37 Instantons in quantum mechanics (QM)

In general, we calculate Euclidean functional integrals by the steepest-descent method always looking, in the absence of external sources, for saddle points in the form of constant solutions to the classical field equations. However, classical field equations may have non-constant solutions. In Euclidean stable field theories, non-constant solutions always have an action larger than the action of minimal constant solutions, because the gradient term gives an additional positive contribution.

In what follows, we are mainly interested in the structure of the ground state, and thus in the zero-temperature limit of the partition function. For a given constant solution, we will focus on the non-constant solutions whose relative action remains finite in this limit. These solutions are called *instanton* solutions, and are the saddle points relevant for a calculation, by the steepest-descent method, of *barrier penetration effects* [373, 374]. In this chapter, we consider the simple example of non-relativistic QM, where instanton calculus is an alternative to the semi-classical Wentzel–Kramers–Brillouin (WKB) method but, in the coming chapters, we show how the instanton method can be generalized to field theory.

We explain the role of instantons in some metastable systems in QM. In particular, we show that instantons determine, in the semi-classical limit, the decay rate of metastable states initially confined in a relative minimum of a potential and decaying through barrier penetration.

Using the technical tools developed in Ref. [375], we first discuss the quartic anharmonic oscillator with negative coupling and calculate the contributions of instantons at leading order. We then generalize the method to a large class of analytic potentials, and obtain explicit expressions, at leading order, for one-dimensional systems.

In the appendix, we give an exact expression for the Jacobian, due to collective coordinates, in the case of path integrals. We describe how semi-classical expressions can be derived from calculations based on the WKB method.

Finally, let us point out that, although we only deal here with Euclidean theories, many aspects of the techniques we describe also apply to the calculation of effects coming from finite energy solutions of the real-time field equations, called *soliton* solutions in the literature.

37.1 The quartic anharmonic oscillator for negative coupling

We consider the quantum Hamiltonian of the quartic anharmonic oscillator (2.74),

$$H = -\tfrac{1}{2}\left(\mathrm{d}/\mathrm{d}q\right)^2 + \tfrac{1}{2}q^2 + \tfrac{1}{4}gq^4, \tag{37.1}$$

where, initially, g is a positive parameter. The ground state energy $E_0(g)$ can be obtained from the large β limit of the partition function $\operatorname{tr} \mathrm{e}^{-\beta H}$ (β is the inverse temperature),

$$E_0(g) = \lim_{\beta\to+\infty} -\frac{1}{\beta} \ln \operatorname{tr} \mathrm{e}^{-\beta H} .$$

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Moreover, a systematic expansion of the partition function for β large also yields the whole spectrum (for rigorous results concerning the spectrum, see Refs. [376]).

Since the partition function has the path integral representation (equation (2.33)),

$$\operatorname{tr} \mathrm{e}^{-\beta H} = \int_{q(-\beta/2)=q(\beta/2)} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}\big(q(t)\big)\right], \tag{37.2}$$

where $\mathcal{S}(q)$ is the Euclidean action ($\dot{q} \equiv \mathrm{d}q/\mathrm{d}t$):

$$\mathcal{S}(q) = \int_{-\beta/2}^{\beta/2} \left[\tfrac{1}{2}\dot{q}^2(t) + \tfrac{1}{2}q^2(t) + \tfrac{1}{4}gq^4(t)\right] \mathrm{d}t\,, \tag{37.3}$$

we can use it to calculate the eigenvalues of H.

A generalization of arguments applicable to finite dimensional integrals, alternative to methods based on the Schrödinger equation [377], indicates that the path integral (37.2) defines a function of g analytic in the half plane $\mathrm{Re}(g) > 0$. In this domain, for g small, the path integral is dominated by the saddle point $q(t) \equiv 0$. Therefore, it can be calculated by expanding the integrand in powers of g and integrating term by term (Section 2.7). This generates the perturbative expansion of the partition function, and thus of the ground state $E_0(g)$ by taking the large β limit.

Remarks

(i) We always expand in g before taking the large β limit. Since $E_N(g)$, the Nth eigenvalue of H, satisfies

$$E_N(g) = N + \tfrac{1}{2} + O(g),$$

the perturbative expansion can be written as

$$\operatorname{tr} \mathrm{e}^{-\beta H} = \sum_{N=0} \mathrm{e}^{-\beta E_N(g)} = \sum_{N=0} \mathrm{e}^{-(N+1/2)\beta} \sum_{k=0} \frac{1}{k!}(-\beta)^k \left(E_N - \tfrac{1}{2} - N\right)^k. \tag{37.4}$$

We note that $E_N(g)$ can be inferred from the coefficient of $\mathrm{e}^{-(N+1/2)\beta}$, that the coefficient of g^k is a polynomial of degree k in β.

(ii) As we have already mentioned when discussing the ϕ^4 field theory, by the rescaling

$$q(t) \mapsto q(t)g^{-1/2},$$

we factorize the whole dependence in g in front of the action:

$$\mathcal{S}(q, g) = \frac{1}{g}\mathcal{S}(q\sqrt{g}). \tag{37.5}$$

The coupling constant g plays the same formal role as $\hbar$ in the semi-classical or loop expansion. Thus, for $g \to 0$, the integral can be evaluated by the steepest-descent method.

Continuation to negative coupling. For $g < 0$, the Hamiltonian is unbounded from below for all values of g. Therefore, the energy levels, considered as analytic functions of g, must have a singularity at $g = 0$: the perturbative expansion in powers of g is always a divergent series [377].

A quantum state, initially localized at time $t = 0$ (t is here the *real physical time* of the Schrödinger equation) in the well of the potential near $q = 0$, then decays due to barrier penetration. To determine the decay rate, in the semi-classical approximation, we can use the following method: we calculate the ground state energy E_0, and the corresponding time-dependent wave function $\psi_0(t)$ for g positive. The time-dependence of the solution $\psi_0(t, q)$ of the Schrödinger equation is

$$\psi_0(t, q) \propto \mathrm{e}^{-iE_0 t}\,.$$

We then proceed by analytic continuation in the complex g plane from $g > 0$ to $g < 0$, in the direction such that $\operatorname{Im} E$ remains negative. After analytic continuation, E_0 becomes complex, and thus $\|\psi_0(t)\|$ decreases exponentially with time at a rate

$$\|\psi_0(t)\| \sim \mathrm{e}^{-|\operatorname{Im} E_0| t}\,.$$

$|\operatorname{Im} E_0|$ is the inverse lifetime of the wave function $\psi_0(t,q)$. Actually, the decay of $\psi(t,q)$ also involves the imaginary parts of the continuations of all excited states. However, we expect on intuitive grounds that, when the real part of the energy increases, the corresponding lifetime decreases (this can easily be verified by examples). Thus, at large times, only the component corresponding to the ground state survives. Therefore, hereafter we calculate $\operatorname{Im} E_0$ for g small and negative.

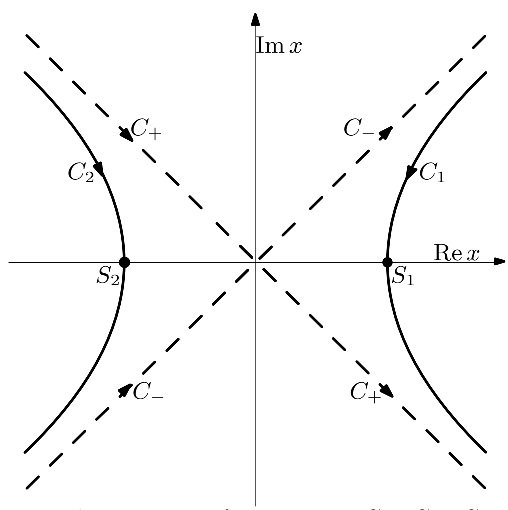

Fig. 37.1 The contours of integration C_+, C_-, C_1, and C_2

37.2 A toy model: A simple integral

To give an idea of how $E_0(g)$ can be defined and evaluated for g negative, we consider a simple integral with an analogous structure: the 'zero-dimensional ϕ^4 field theory'. The coefficients of the expansion of the integral

$$I(g) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\left(x^2/2 + gx^4/4\right)}\, \mathrm{d}x\,, \tag{37.6}$$

in powers of g, count the number of Feynman diagrams contributing to the partition function (or vacuum amplitude) in the general ϕ^4 field theory.

