, in a *loop expansion* the boson contributions dominates the large order behaviour.

Alternatively, it is also consistent with renormalization to consider the ϕ^4 coupling as being of order g^2, as expression (7.40) shows. Then, both interaction terms $\bar\psi\psi\phi$ and ϕ^4 give similar contributions to the large order behaviour, up to powers of logarithm.

7.4.5 The QED problem

A potentially interesting application of the fermion analysis is QED in four dimensions. The action has formally the same structure, but one additional complication then arises. The fermion action is

$$\mathcal{S}_{\mathrm{F}} = \int \mathrm{d}^d x\, \bar{\psi}(x)\, (\not{D} + m)\, \psi(x),$$

where

$$\not{D} = D_\mu \gamma_\mu\,, \quad D_\mu = \partial_\mu + ieA_\mu\,.$$

(D_μ is the covariant derivative). The fermion integration yields the contribution to the action

$$\Sigma = -\ln\det(\not{D} + m)\,. \tag{7.49}$$

However, this expression is gauge invariant and the concept of large gauge dependent quantity A_μ is not meaningful. Moreover, the gauge degree of freedom of the gauge field cannot be considered as slowly varying. Thus, one must fix the gauge. It is convenient to choose a gauge linear in A_μ and covariant. This leads to the choice

$$\partial_\mu A_\mu(x) = 0 \;\Rightarrow\; [D_\mu, A_\mu] = 0\,.$$

In $d = 2$ dimensions, we already know from the solution of the massless Schwinger model, and from the bosonisation of the massive model, that the origin is not an essential singularity: for $m = 0$ the determinant can be calculated exactly and is related to the Abelian anomaly:

$$\Sigma(A) \equiv -\ln\det(\not{D}) = -\frac{e^2}{2\pi}\int \mathrm{d}^2 x\, A_\mu^2(x).$$

More generally, on the basis of studying the determinant for special gauge fields, it has been conjectured, that the determinant is equivalent for large e to [38, 39]

$$\Sigma(A) \sim -C(d)\int \mathrm{d}^d x\, |eA_\mu(x)|^d\,; \quad C^{-1}(d) = d(4\pi)^{(d-1)/2}\Gamma\big((d+1)/2\big).$$

This expression is local in the $\partial_\mu A_\mu = 0$ gauge but non-local otherwise. It agrees for $d = 2$ with the exact result obtained from the Abelian anomaly ($C(2) = 1/2\pi$). For $d = 4$, the case of physical interest, $C(4) = 1/12\pi^2$. The effective classical field theory then is scale invariant. Arguments related to conformal invariance can be used to construct some ansatz for the instanton solutions. Two kind of solutions have been explored [38, 39]. Taking the minimal action solution one obtains an evaluation of the form

$$\mathcal{Z}_k \sim (-1)^k A^{-k}\Gamma(k/2)\,, \quad A = 4.886\,, \tag{7.50}$$

the expansion parameter being $\alpha = e^2/4\pi$. It should be pointed out that this evaluation is probably not very useful as a practical mean to predict new orders in QED for several reasons. First, the theory is not asymptotically free and thus has a potential renormalon problem, which can be understood by inserting in a Feynman diagram the one-loop corrected photon propagator. Second, the cancellation coming from the sign of fermion loops does not seem to be very effective at low orders. Therefore, an alternative calculation, which leads to a large order behaviour at a fixed number of fermion loops, seems to be more useful. Predictions of this kind made for diagrams with one fermion loop, seem to agree well with numerical estimates.

7.5 Divergent series, Borel summability

As we have shown, most perturbative expansions in quantum field theory lead to divergent series. An important issue is whether a function can be determined from the knowledge of such a series. This is the case, in particular, if the series is Borel summable.