The integral defines the function for $\operatorname{Re} g \geq 0$, but the function $I(g)$ is analytic in a cut plane. Its analytic continuation to $\operatorname{Re} g < 0$ can be obtained by rotating the contour of integration C in the complex plane as one changes the argument of g:

$$C: \ \arg x = -\tfrac{1}{4} \arg g \qquad (\mathrm{mod}\ \pi)\,,$$

so that $\operatorname{Re}(gx^4)$ remains positive.

In this way, one obtains two different expressions for $I(g)$ depending on the direction of rotation in the g-plane:

$$\text{for } g = -|g| + i0: \ I(g) = \int_{C_+} e^{-(x^2/2+gx^4/4)}\,dx\,, \ \text{with } C_+ : \arg x = -\frac{\pi}{4} \pmod{\pi},$$

$$\text{for } g = -|g| - i0: \ I(g) = \int_{C_-} e^{-(x^2/2+gx^4/4)}\,dx\,, \ \text{with } C_- : \arg x = \frac{\pi}{4} \pmod{\pi}.$$

For g positive and small, the integral is dominated by the saddle point at $x = 0$, and $I(g) = 1 + O(g)$. For $g \to 0_-$, the two integrals are still dominated by the saddle point at the origin, since the contribution of the other saddle points:

$$x + gx^3 = 0 \Rightarrow x^2 = -1/g \tag{37.7}$$

are of the order of

$$e^{-(x^2/2+gx^4/4)} \sim e^{1/4g} \ll 1\,. \tag{37.8}$$

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

$$I(g+i0) - I(g-i0) = 2i\,\mathrm{Im}\,I(g) = \frac{1}{\sqrt{2\pi}}\int_{C_+ - C_-} e^{-\left(x^2/2+gx^4/4\right)}\,dx\,. \tag{37.9}$$

It corresponds to the contour $C_+ - C_-$ which, as Fig. 37.1 shows, can be deformed into the sum of the contours C_1 and C_2, which are dominated by the lower non-trivial saddle points S_1 and S_2: $x = \pm 1/\sqrt{-g}$. This implies that the contribution of the saddle point at $x = 0$ cancels. The contributions of the saddle points S_1 and S_2 then yields

$$\mathrm{Im}\,I(g) \sim 2^{-1/2}\,e^{1/4g}\,. \tag{37.10}$$

Thus, for g negative and small, the real part of the integral is given by perturbation theory, while the exponentially small imaginary part is given by the contribution of non-trivial saddle points.

37.3 QM: Instantons

The method used in the example of the integral (37.6) can be adapted to the path integral (37.2). We rotate the contour in the functional $q(t)$ space, as we change the argument g from g positive to g negative:

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

in which θ is time independent. Returning to the definition of the path integral as a limit of integrals in a discretized time (see Chapter 2), one can verify that this procedure makes sense.

However, there is one difference with respect to the simple integral: the contour has to stay within the domain in which $\mathrm{Re}\left[\dot q^2(t)\right] > 0$, since, as we have discussed in Chapter 2, the kinetic part $\int \dot q^2(t)dt$ selects continuous paths and ensures, therefore, the existence of the continuum limit of the discretized path integral.

For g negative, we thus integrate along a path

$$\arg q(t) = -\theta\,, \quad \text{with } \tfrac{1}{8}\pi < \theta < \tfrac{1}{4}\pi\,, \tag{37.11}$$

which satisfies the two conditions

$$\mathrm{Re}\left[gq^4(t)\right] > 0\,, \quad \mathrm{Re}\left[\dot q^2(t)\right] > 0\,. \tag{37.12}$$

For $g \to 0_-$, the path integrals corresponding to the two analytic continuations are still dominated by the saddle point at the origin $q(t) = 0$ but, in the difference, this contribution cancels. We have to look for non-trivial saddle points, which are solutions of the Euclidean classical equation of motion for $g < 0$,

$$-\ddot{q}(t) + q(t) + gq^3(t) = 0\,, \tag{37.13}$$

$$\text{with } q(-\beta/2) = q(\beta/2). \tag{37.14}$$

The contribution of the constant saddle point $q^2(t) = -1/g$ is of the order of $\mathrm{e}^{\beta/4g}$ and, therefore, negligible in the large β limit. We have to look for solutions that have an action that remains finite for $\beta \to +\infty$. These are called *instantons*.

The solutions of equations (37.13, 37.14) correspond to a periodic motion in *real-time* in the potential $-V(q)$

$$V(q) = \tfrac{1}{2}q^2 + \tfrac{1}{4}gq^4. \tag{37.15}$$

Solutions exist which correspond to oscillations around each of the minima $q = \pm\sqrt{-1/g}$ of $-V$. Integrating once equation (37.13), one obtains

$$\tfrac{1}{2}\dot{q}^2(t) - \tfrac{1}{2}q^2(t) - \tfrac{1}{4}gq^4(t) = \epsilon\,,$$

where the constant ϵ is negative.

Denoting by q_0 and q_1 the points, with $q > 0$, where the velocity $\dot{q}$ vanishes, one finds for the period of such a solution,

$$\beta = 2\int_{q_0}^{q_1} \frac{\mathrm{d}q}{\sqrt{q^2 + \frac{1}{2}gq^4 + 2\epsilon}}\,.$$

β can only become large if the constant ϵ, and thus q_0 go to 0. With increasing β, the classical trajectory comes closer to the origin. In the infinite β limit, the classical solution becomes

$$q_c(t) = \pm\left(-\frac{2}{g}\right)^{1/2} \frac{1}{\cosh(t - t_0)}\,. \tag{37.16}$$

The corresponding classical action is

$$\mathcal{S}(q_c) = -\frac{4}{3g} + O\left(\mathrm{e}^{-\beta}/g\right). \tag{37.17}$$

Since the Euclidean action is invariant under time translations, the classical solution depends on a free parameter t_0, which, for β, finite varies between 0 and β: $0 \le t_0 < \beta$. Therefore, in contrast to the simple integral, we do not find two degenerate saddle points, but *two one-parameter families*.

We could have also considered trajectories oscillating n times around $q^2 = -1/g$ in the time interval β. It is easy to verify that the corresponding action in the infinite β limit becomes

$$\mathcal{S}(q_c) = -n\frac{4}{3g}\,, \tag{37.18}$$

and yields, therefore, a contribution proportional to $\mathrm{e}^{n4/3g}$. For g small, the path integral is dominated by the term $n = 1$. Similarly, trajectories with $\epsilon > 0$ degenerate into the sum of two solutions with an action $-n8/3g$.

Remark. Although we emphasize the role of finite action configurations, the action corresponding to the paths that contribute to the path integral is always infinite, because the paths are not differentiable and, thus, the kinetic term diverges. However, the leading configurations are close to the saddle points.

37.4 Instanton contributions at leading order

The Gaussian approximation. To evaluate the contribution of the saddle points at leading order, the usual strategy consists in expanding the action around a saddle point, setting

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

and calculating for $g \to 0_-$, $\beta \to \infty$ the Gaussian integral (one-loop order):

$$\begin{aligned} \operatorname{Im} \operatorname{tr} \mathrm{e}^{-\beta H} &= \frac{1}{i}\, \mathrm{e}^{4/3g} \int [\mathrm{d}r(t)] \exp\left[-\tfrac{1}{2}\int \mathrm{d}t \big(\dot{r}^2(t) + r^2(t) + 3gq_c^2(t) r^2(t)\big)\right], \\ &\equiv \frac{1}{i}\, \mathrm{e}^{4/3g} \int [\mathrm{d}r(t)] \exp\left(-\tfrac{1}{2}\int \mathrm{d}t_1 \mathrm{d}t_2\, r(t_1) M(t_1,t_2) r(t_2)\right), \end{aligned}$$

where M is the differential operator,

$$M(t_1,t_2) = \left.\frac{\delta^2 \mathcal{S}}{\delta q(t_1)\delta q(t_2)}\right|_{q=q_c} = \left[-\left(\mathrm{d}_{t_1}\right)^2 + 1 + 3gq_c^2(t_1)\right] \delta(t_1 - t_2). \tag{37.19}$$

The path integral is normalized by dividing it by the partition function of the harmonic oscillator.

The zero mode. Differentiating equation (37.13) with respect to t, one finds

$$-(\mathrm{d}_t)^2 \dot{q}_c(t) + \dot{q}_c(t) + 3gq_c^2(t)\dot{q}_c(t) \equiv [M\dot{q}](t) = 0\,. \tag{37.20}$$

Since the function $\dot{q}_c(t)$ is square integrable, this equation implies that $\dot{q}_c(t)$ is an eigenvector of M with eigenvalue 0. Hence, the naive Gaussian approximation yields a result proportional to $(\det M)^{-1/2}$, which is infinite!

The problem should have been expected: as we have noted previously, translation invariance in time implies the existence of two one-parameter families of continuously connected degenerate saddle points. An infinitesimal variation of $q(t)$ that corresponds to a variation of the parameter t_0, that is, proportional to $\dot{q}_c$ leaves the action unchanged. The problem that we face here is by no means special to path integrals, as the following example shows.

Zero modes in finite-dimensional integrals. We consider the integral,

$$I_2(g) = \int_{\mathbb{R}^\nu} \mathrm{d}^\nu \mathbf{x}\; \mathrm{e}^{\mathbf{x}^2 - g(\mathbf{x}^2)^2}, \quad \text{with } g > 0\,, \tag{37.21}$$

in which $\mathbf{x}$ is a ν-component vector ($\nu > 1$), and the integrand is $O(\nu)$ invariant. For g small, this integral can be calculated by the steepest-descent method. The saddle points are given by

$$\mathbf{x}_c \left(1 - 2g\mathbf{x}_c^2\right) = 0\,, \tag{37.22}$$

and, since $\mathbf{x}_c = 0$ corresponds to a minimum, the relevant solutions are $|\mathbf{x}_c| = (2g)^{-1/2}$. We find a $(\nu - 1)$ parameter family of degenerate saddle points, since the saddle point equation determines only the length of the vector $\mathbf{x}_c$. If we single out one saddle point and evaluate its contribution in the Gaussian approximation, we are led to calculate the determinant of the matrix

$$M_{\alpha\beta} = 8gx_\alpha x_\beta\,, \tag{37.23}$$

which is the projector on $\mathbf{x}$ and has, therefore, $(\nu - 1)$ vanishing eigenvalues.

Here, it is clear how to solve the problem: it is necessary to factorize the integration measure into a measure corresponding to angular variables, and a measure for the integration over the radial variable. The integration over angular variables has to be done exactly; only the integral over the radial variable can be evaluated by the steepest-descent method.

Similarly, in the case of the path integral, it is necessary to factorize the integration measure over the integration constants that parametrize the saddle points, in the preceding example, the time-translation constant. Then, the integration over these parameters has to be done exactly. The integration over the other path modes can be done by the steepest-descent method. This is the method of so-called *collective coordinates* [378].

Remark. We have already studied theories invariant under a continuous symmetry group in which the classical minimum is not invariant under the group, for example, the $O(N)$-symmetric $(\boldsymbol{\phi}^2)^2$ field theory in the ordered phase:

$$\mathcal{S}(\boldsymbol{\phi}) = \frac{1}{2}\int \mathrm{d}^d x \left[\tfrac{1}{2}\bigl(\nabla\boldsymbol{\phi}(x)\bigr)^2 + \tfrac{1}{2}r\boldsymbol{\phi}^2(x) + \tfrac{1}{4!}g\bigl(\boldsymbol{\phi}^2(x)\bigr)^2\right], \quad \text{for } r<0\,. \tag{37.24}$$

In such a situation, we have generally chosen one classical minimum, and made a systematic expansion around it. However, this procedure is justified only if the *symmetry is spontaneously broken.* Actually, we have noted in Chapter 19 that the absence of symmetry breaking manifests itself, in perturbation theory, by the appearance of infrared singularities. In the case of instanton solutions, the propagator M^{-1} in an instanton background has an isolated pole at the origin, which also leads to divergences in perturbation theory. We conclude that time-translation symmetry is not spontaneously broken, and that it is necessary to sum over all degenerate saddle points (see also Chapter 14).

37.4.1 Collective coordinates and Gaussian integration

The problem of factorizing the measure corresponding to the time-translation variable (a *collective coordinate*) is slightly more subtle than in the case of simple integrals, because a path corresponds to an infinite number of variables. A method, inspired by the Faddeev–Popov quantization method of gauge theories [219] can be used. We call t_0 the time-collective coordinate and start from the identity

$$1 = \int \frac{\mathrm{d}t_0}{\sqrt{2\pi\xi}}\left[\int \mathrm{d}t\,\dot q_c(t)\dot q(t+t_0)\right]\exp\left\{-\frac{1}{2\xi}\left[\int \mathrm{d}t\,\dot q_c(t)\bigl(q(t+t_0)-q_c(t)\bigr)\right]^2\right\}, \tag{37.25}$$

which one can verify by changing variables,

$$t_0 \mapsto \lambda\,, \text{ with } \lambda = \int \mathrm{d}t\,\dot q_c(t)\bigl(q(t+t_0)-q_c(t)\bigr).$$

The constant ξ has been introduced mainly for cosmetic reasons, but is of order g.

We insert the identity (37.25) into the path integral. The new action

$$\mathcal{S}(q) + \frac{1}{2\xi}\left[\int \mathrm{d}t\,\dot q_c(t)\bigl(q(t+t_0)-q_c(t)\bigr)\right]^2$$

is no longer time-translation invariant. It leads to the saddle point equation

$$\frac{\delta\mathcal{S}}{\delta q(t)} + \frac{1}{\xi}\dot q_c(t-t_0)\int \mathrm{d}t'\,\dot q_c(t'-t_0)\bigl(q(t')-q_c(t'-t_0)\bigr) = 0\,. \tag{37.26}$$

The equation is clearly satisfied for $q(t) = q_c(t - t_0)$. The determinant generated by the Gaussian integration around the saddle point is the determinant of the modified operator,

$$M'(t_1, t_2) = M(t_1, t_2) + \frac{1}{\xi}\dot{q}_c(t_1 - t_0)\dot{q}_c(t_2 - t_0),$$

or in the bra–ket notation of QM,

$$M' = M + \mu \left|1\right\rangle \left\langle 1\right| , \tag{37.27}$$

where we have denoted by $|1\rangle$ the eigenvector proportional to $\dot{q}_c$ with unit norm, and μ is given by

$$\mu = \left\|\dot{q}_c\right\|^2 / \xi \,.$$

All the eigenvalues of the operators M' and M (equation (37.19)) are the same, except one: the eigenvalue that corresponds to the eigenvector $\dot{q}_c$ is $\|\dot{q}_c\|^2/\xi$, instead of 0.

To normalize the path integral, we compare it to its value at $g = 0$, which is the partition function $\mathcal{Z}(\beta)$ of the harmonic oscillator, and which, in the large β limit, reduces to $\mathrm{e}^{-\beta/2}$. At $g = 0$, the operator M reduces to the operator

$$M_0(t_1, t_2) = \left[-\left(\mathrm{d}_{t_1}\right)^2 + 1\right] \delta(t_1 - t_2). \tag{37.28}$$

As we explain in Section 37.4.2, a well-defined quantity that can be calculated is the determinant of the ratio of operators $\det\left(M + \varepsilon\right)\left(M_0 + \varepsilon\right)^{-1}$, where ε is an arbitrary constant. For $\varepsilon \to 0$, it vanishes like ε, and we thus set

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \det\left(M + \varepsilon\right)\left(M_0 + \varepsilon\right)^{-1} \equiv \det{}' M M_0^{-1}. \tag{37.29}$$

By contrast, the quantity that one needs to evaluate has the form

$$\det(M + \mu \left|1\right\rangle \left\langle 1\right|) M_0^{-1} = \lim_{\varepsilon \to 0} \det\left(M + \varepsilon + \mu \left|1\right\rangle \left\langle 1\right|\right)\left(M_0 + \varepsilon\right)^{-1}.$$

Then,

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

One thus finds

$$\det{}' M M_0^{-1} \, \|\dot{q}_c\|^2/\xi \,.$$

Note that all functions depend only on $t - t_0$ and, therefore, t_0 can be eliminated from the determinant. In the first factor in (37.25), at leading order, we replace $q(t + t_0)$ by $q_c(t)$. The integral does not depend on t_0 anymore, and we find the factor

$$\frac{1}{\sqrt{2\pi\xi}} \beta \left\|\dot{q}_c\right\|^2 .$$

Therefore, the result of the integration over the fluctuations around the saddle point is

$$\frac{\beta}{\sqrt{2\pi}} \mathcal{Z}_0(\beta) \|\dot{q}_c\| (\det{}' M M_0^{-1})^{-1/2}.$$

Taking into account the two families of saddle points and dividing by $2i$ to obtain the imaginary part, we find for $\beta \to \infty$:

$$\operatorname{Im} \operatorname{tr} \mathrm{e}^{-\beta H} \sim \frac{2}{2i} \frac{\beta}{\sqrt{2\pi}} \, \mathrm{e}^{-\beta/2} \left\|\dot{q}_c\right\| \left[\det{}' M \left(\det M_0\right)^{-1}\right]^{-1/2} \mathrm{e}^{4/3g} \,. \tag{37.30}$$