7.5.1 Asymptotic series

Let us consider a function $f(z)$, analytic in the sector S of the complex plane defined by

$$|\operatorname{Arg} z| \le \alpha/2\,, \quad |z| \le |z_0|. \tag{7.51}$$

We say that $f(z)$ has in S the asymptotic expansion

$$f(z) = \sum_{0}^{\infty} f_k z^k \tag{7.52}$$

if the series in the right hand side of (7.52) diverges for all $z \neq 0$ and if in S the truncated series satisfies the bound

$$\left| f(z) - \sum_{k=0}^{N} f_k z^k \right| \le F_{N+1} |z|^{N+1} \quad \forall\, N\,. \tag{7.53}$$

(This implies $F_N \ge |f_N|$.) Though the series (7.52) diverges, it is possible to use it to estimate the function $f(z)$ for $|z|$ small. At $|z|$ fixed, we can look for a minimum in the bound (7.53) when N varies. If $|z|$ is small enough, the bound first decreases with N and then, since the series is divergent, finally increases. If we truncate the series at the minimum, we get the best possible estimate of $f(z)$, with a finite error $\varepsilon(z)$. Let us assume for definiteness that the coefficients F_N have the form

$$F_N = M\, A^{-N} (N!)^{\beta}. \tag{7.54}$$

We can then estimate $\varepsilon(z)$ explicitly and find

$$\varepsilon(z) = \min_{\{N\}} F_N |z|^N \sim \exp\left[-\beta (A/|z|)^{1/\beta}\right]. \tag{7.55}$$

Therefore, an asymptotic series does not in general define a unique function. Indeed, if one function has been found that satisfies the bounds (7.53), we can add to it any function analytic in the sector (7.51) and bounded by $\varepsilon(z)$ in the whole sector. The new function still satisfies the bounds (7.53). However, there is one situation in which the asymptotic series defines a unique function. If the angle α satisfies: $\alpha \geq \pi\beta$, then a classical theorem about analytic functions tells us that a function analytic in the sector and bounded by $\varepsilon(z)$ in the whole sector vanishes identically.

7.5.2 Borel transformation

Loopwise expansion. Even though most arguments can be easily generalized, from now on we specialize to the case $\beta = 1$, which is typical for the steepest descent method and, thus, also for perturbative expansions in quantum field theory in a loopwise expansion. One then finds

$$\alpha \geq \pi\,. \tag{7.56}$$

In the marginal case in which the series is asymptotic only in the open interval $|\operatorname{Arg} z| \in (-\pi\beta/2, \pi\beta/2)$, additional conditions have to be imposed to prove uniqueness.

Under the condition (7.56), the function $f(z)$ is uniquely defined by the series. Moreover, there then exist methods to 'sum' the series, which means that one can derive from the knowledge of the series a sequence converging to the function. One set of methods is based upon the Borel transformation.

The Borel transform $B_f(z)$ of $f(z)$ is defined by

$$B_f(z) = \sum_0^{\infty} B_k z^k \equiv \sum_0^{\infty} \frac{f_k}{k!} z^k . \tag{7.57}$$

The bounds (7.53) and the form (7.54) imply

$$|f_k/k!| < M\, A^{-k}. \tag{7.58}$$

Thus $B_f(z)$ is analytic at least in a circle of radius A and uniquely defined by the series. Furthermore, in the sense of formal power series

$$f(z) = \int_0^{\infty} \mathrm{e}^{-t}\, B_f(zt) \mathrm{d}t\,. \tag{7.59}$$

As a consequence of the inequality (7.56), it can be shown that $B_f(z)$ is also analytic in a sector

$$|\operatorname{Arg} z| \in [0, \tfrac{1}{2}(\alpha - \pi)[\,, \tag{7.60}$$

and does not increase faster than an exponential in the sector, so that integral (7.59) converges for $|z|$ small enough and inside the sector

$$|\operatorname{Arg} z| < \alpha/2\,.$$

In addition, it can be shown that the right hand side of equation (7.59) satisfies a bound of type (7.53). Hence, this integral representation yields the unique function which has the asymptotic expansion (7.52) in the domain (7.51).