37.4.2 The result at leading order

In Section 37.6.1, we calculate the determinant for a general, analytic potential in one-dimensional systems and, in Section A37.2, we compare this calculation with the corresponding WKB calculation. We show indirectly that, for all systems for which we can solve explicitly the classical equations of motion with arbitrary boundary conditions, we can also explicitly calculate the determinant of the operator governing the small fluctuations around the classical trajectory. In the special case considered here, M is a Hamiltonian with a Bargmann potential, whose spectrum is known exactly, and one finds [379],

$$\det(M+\varepsilon)(M_0+\varepsilon)^{-1} = \frac{\sqrt{1+\varepsilon}-1}{\sqrt{1+\varepsilon}+1}\frac{\sqrt{1+\varepsilon}-2}{\sqrt{1+\varepsilon}+2}\,. \tag{37.31}$$

General arguments show that the ground-state wave function has no node, the wave function of the first excited state one node, and so on. The wave function $\dot{q}_c(t)$ vanishes once at the turning point and corresponds to the first excited state. Therefore, M has one negative eigenvalue corresponding to the ground state, as expression (37.31) confirms.

Then,

$$\det{}' M\,(\det M_0)^{-1} = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\det(M+\varepsilon)(M_0+\varepsilon)^{-1} = -\frac{1}{12}\,. \tag{37.32}$$

The square root of the determinant thus is imaginary, and the final result is real, as expected. However, the sign of the square root of expression (37.31) can only be resolved by following the analytic continuation from g positive to g negative.

The norm $\|\dot{q}_c\|$ is easily calculable. It has an important property: it is proportional to $1/\sqrt{g}$. As we shall note later, this is the first example of a general situation: when the instanton solution breaks a continuous symmetry of the classical action, the solution depends on parameters generated by the action of the symmetry group on the solution. Each parameter has to be taken as an integration variable, and the corresponding Jacobian generates as a factor the loop expansion parameter to the power $-1/2$. Here, we find

$$\|\dot{q}_c\| = \frac{2}{\sqrt{3}}\frac{1}{\sqrt{-g}}. \tag{37.33}$$

The expression then becomes

$$\operatorname{Im}\operatorname{tr} \mathrm{e}^{-\beta H} = -\beta\,\mathrm{e}^{-\beta/2}\,\frac{4}{\sqrt{2\pi}}\frac{1}{\sqrt{-g}}\,\mathrm{e}^{4/3g}\left[1+O\left(g,\mathrm{e}^{-\beta}\right)\right], \ \text{for } g\to 0_-\,,\ \beta\to\infty\,. \tag{37.34}$$

For β large, the left-hand side has the form

$$\operatorname{Im}\operatorname{tr}\mathrm{e}^{-\beta H} \sim \operatorname{Im}\mathrm{e}^{-\beta E_0(g)} \equiv \operatorname{Im}\mathrm{e}^{-\beta(\operatorname{Re}E_0(g)+i\operatorname{Im}E_0(g))}, \quad \text{for } g\to 0_-\,,\ \beta\to\infty\,. \tag{37.35}$$

For g-small, the imaginary part of E_0 is exponentially small. Since the small g limit has always to be taken before the large β limit, we can write

$$\operatorname{Im}\operatorname{tr}\mathrm{e}^{-\beta H} \sim -\beta\operatorname{Im}(E_0(g))\,\mathrm{e}^{-\beta\operatorname{Re}E_0(g)} \sim -\beta\,\mathrm{e}^{-\beta/2}\operatorname{Im}E_0\,. \tag{37.36}$$

Equation (37.34) then leads to

$$\operatorname{Im}E_0(g) = \frac{4}{\sqrt{2\pi}}\frac{\mathrm{e}^{4/3g}}{\sqrt{-g}}\left[1+O(g)\right], \quad g\to 0_-\,. \tag{37.37}$$

Remark. We have derived the behaviour of the imaginary part of the ground state energy for g small and negative and, therefore, the decay rate of a metastable state localized in the unbounded potential corresponding to the anharmonic oscillator with negative coupling. In Section 40.1.1, we derive from this result an evaluation of the large-order behaviour of perturbation series for the quartic anharmonic oscillator.

37.5 General analytic potentials: Instanton contributions

WE now generalize the methods described in previous sections to a general class of one-dimensional analytic potentials. We calculate, at leading order in the semi-classical limit, the decay rate of a quantum state located at initial time around a relative minimum of a potential and decaying through barrier penetration.

To guide the intuition, we imagine that we start from a situation in which a given minimum of a potential is an absolute minimum, and after an analytic continuation, becomes a relative minimum of the potential. As we have argued in Section 37.1, the corresponding ground state energy becomes complex in the analytic continuation, and its imaginary part yields the inverse lifetime of a state initially concentrated around the relative minimum of the potential. In the semi-classical limit, the imaginary part is again related to finite action, that is, instanton solutions of the Euclidean classical equations of motion.

The instanton solution. We consider Hamiltonians of the form [380],

$$H = -\tfrac{1}{2}\left(\mathrm{d}/\mathrm{d}q\right)^2 + g^{-1}V(q\sqrt{g}), \tag{37.38}$$

where $V(q)$ is an analytic function of q, which, for q small, behaves like

$$V(q) = \tfrac{1}{2}q^2 + O\left(q^3\right). \tag{37.39}$$

We assume that $q = 0$ corresponds to a *relative minimum* of the potential.

Again, in the Hamiltonian (37.38) the potential has been parametrized in such a way that g plays the formal role of $\hbar$ and is a loop expansion parameter.

The path integral representation of the partition function is

$$\operatorname{tr} \mathrm{e}^{-\beta H} = \int_{q(-\beta/2)=q(\beta/2)} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}(q)\right], \text{ with} \tag{37.40}$$

$$\mathcal{S}(q) = \int_{-\beta/2}^{\beta/2} \left[\tfrac{1}{2}\dot{q}^2(t) + g^{-1}V(q(t)\sqrt{g})\right] \mathrm{d}t\,. \tag{37.41}$$

In the situation that we are considering, we know that instanton solutions exist. Because $q = 0$ is only a relative minimum of the potential, the function $V(q)$, which we have assumed to be analytic and thus continuous has at least another zero. For β infinite, an instanton solution $q_c(t)$ starts from the origin at time $-\infty$, is reflected on a zero of the potential and returns to the origin at time $+\infty$.

A variation of $\mathcal{S}(q)$ yields the Euclidean equation of motion

$$\ddot{q}_c(t) = \frac{1}{\sqrt{g}} V'\big(q_c(t)\sqrt{g}\big). \tag{37.42}$$

Integrating once, we obtain for a finite action solution (for $\beta = \infty$):

$$\tfrac{1}{2}\dot{q}_c^2(t) - g^{-1}V\big(q_c(t)\sqrt{g}\big) = 0\,. \tag{37.43}$$

Denoting by x_0 the relevant zero of $V(x)$, we can write the corresponding action as

$$\mathcal{S}(q_c) = \int_{-\infty}^{+\infty} \dot{q}_c^2(t)\mathrm{d}t = \frac{a}{g}, \quad \text{with } a = 2\int_0^{x_0} \sqrt{2V(x)}\mathrm{d}x\,. \tag{37.44}$$

We note that the classical action is positive and proportional to $1/g$.

The Gaussian integration. To calculate the instanton contribution at leading order, we have to integrate over the paths close to the saddle point $q_c(t)$, in the Gaussian approximation. However, as we have explained in Section 37.4, we must first separate a collective coordinate corresponding to time translation and restrict the Gaussian integration to the other modes. The zero mode yields a factor β and, at leading order, the Jacobian

$$J = \left[\int_{-\infty}^{+\infty} \dot{q}_c^2(t)\mathrm{d}t\right]^{1/2} = \left(\frac{a}{g}\right)^{1/2}. \tag{37.45}$$

Since $\dot{q}_c(t)$, which is an eigenfunction of the operator $\delta^2\mathcal{S}/\delta q(t_1)\delta q(t_2)$ has a node at the turning point $x_0/\sqrt{g}$, there exists one eigenfunction with negative eigenvalue. Therefore, the determinant of the operator $\delta^2\mathcal{S}/\delta q(t_1)\delta q(t_2)$ from which the eigenvalue 0 has been removed is negative.

Collecting all factors, one obtains

$$\begin{aligned} \operatorname{Im}\operatorname{tr}\mathrm{e}^{-\beta H} &\sim \frac{1}{2}\frac{\beta}{\sqrt{2\pi}}\,\mathrm{e}^{-\beta/2}\sqrt{\frac{a}{g}}\left[\det M_0\left(-\det{}'M\right)^{-1}\right]^{1/2}\mathrm{e}^{-a/g} \\ &\text{for } g\to 0\,,\quad \beta\to\infty\,, \end{aligned} \tag{37.46}$$

with M_0 and M given by

$$M(t_1,t_2) = \delta^2\mathcal{S}\,/\delta q(t_1)\delta q(t_2)\big|_{q=q_c}\,,\quad M_0(t_1,t_2) = \left[-\left(\mathrm{d}_{t_1}\right)^2+1\right]\delta(t_1-t_2), \tag{37.47}$$

and $\det'$ means determinant in the subspace orthogonal to $\dot{q}_c$ (see also Section 37.4).

One infers the imaginary part of the 'ground state' energy E_0 of the metastable state:

$$\operatorname{Im}E_0 = \frac{1}{2}\sqrt{\frac{a}{2\pi g}}\left[\det M_0\left(-\det{}'M\right)^{-1}\right]^{1/2}\mathrm{e}^{-a/g}\,. \tag{37.48}$$

An expansion around the saddle point then generates an expansion in powers of g.

37.6 Evaluation of the determinant: The shifting method

To determine $\det'M$, we calculate the Gaussian integral explicitly using the *shifting method* [381], a calculation which can always be done in one-dimensional systems and, more generally, in classically integrable systems. The main drawback of the method is that it involves a dangerous change of variables, and the final result is at first sight undefined. On the other hand, it makes a rather straightforward evaluation of the determinant possible. The idea behind the calculation is that, if we know the solutions of the classical equation of motion for arbitrary boundary conditions, we can construct a canonical transformation that maps any Hamiltonian system onto a standard one (here we choose a free Hamiltonian). For details, see Section A3.2.

In Section A37.2, for a comparison, we describe the calculation with the use of the WKB method (solving the Schrödinger equation for $\hbar\to 0$).

37.6.1 The shifting method

For reasons that will become apparent later, we first calculate the general matrix element

$$\left\langle x' \left| \mathrm{e}^{-\beta H} \right| x \right\rangle = \int_{q(-\beta/2)=x'}^{q(\beta/2)=x} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}(q)\right] \tag{37.49}$$

(we have used the quantum bra–ket notation). We denote by $q_c(t)$ a classical solution satisfying the boundary conditions $q_c(-\beta/2) = x'$ and $q_c(\beta/2) = x$, and by

$$\mathcal{S}_c(x', x; \beta) = \int_{-\beta/2}^{\beta/2} \left[\tfrac{1}{2}\dot{q}_c^2(t) + g^{-1}V\big(q_c(t)\sqrt{g}\big)\right] \mathrm{d}t\,, \tag{37.50}$$

the corresponding classical action. Setting

$$q(t) = q_c(t) + r(t)\,, \quad \Rightarrow \; r(\pm\beta/2) = 0\,, \tag{37.51}$$

we obtain, at leading order, the path integral

$$\begin{aligned} \left\langle x' \left| \mathrm{e}^{-\beta H} \right| x \right\rangle &\sim \mathrm{e}^{-\mathcal{S}_c} \int_{r(-\beta/2)=0}^{r(\beta/2)=0} [\mathrm{d}r(t)] \exp\left[-\Sigma(r)\right], \quad \text{with} \\ \Sigma(r) &= \int_{-\beta/2}^{\beta/2} \tfrac{1}{2}\left[\dot{r}^2(t) + V''(q_c\sqrt{g})r^2(t)\right] \mathrm{d}t\,. \end{aligned} \tag{37.52}$$

We then set

$$V''\big(\sqrt{g}q_c(t)\big) = \ddot{\kappa}(t)/\kappa(t). \tag{37.53}$$

We know at least one solution $\kappa(t)$. Differentiating the equation of motion (37.42), we obtain

$$\frac{\mathrm{d}^2}{(\mathrm{d}t)^2}\dot{q}_c(t) = V''\big(q_c(t)\sqrt{g}\big)\dot{q}_c(t)\,. \tag{37.54}$$

If $\dot{q}_c(t)$ does not vanish on the classical trajectory, we can choose $\kappa(t) = \dot{q}_c(t)$. Otherwise, we look for a linear combination of the two independent solutions of equation (37.53), $\dot{q}_c(t)$ and

$$\dot{q}_c(t) \int^t \frac{\mathrm{d}\tau}{\left[\dot{q}_c(\tau)\right]^2},$$

that does not vanish on the classical trajectory.

The action in expression (37.52) then can be written as

$$\int_{-\beta/2}^{\beta/2} \frac{1}{2}\left(\dot{r}^2(t) + \frac{\ddot{\kappa}(t)}{\kappa(t)}r^2(t)\right) \mathrm{d}t = \int_{-\beta/2}^{\beta/2} \frac{1}{2}\left(\dot{r}(t) - \frac{\dot{\kappa}(t)}{\kappa(t)}r(t)\right)^2 \mathrm{d}t\,. \tag{37.55}$$

This can be verified by integrating by parts the cross term in the expansion of the square in the right-hand side and using the boundary conditions $r(\pm\beta/2) = 0$. Then, after the linear change of variable, $r(t) \mapsto \sigma(t)$, with

$$\dot{r}(t) - \frac{\dot{\kappa}(t)}{\kappa(t)}r(t) = \dot{\sigma}(t)\,, \quad \sigma(-\beta/2) = 0\,, \tag{37.56}$$

the action for a time-dependent harmonic oscillator transforms into a free action:

$$\int_{-\beta/2}^{\beta/2} \tfrac{1}{2}\left(\dot{r}^2(t) + \frac{\ddot{\kappa}(t)}{\kappa(t)}r^2(t)\right) \mathrm{d}t = \int_{-\beta/2}^{\beta/2} \tfrac{1}{2}\dot{\sigma}^2(t)\mathrm{d}t\,. \tag{37.57}$$

The transformation (37.56) has the form of a Langevin equation (34.1), $r(t)$ corresponding to the trajectory and $\dot{\sigma}(t)$ to the noise. Therefore, the same difficulty as in naive continuum derivations of the Fokker–Planck (FP) equation is encountered. Indeed, integrating equation (37.56), one obtains

$$r(t)=\kappa(t)\int_{-\beta/2}^{t}\mathrm{d}\tau\,\frac{\dot{\sigma}(\tau)}{\kappa(\tau)}=\sigma(t)+\kappa(t)\int_{-\beta/2}^{t}\mathrm{d}\tau\,\sigma(\tau)\frac{\dot{\kappa}(\tau)}{\kappa^2(\tau)}\,. \tag{37.58}$$

The Jacobian J of this transformation is formally the determinant of the kernel (see Section 35.2.1),

$$J=\frac{\delta r(t_2)}{\delta\sigma(t_1)}=\det\left[\delta(t_1-t_2)+\theta(t_2-t_1)\kappa(t_2)\frac{\dot{\kappa}(t_1)}{\kappa^2(t_1)}\right], \tag{37.59}$$

where $\theta(t)$ is the step function ($\theta(t)=0$ for $t<0$, $\theta(t)=1$ for $t>0$).