7.6 Large order behaviour and Borel summability

We have learned that, for a large class of potentials in quantum mechanics and for a number of field theories, instanton contributions for small values of the loop expansion parameter g behave like

$$Cg^{-b}\,\mathrm{e}^{-a/g}\,. \tag{7.61}$$

The corresponding contribution to the perturbative coefficients for large order k of the loop expansion is then,

$$(C/\pi)k^{b-1}a^k k!\,. \tag{7.62}$$

Therefore, the coefficients B_k of the Borel transform $B(z)$ (equation (7.57)) behave as

$$B_k \sim (C/\pi)k^{b-1}a^k. \tag{7.63}$$

This asymptotic estimate tells us that the singularity of $B(z)$ closest to the origin is located at the point $z = 1/a$. More precisely, the Borel transform $B(z)$ has an algebraic singularity of the form

$$\frac{C}{\pi}\int_0 \frac{\mathrm{d}g\,\mathrm{e}^{-a/g}}{g^{b+1}}\sum_k \frac{1}{k!}\left(\frac{z}{g}\right)^k = \frac{C}{\pi}\int_0 \frac{\mathrm{d}g\,\mathrm{e}^{-(a-z)/g}}{g^{b+1}} = (C/\pi)\Gamma(b)(a-z)^{-b}.$$

Therefore, the integral (7.59) does not exist if the classical action $A = 1/a$ is positive. The perturbation series in such theories is not Borel summable. This observation has the following implications when applied to the various situations we have encountered:

(i) The field equations have no real instanton solutions. This is, in particular, the case if we have expanded around the unique absolute minimum of the potential. If complex instanton solutions exist, the corresponding classical action is non-positive, and the perturbative expansion is presumably Borel summable. It is only a presumption because various features of the perturbative expansion, invisible at large orders, could prevent still Borel summability. The perturbative expansion could contain for instance contributions all of the same sign, growing faster than any exponential of the order k, but much smaller than $k!$ (for example $\sqrt{k!}$). Then, $B(z)$ would grow too rapidly for large argument z ($\ln B(z) \sim z^2$ in the example) and the Borel integral would not converge at infinity.

(ii) We have found real instantons in the theory because we expanded around a relative minimum of the potential: the perturbative expansion is not Borel summable.

However, in this case, we can provide one additional piece of information useful for determining the solution: the unstable situation can be considered as coming from a stable situation by analytic continuation. Therefore, a possible solution could be to integrate in the Borel transform just above the cut which is on the real positive axis. As a consequence, from a real perturbative expansion we would obtain a complex result, but this is exactly what we expect. It is easy to verify that the imaginary part is for g small exactly what we have calculated directly. Actually, this is only the solution of the problem in the simplest case, when no other instanton singularities cross the contour of integration in the analytic continuation.

(iii) There are real instantons connecting degenerate classical minima.

The theory is not Borel summable. Integration above or below the axis yields a complex result for a real quantity. This cannot be the correct prescription. The half sum of the integral above and below is real, but even in the simple example of the quartic double well-potential, one can verify numerically, and argue analytically, that it is not the correct solution. In the example of one-dimensional potentials that are entire functions, one can show that the additional information needed to determine the sum of the perturbative expansion is provided by the consideration of multi-instanton contributions. The corresponding problem has not been solved in field theory examples yet.

Remarks. We have given field theory examples of such a situation in sections 6.2, 6.3: the two-dimensional $CP(N-1)$ models and four-dimensional $SU(2)$ gauge theory. In these models real instantons connect degenerate minima of the classical action and the corresponding classical action is positive. Therefore, the coefficients of the perturbative expansion contain a non-Borel summable contribution. This contribution does not necessarily dominate the large order behaviour, because, as the example of of the ϕ^4_4 massless field theory (see section 7.3.2) illustrates, when a field theory is classically scale invariant, the perturbative expansion might be dominated by contributions unobtainable by semi-classical methods, and related to the UV or IR singularities.

7.7 Practical summation methods

Various practical summation methods rely upon a Borel transformation.