Expanding

$$\ln\det(1+M)=\operatorname{tr}\ln(1+M)=\operatorname{tr}M-\tfrac{1}{2}\operatorname{tr}M^2+\cdots\ , \tag{37.60}$$

one verifies that only the first term does not vanish, but has the ambiguous form

$$\ln J=\theta(0)\int_{-\beta/2}^{\beta/2}\mathrm{d}t\frac{\dot{\kappa}(t)}{\kappa(t)}=\theta(0)\ln\left[\kappa(\beta/2)/\kappa(-\beta/2)\right]. \tag{37.61}$$

For reasons we have discussed in Section 3.3.1 (commutation of derivative and expectation value, which is required to justify the identity (37.55) within the path integral), the suitable prescription is $\theta(0)=\frac{1}{2}$, and the Jacobian becomes

$$J=\sqrt{\frac{\kappa(\beta/2)}{\kappa(-\beta/2)}}\,. \tag{37.62}$$

In the path integral, we still have to impose the boundary condition:

$$0=r(\beta/2)=\kappa(\beta/2)\int_{-\beta/2}^{\beta/2}\mathrm{d}t\,\frac{\dot{\sigma}(t)}{\kappa(t)}\,. \tag{37.63}$$

This condition can be implemented by introducing a δ-function for which we use the Fourier representation

$$\delta\bigl(r(\beta/2)\bigr)=\frac{1}{\kappa(\beta/2)}\int\frac{\mathrm{d}\lambda}{2\pi}\exp\left(i\lambda\int_{-\beta/2}^{\beta/2}\mathrm{d}t\,\frac{\dot{\sigma}(t)}{\kappa(t)}\right).$$

The complete expression then reads

$$\left\langle x'\left|\mathrm{e}^{-\beta H}\right|x\right\rangle\sim\mathrm{e}^{-\mathcal{S}_c}\int_{\sigma(-\beta/2)=0}[\mathrm{d}\sigma(t)]\,\frac{\mathrm{d}\lambda}{2\pi}\frac{1}{\sqrt{\kappa(\beta/2)\kappa(-\beta/2)}}\,\mathrm{e}^{-\mathcal{S}(\sigma,\lambda)}, \tag{37.64}$$

with

$$\mathcal{S}(\sigma,\lambda)=\int_{-\beta/2}^{\beta/2}\mathrm{d}t\left(\frac{1}{2}\dot{\sigma}^2(t)-i\lambda\frac{\dot{\sigma}(t)}{\kappa(t)}\right). \tag{37.65}$$

To eliminate the term linear in $\dot{\sigma}(t)$ in equation (37.65), we shift $\dot{\sigma}(t)$,

$$\sigma(t) \mapsto \varsigma(t), \text{ with } \dot{\sigma}(t) = i\frac{\lambda}{\kappa(t)} + \dot{\varsigma}(t)\,. \tag{37.66}$$

After the shift, the path integral becomes

$$\left\langle x' \left| \mathrm{e}^{-\beta H} \right| x \right\rangle \sim \mathrm{e}^{-\mathcal{S}_c} \int_{\varsigma(-\beta/2)=0} [\mathrm{d}\varsigma(t)]\, \frac{\mathrm{d}\lambda}{2\pi} \frac{1}{\sqrt{\kappa(\beta/2)\kappa(-\beta/2)}} \\ \times \exp\left[-\frac{1}{2}\lambda^2 \int_{-\beta/2}^{\beta/2} \frac{\mathrm{d}t}{\kappa^2(t)} - \frac{1}{2}\int_{-\beta/2}^{\beta/2} \dot{\varsigma}^2(t)\mathrm{d}t\right]. \tag{37.67}$$

The integration over λ yields

$$\left\langle x' \left| \mathrm{e}^{-\beta H} \right| x \right\rangle \sim \mathrm{e}^{-\mathcal{S}_c(x',x;\beta)} \left[\kappa(\beta/2)\kappa(-\beta/2) \int_{-\beta/2}^{\beta/2} \frac{\mathrm{d}t}{\kappa^2(t)}\right]^{-1/2} \mathcal{N}(\beta). \tag{37.68}$$

The constant $\mathcal{N}(\beta)$ does not depend on x and x', and is proportional to the matrix element $\langle 0|\, \mathrm{e}^{-\beta H_0}\, |0\rangle$, in which H_0 is the free Hamiltonian:

$$\left\langle x' \left| \mathrm{e}^{-\beta H_0} \right| x \right\rangle = (2\pi\beta)^{-1/2}\, \mathrm{e}^{-(x'-x)^2/2\beta}\,. \tag{37.69}$$

To determine $\mathcal{N}(\beta)$, we set $H = H_0$ in equation (37.68) and note that in this case $\kappa(t)$ is a constant. The final result is

$$\left\langle x' \left| \mathrm{e}^{-\beta H} \right| x \right\rangle \sim \mathrm{e}^{-\mathcal{S}_c(x',x;\beta)} \left[2\pi\kappa(\beta/2)\kappa(-\beta/2) \int_{-\beta/2}^{\beta/2} \frac{\mathrm{d}t}{\kappa^2(t)}\right]^{-1/2}. \tag{37.70}$$

We leave as an exercise to show that the result (37.70) is formally independent of the particular linear combination of the two solutions of equation (37.53) that has been chosen. To obtain a more explicit expression, we then substitute for example $\kappa(t) = \dot{q}_c(t)$. We integrate the equation of motion (37.42), taking into account the boundary conditions,

$$\tfrac{1}{2}\dot{q}_c^2(t) = g^{-1}\left[V\big(q_c(t)\sqrt{g}\big) + E\right], \tag{37.71}$$

and, therefore,

$$\beta = \int_{x'\sqrt{g}}^{x\sqrt{g}} \frac{\mathrm{d}q}{\left[2\big(E + V(q)\big)\right]^{1/2}}\,. \tag{37.72}$$

Differentiating equation (37.72) with respect to β, we obtain the equation

$$1 = -\int_{x'\sqrt{g}}^{x\sqrt{g}} \frac{\mathrm{d}q}{\left[2\big(E + V(q)\big)\right]^{3/2}} \frac{\partial E}{\partial \beta}, \tag{37.73}$$

which can be written as

$$\frac{\partial E}{\partial \beta} = -\left[\int_{-\beta/2}^{\beta/2} \frac{\mathrm{d}t}{\kappa^2(t)}\right]^{-1}. \tag{37.74}$$

The result (37.70) can then also be expressed as

$$\left\langle x' \left| \mathrm{e}^{-\beta H} \right| x \right\rangle \sim \mathrm{e}^{-\mathcal{S}_c(x',x;\beta)} \frac{1}{\sqrt{2\pi \dot{q}_c(\beta/2)\dot{q}_c(-\beta/2)}} \left(-\frac{\partial E}{\partial \beta}\right)^{1/2}. \tag{37.75}$$

We leave as an exercise to verify the identity

$$\kappa(\beta/2)\kappa\,(-\beta/2) \int_{-\beta/2}^{\beta/2} \frac{\mathrm{d}t}{\kappa^2(t)} = \left(-\frac{\partial^2 \mathcal{S}_c}{\partial x \partial x'}\right)^{-1}. \tag{37.76}$$

Substituting equation (37.76) into equation (37.70), one then obtains Van Vleck's formula [382] (Section A37.2) in imaginary time:

$$\left\langle x' \left| \mathrm{e}^{-\beta H} \right| x \right\rangle \sim \left(-\frac{1}{2\pi} \frac{\partial^2 \mathcal{S}_c}{\partial x \partial x'}\right)^{1/2} \exp\left[-\mathcal{S}_c(x', x; \beta)\right]. \tag{37.77}$$

Several component paths. The calculation of the instanton contribution by the shifting method can be generalized to $\nu > 1$ component vectors $\mathbf{q}$, provided one can find a non-singular $\nu \times \nu$ matrix $\mathbf{K}$, solution of the equation

$$\ddot{K}_{ij}(t) = \sum_k \frac{\partial V\big(\mathbf{q}_c(t)\big)}{\partial q_i \partial q_k} K_{kj}(t). \tag{37.78}$$

The change of variables (37.56) then takes the form

$$\dot{\mathbf{r}}(t) - \dot{\mathbf{K}}(t)\mathbf{K}^{-1}(t)\mathbf{r}(t) = \dot{\boldsymbol{\sigma}}(t). \tag{37.79}$$

The matrix $\mathbf{K}$ can be chosen in such a way that $\dot{\mathbf{K}}\mathbf{K}^{-1}$ is symmetric. It is easy to verify that all arguments can then be repeated and, finally, one obtains an expression similar to equation (37.75):

$$\begin{aligned}\left\langle \mathbf{x}' \left| \mathrm{e}^{-\beta H} \right| \mathbf{x} \right\rangle \sim \left\{ (2\pi)^d \det \left[\mathbf{K}(\beta/2)\mathbf{K}(-\beta/2) \int_{-\beta/2}^{\beta/2} \mathrm{d}t\, \left(\mathbf{K}^T\right)^{-1} \mathbf{K}^{-1} \right] \right\}^{-1/2} \\ \times \exp\left[-\mathcal{S}_c(\mathbf{x}', \mathbf{x}; \beta)\right].\end{aligned} \tag{37.80}$$

This expression is again equivalent to Van Vleck's formula (see Section A37.2), and can be derived in the same conditions, that is, if the classical equations of motion can be solved for arbitrary initial and final conditions. For more than one degree of freedom, this is no longer the generic situation, and it corresponds only to the special class of integrable Hamiltonians. Simple examples are provided by $O(N)$-symmetric potentials.