The Borel transformation reduces the problem of determining the function to the analytic continuation of the Borel transform. The Borel transform is given by a Taylor series in a circle and an analytic continuation of the series on the real positive axis is required. This analytic continuation can be performed by various methods and the optimal choice depends somewhat on the additional information one possesses about the function. We give here two examples.

We give also an example of a method that does not involve a Borel transformation, the order-dependent mapping (ODM).

7.7.1 Padé approximants

In the absence of a precise knowledge of the location of the singularities of the Borel transform in the complex plane, one can use the Padé approximation [32, 33]. From the series, one derives Padé approximants which are rational functions P_M/Q_N satisfying

$$B_f(z) = \frac{P_M(z)}{Q_N(z)} + O\left(z^{N+M+1}\right), \tag{7.64}$$

where P_M and Q_N are polynomials of degrees M and N, respectively. If one knows $K+1$ terms of the series, one can construct all $[M, N]$ Padé approximants with $N+M \le K$. This method is well adapted to meromorphic functions. The main disadvantage of the method is that for a rather general class of functions, Padé approximants are known to converge only in measure and thus spurious poles may occasionally appear close to or on the real positive axis.

Even if Padé approximants converge, this property may be the source of some instabilities in the results, and, therefore, make the empirical evaluation of errors difficult.

7.7.2 Conformal mapping

If the domain of analyticity of the Borel transform is known, one can find a mapping that preserves the origin, and maps the domain of analyticity onto a circle. In the transformed variable, the new series converges in the whole domain of analyticity.

As an example, we assume that the Borel transform is analytic in a cut-plane, the cut running along the real negative axis from $-\infty$ to $-1/a$. To map the cut-plane onto a circle of radius 1, we set [34, 35]

$$z \mapsto u, \quad u(z) = \frac{\sqrt{1+az}-1}{\sqrt{1+az}+1}\,. \tag{7.65}$$

From the original series for the Borel transform, we derive a series in powers of the new variable u:

$$B_f(z) = \sum \frac{f_k}{k!} z^k, \qquad B_f[z(u)] = \sum_0^\infty B_k u^k. \tag{7.66}$$

Introducing this expansion in the Borel transformation, we obtain a new expansion for $f(z)$,

$$f(z) = \sum_0^\infty B_k I_k(z)\,, \tag{7.67}$$

in which the functions $I_k(z)$ have the integral representation:

$$I_k(z) = \int_0^\infty \mathrm{e}^{-t}\,[u(zt)]^k\,\mathrm{d}t\,. \tag{7.68}$$

It is possible to study the natural domain of convergence of this new expansion. One verifies that $I_k(z)$ for k behaves large as [26]

$$I_k(z) \sim \exp\left[-3k^{2/3}/(az)^{1/3}\right]. \tag{7.69}$$

Three situations can then arise:

(i) The coefficients B_k either decrease or at least do not grow too rapidly,

$$|B_k| < M\,\mathrm{e}^{\varepsilon k^{2/3}} \quad \text{for all } \varepsilon > 0\,.$$

Then, the expansion (7.67) converges at least in the region

$$\operatorname{Re} z^{-1/3} > 0 \ \Rightarrow\ |\operatorname{Arg} z| < 3\pi/2\,. \tag{7.70}$$

In particular, this implies that the function $f(z)$ must be analytic in the corresponding region which contains a part of the second sheet.

(ii) The coefficients behave like

$$B_k \sim \exp\left(ck^{2/3}\right) \quad \text{for } k \text{ large}. \tag{7.71}$$

The domain of convergence is, then,

$$\operatorname{Re} z^{-1/3} > \tfrac{1}{3}ca^{1/3}. \tag{7.72}$$

This condition implies analyticity in a finite domain containing a part of the second sheet since for $|z|$ small, the right hand side is negligible.

(iii) The coefficients B_k grow faster than $\exp(ck^{2/3})$. This is quite possible since the only constraint on the coefficients B_k is that the series (7.66) has a radius of convergence 1. For instance the coefficients B_k could grow like $\exp(ck^{4/5})$. In such a situation, the new series is also divergent. Such a situation arises when the singularities on the boundary of the domain of analyticity are too strong. One should map a smaller part of the domain of analyticity onto a circle.

Application to the calculation of critical exponents. In the summation method based on Borel transformation and mapping, it is easy to take into account the large order behaviour. This is one reason why it has been used quite systematically in the framework of the ϕ^4 field theory to calculate critical exponents and other universal quantities [35, 36]. Critical exponents have been calculated by applying variants of the Borel summation method to the known terms of the perturbative expansion, that is, six successive terms in fixed dimension 3 and up to order ε^5 for the ε-expansion.

Let us now summarize the information available in the ϕ^4 field theory that justifies the use of this summation method.

(i) The Borel summability of perturbation theory in the ϕ^4_2 and ϕ^4_3 theories has been rigorously established.

(ii) The large order behaviour has been determined in all cases and compares favourably with the first terms of the series available (see section 7.2).

(iii) Since all known instanton solutions in the ϕ^4 theory give negative actions, it is plausible that the Borel transform is analytic in a cut-plane, the location and nature of the singularity closest to the origin being given by the large order estimates.

Consequently, the methods based upon a Borel transformation and a conformal mapping of the cut-plane onto a circle, have appeared as excellent candidates to sum the perturbation series and the ε-expansion.

For completeness, let us finally give one example of a summation method not based on a Borel transformation.

7.7.3 Order dependent mappings (ODM)

The ODM method [40--44] requires, to be applicable, some knowledge (or educated guess) of the analyticity properties of the function itself. As we have discussed, the series diverge because the function has singularities accumulating at the origin. However, the strengths of the singularities have to decrease fast enough for the function to have a series expansion. In the examples we have met, the discontinuity of the function decreases exponentially near the origin. The idea is then to pretend that the function is analytic, in addition to its true domain of analyticity, in a small circle centred at the origin of adjustable radius ρ and to map this extended domain onto a circle centred at the origin, keeping the origin fixed. If the function would really be analytic in such a domain, the expansion in the transformed variable would converge in the whole domain of analyticity and our problem would be solved. Since the original series is in fact only asymptotic, the series in the transformed variable is also asymptotic. However, as a result of this transformation, the coefficients of the new series now depend on an adjustable parameter ρ.

Let us assume for instance that $f(z)$ is analytic in a cut-plane. We then use the mapping

$$z = 4\rho u/(1-u)^2. \tag{7.73}$$

The transformed series has the form

$$f\bigl(z(u)\bigr) = \sum_0^\infty P_k(\rho) u^k, \tag{7.74}$$

in which the coefficients $P_k(\rho)$ are polynomials of degree k in the parameter ρ. The kth order approximation is obtained by truncating the series at order k, and choosing ρ as one of the zeros of the polynomial $P_k(\rho)$. The zero cannot actually be chosen arbitrarily, but roughly speaking must be the zero of largest modulus for which the derivative $P'_k(\rho)$ is small. The idea behind the method is the following: with the original series, the best approximation is obtained by truncating the series at z fixed, at an order dependent on z such the modulus of the last term taken into account is minimal. By introducing an additional parameter, one modifies the situation: one can choose first the order of truncation and then try to adjust the parameter ρ in such a way that, at z again fixed, the last term taken into account is minimal.

The kth order approximant has the form

$$\{f(z)\}_k = \sum_{l=0}^{k} P_l(\rho_k)\,[u(z)]^l\,, \qquad P_k(\rho_k) = 0\,. \tag{7.75}$$

It can be shown under some conditions that if the terms f_k of the original series grow like $(k!)^\beta$ then the sequence ρ_k decreases like $1/k^\beta$. Such a method has been successfully applied to test problems like the quartic anharmonic oscillator and the imaginary cubic potential, and to one physical example, the hydrogen atom in a strong magnetic field.

A review about various summation methods can also be found in reference [45].

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