37.6.2 The partition function

In order to calculate $\operatorname{tr} \mathrm{e}^{-\beta H}$, we now impose periodic boundary conditions. Then,

$$\left[\dot{q}_c(\beta/2)\dot{q}_c(-\beta/2)\right]^{-1/2} = \left\{ \frac{2}{g} \left[V(x\sqrt{g}) + E \right] \right\}^{-1/2}. \tag{37.81}$$

Integrating over x, we obtain the trace. Using equation (37.72), we find

$$\int \mathrm{d}x \left[\frac{2}{g}\big(V(x\sqrt{g})+E\big)\right]^{-1/2} = \beta\,. \tag{37.82}$$

Collecting all factors, we obtain the more explicit expression

$$\operatorname{Im}\operatorname{tr}\mathrm{e}^{-\beta H} \sim \frac{\beta}{2i}\left(-\frac{\partial E}{\partial\beta}\frac{1}{2\pi g}\right)^{1/2}\mathrm{e}^{-A(\beta)/g}, \tag{37.83}$$

where $E(\beta)$ and $A(\beta)$ are defined by

$$\beta = 2\int_{x_-}^{x_+}\frac{\mathrm{d}x}{\left[2\left(E(\beta)+V(x)\right)\right]^{1/2}}, \tag{37.84}$$

$$A(\beta) = 2\int_{x_-}^{x_+}\mathrm{d}x\left[2\left(E(\beta)+V(x)\right)\right]^{1/2} - \beta E(\beta). \tag{37.85}$$

The quantities x_+ and x_- are the zeros of $E(\beta)+V(x)$. Note the useful relation

$$\partial A/\partial\beta = -E(\beta). \tag{37.86}$$

It is clear that, at least for β large enough, $E(\beta)$ is a negative increasing function of β. Therefore, $-\partial E/\partial\beta$ is negative, and the result

$$\operatorname{Im}\operatorname{tr}\mathrm{e}^{-\beta H} \sim -\frac{\beta}{2}\left(\frac{\partial E}{\partial\beta}\frac{1}{2\pi g}\right)^{1/2}\mathrm{e}^{-A(\beta)/g} \quad \text{for } g\to 0 \tag{37.87}$$

is real, as expected. This completes the calculation for finite β.

Remark. At β finite, the calculation is valid only above some critical value β_c. Indeed, when β decreases, x_+ and x_- approach a common value x_0, which corresponds to a maximum of $V(x)$:

$$\begin{cases} V(x) \sim V_0 - \frac{1}{2}\omega^2(x-x_0)^2 + O\left[(x-x_0^3\right], \\ \quad V_0 > 0\,. \end{cases} \tag{37.88}$$

Let us parametrize E, x_+ and x_-,

$$E = -V_0 + \tfrac{1}{2}\omega^2\varepsilon^2, \quad x_\pm = x_0 \pm \varepsilon\,. \tag{37.89}$$

Then,

$$\beta = \int_{x_0-\varepsilon}^{x_0+\varepsilon}\frac{\mathrm{d}x}{\left[\omega^2\varepsilon^2-\omega^2\left(x-x_0\right)^2\right]^{1/2}}, \;\Rightarrow\; \lim_{\varepsilon\to 0}\beta = \beta_c = 2\pi/\omega\,. \tag{37.90}$$

For $\beta \le \beta_c$, no instanton solution can be found, and, by contrast, it is the perturbative expansion around the classical extremum $x = x_0$ of the potential that becomes relevant.

37.7 Zero temperature limit: The ground state

Rewriting equation (37.84) as

$$\beta = 2\int_{x_-}^{x_+} \left\{ [2\,(V(x)+E)]^{-1/2} - \left(x^2+2E\right)^{-1/2} + \left(x^2+2E\right)^{-1/2} \right\} \mathrm{d}x\,, \tag{37.91}$$

we can explicitly evaluate the last term, and neglect E in the difference between the first two terms. This leads to

$$E(\beta) \sim -2C\,\mathrm{e}^{-\beta}, \quad \text{with} \quad C = x_+^2 \exp\left[2\int_0^{x_+} \left(\frac{1}{\sqrt{2V(x)}} - \frac{1}{x}\right) \mathrm{d}x\right], \tag{37.92}$$

where now x_+ is the zero of the potential. Equation (37.85) has a large β expansion of the form

$$A(\beta) = a - 2C\,\mathrm{e}^{-\beta} + O\left(\mathrm{e}^{-2\beta}\right), \quad \text{with } a = 2\int_0^{x_+} \sqrt{2V(x)}\,. \tag{37.93}$$

Substituting into equation (37.87), one obtains at leading order,

$$\mathrm{Im}\,\mathrm{e}^{-\beta E_0(g)} \underset{g\to 0}{\sim} \frac{\beta}{2}\,\mathrm{e}^{-\beta/2} \left(\frac{C}{\pi g}\right)^{1/2} \mathrm{e}^{-a/g}, \tag{37.94}$$

and thus,

$$\mathrm{Im}\,E_0(g) \underset{g\to 0}{\sim} -\frac{1}{2}\left(\frac{C}{\pi g}\right)^{1/2} \mathrm{e}^{-a/g}\,. \tag{37.95}$$

Here we have calculated only the imaginary part of the would-be ground state energy. To derive the imaginary part of the excited levels, we have to keep the correction of order $\mathrm{e}^{-\beta}$ in $A(\beta)$ for β large. We then expand $\exp[-g^{-1}A(\beta)]$ in powers of $\mathrm{e}^{-\beta}$. The coefficient of $\mathrm{e}^{-N\beta}$ in the expansion yields the imaginary part of the Nth level, at leading order.

Two remarks

(i) We have assumed that we have only one instanton solution corresponding to a given zero of the potential. If we find other instanton solutions corresponding to other zeroes of the potential, we have to look for the solution of minimal action, which gives the largest contribution in the small-coupling limit.

(ii) In Section 37.1, we have argued that the imaginary part of the energy levels which we evaluate is the inverse lifetime of a state whose wave function is originally concentrated near the bottom of the metastable minimum of the potential. This interpretation is not problematic for potentials which are either unbounded, or have a continuous spectrum, in which case the complex energy level corresponds to a resonance in the potential. For potentials which have a pure discrete spectrum (and all eigenvalues are real), the situation appears more puzzling. First, the energy of the initial state, which is large compared to the energy of true ground state, corresponds in the semi-classical limit to an almost continuous spectrum outside the well. Moreover, in the semi-classical limit, the lifetime of the metastable state is very long. For times that are not too long, the decay process is exponential, and ignores effects coming from the shape of the potential outside of the barrier. Eventually inverse tunnelling will occur, and the decay law will be modified.

A37 Exact Jacobian. WKB method.

We give here, *without proof, explicit exact expressions*, beyond the leading-order approximation used in the chapter, for the Jacobians generated by the method of collective coordinates [383]. The generalization to quantum field theory (QFT) is simple.

We then discuss semi-classical calculations, using the WKB method, in the framework of the Schrödinger equation, under the assumption that the classical equations of motion can be solved for arbitrary boundary conditions (see Section A3.2).

A37.1 The exact Jacobian

We denote by $\mathbf{q}(t)$, $t \in \mathbb{R}$, the N-component path over which one integrates, and $\mathbf{q}_c(t)$ the instanton solution. In terms of complete set of collective coordinates τ_i, the Jacobian can be written as

$$\mathcal{J} = \det \mathbf{J}(\mathbf{q}) / \det^{1/2} \mathbf{J}(\mathbf{q}_c)\,, \tag{A37.1}$$

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

$$J_{ij}(\mathbf{q}) = \int \mathrm{d}t\, \frac{\partial \mathbf{q}}{\partial \tau^i} \cdot \frac{\partial \mathbf{q}_c}{\partial \tau^j}. \tag{A37.2}$$

A37.1.1 Example: Time translation

We first assume that $q(t)$ has one component, and the instanton solution breaks the symmetry of the action under time translation. Then, the function $J(q)$ in equation ($A37.2$) reduces to the expression

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

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),

$$J(q) = J(q_c) - \int \mathrm{d}t\, \ddot{q}_c(t) r(t).$$

A37.1.2 Time translation and $O(N)$ internal rotations

We now consider a path integral where the integrand is both invariant under time translation and internal $O(N)$ group transformations. We assume that the general instanton solution takes the form

$$\mathbf{q}_c(t) = \mathbf{u}\, q_c(t + t_0), \tag{A37.3}$$

where $\mathbf{u}$ is a time-independent unit vector: $\mathbf{u}^2 = 1$, a form that breaks both time-translation and $O(N)$ invariance. Parametrizing the sphere by collective coordinates τ_i, we then set

$$\mathbf{q}(t) = q_{\mathrm{L}}(t + t_0)\mathbf{u}(\boldsymbol{\tau}) + \mathbf{q}_{\mathrm{T}}(t + t_0), \tag{A37.4}$$

where

$$\mathbf{u} \cdot \mathbf{q}_{\mathrm{T}}(t) = 0\,. \tag{A37.5}$$

The Jacobian can then be written as (g_{ij} is the metric on the sphere S_{N-1})

$$\mathcal{J} = (\det g_{ij})^{1/2} \left[\int \mathrm{d}t\, \mathbf{q}_c^2(t)\right]^{(1-N)/2} \left[\int \mathrm{d}t\, \dot{\mathbf{q}}_c^2(t)\right]^{-1/2} \left[\int \mathrm{d}t\, \mathbf{q}(t)\cdot\mathbf{q}_c(t)\right]^{N-2}$$
$$\times \int \mathrm{d}t\,\mathrm{d}t' \left[\dot{\mathbf{q}}(t)\cdot\dot{\mathbf{q}}_c(t)\mathbf{q}(t')\cdot\mathbf{q}_c(t') - \dot{q}_c(t)\dot{q}_c(t')\mathbf{q}_{\mathrm{T}}(t)\cdot\mathbf{q}_{\mathrm{T}}(t')\right]. \qquad (A37.6)$$

A37.2 The WKB method

We reintroduce the quantity $\hbar$, which we often elsewhere set equal to 1, to make the expansion parameter explicit. We explicitly write the Schrödinger equation (in real time) for the evolution operator as

$$H\left(\frac{\hbar}{i}\frac{\partial}{\partial\mathbf{x}},\mathbf{x};t\right)U(\mathbf{x},\mathbf{x}';t) = i\hbar\frac{\partial U}{\partial t}(\mathbf{x},\mathbf{x}';t), \qquad (A37.7)$$

with the definition $U(\mathbf{x},\mathbf{x}';t) = \langle\mathbf{x}\,|\mathbf{U}(t)|\,\mathbf{x}'\rangle$, and the boundary condition

$$\mathbf{U}(t=T') = \mathbf{1}\,. \qquad (A37.8)$$

We assume that, in equation (A37.7), the Hamiltonian is Hermitian, and results from the quantization of a classical Hamiltonian. Thus, we now face the problem of how to associate a quantum operator with a real classical Hamiltonian $H(\mathbf{p},\mathbf{q},;t)$ (see Chapter 3). As an ansatz, we set

$$U(\mathbf{x}',\mathbf{x};t) = G(\mathbf{x},\mathbf{x}';t)\,\mathrm{e}^{iA(\mathbf{x},\mathbf{x}';t)/\hbar}\left[1+O(\hbar)\right]. \qquad (A37.9)$$

Introducing the ansatz into equation (A37.7), and keeping the two first terms in $\hbar$, we obtain two equations. The first equation involves only the classical Hamiltonian. It is the Hamilton–Jacobi equation for the classical action on the classical trajectory,

$$H\left(\frac{\partial A}{\partial\mathbf{x}},\mathbf{x};t\right) = -\frac{\partial A}{\partial t}. \qquad (A37.10)$$

With the boundary conditions implied by the condition (A37.8), it determines A completely. The derivation of the second equation involves some more work. First, we note that

$$H\left(\frac{\hbar}{i}\frac{\partial}{\partial\mathbf{x}},\mathbf{x};t\right)G = GH - i\hbar\sum_i\frac{\partial H}{\partial p_i}\frac{\partial G}{\partial x_i} + O\left(\hbar^2\right). \qquad (A37.11)$$

Here again, only the classical Hamiltonian is needed. The term containing $\partial H/\partial p_i$ is already multiplied by a factor $\hbar$, thus we can replace the operator p_i by $\partial A/\partial x_i$. For the first term, we now use the identity

$$\mathrm{e}^{-iA/\hbar}\,H\,\mathrm{e}^{iA/\hbar} = H\left(\frac{\partial A}{\partial\mathbf{x}},\mathbf{x};t\right) - \frac{i\hbar}{2}\sum_j\frac{\partial^2 H}{\partial p_j\partial q_j}\left(\frac{\partial A}{\partial\mathbf{x}},\mathbf{x};t\right)$$
$$-\frac{i\hbar}{2}\sum_{j,k}\frac{\partial^2 H}{\partial p_j\partial p_k}\left(\frac{\partial A}{\partial\mathbf{x}},\mathbf{x};t\right)\frac{\partial^2 A}{\partial x_j\partial x_k} + O\left(\hbar^2\right). \qquad (A37.12)$$

The second term in the right-hand side comes from commuting all the derivatives completely on the right. It relies on the assumption that the quantum Hamiltonian is Hermitian. Indeed, let us first assume that we have symmetrized all monomials:

$$p^n q^m \to \tfrac{1}{2}\left(p^n q^m + q^m p^n\right). \tag{A37.13}$$

Then, a contribution to this term arises each time an operator p of $p^n q^m$ acts on q^m, and the factor $\frac{1}{2}$ comes from the symmetrization. If we choose another Hermitian quantization procedure, we can start commuting all operators p and q until the Hamiltonian is again a sum of terms (A37.13). Each commutation introduces a factor $i\hbar$. Since the difference between the two expressions is Hermitian, it can only involve $(i\hbar)^2$, which can be neglected at this order.

The third term in expression (A37.12) arises from two derivatives acting on the action. The factor 1/2 is a counting factor. We then obtain the equation for G,

$$\sum_i \frac{\partial H}{\partial p_i}\frac{\partial G}{\partial x_i} + \frac{1}{2}\left(\sum_j \frac{\partial^2 H}{\partial p_j \partial q_j} + \sum_{j,k} \frac{\partial^2 H}{\partial p_j \partial p_k}\frac{\partial^2 A}{\partial x_j \partial x_k}\right) G = -\frac{\partial G}{\partial t}. \tag{A37.14}$$

We introduce the matrix notation

$$M_{ij} = \frac{\partial^2 A}{\partial x'_i \partial x_j}, \quad H_{ij} = \frac{\partial^2 H}{\partial p_i \partial p_j}, \quad \widetilde{H}_{ij} = \frac{\partial^2 H}{\partial p_i \partial q_j}. \tag{A37.15}$$

We now differentiate equation (A37.10) with respect to x'_i and x_j, successively. We find,

$$\sum_k M_{ik}\frac{\partial H}{\partial p_k} = -\frac{\partial^2 A}{\partial t \partial x'_i}, \tag{A37.16}$$

and

$$\sum_k \frac{\partial \mathbf{M}}{\partial x_k}\frac{\partial H}{\partial p_k} + \mathbf{MHM} + \mathbf{M}\widetilde{\mathbf{H}} = -\frac{\partial \mathbf{M}}{\partial t}. \tag{A37.17}$$

All multiplications are meant in a matrix sense. We now multiply equation (A37.17) by $\mathbf{M}^{-1}$ on the left and take the trace:

$$\sum_k \frac{\partial H}{\partial p_k}\operatorname{tr}\mathbf{M}^{-1}\frac{\partial \mathbf{M}}{\partial x_k} + \operatorname{tr}\left(\mathbf{HM} + \widetilde{\mathbf{H}}\right) = -\operatorname{tr}\mathbf{M}^{-1}\frac{\partial \mathbf{M}}{\partial t}. \tag{A37.18}$$

We note that

$$\partial \ln\det\mathbf{M} = \partial \operatorname{tr}\ln\mathbf{M}) = \operatorname{tr}\partial\mathbf{M}\mathbf{M}^{-1}. \tag{A37.19}$$

The equation (A37.18) can then be rewritten as

$$\frac{\partial H}{\partial p_i}\frac{\partial}{\partial x_i}\ln\det\mathbf{M} + \operatorname{tr}\tilde{\mathbf{H}} + \operatorname{tr}\mathbf{MH} = -\frac{\partial}{\partial t}\ln\det\mathbf{M}, \tag{A37.20}$$

while equation (A37.14) can be written as

$$\frac{\partial H}{\partial p_i}\frac{\partial}{\partial x_i}\ln G + \tfrac{1}{2}\operatorname{tr}\tilde{\mathbf{H}} + \tfrac{1}{2}\operatorname{tr}\mathbf{MH} = -\frac{\partial}{\partial t}\ln G\,. \tag{A37.21}$$

Comparing the two equations, we conclude that a solution to equation (A37.21) is

$$\ln G = \tfrac{1}{2}\ln\det\mathbf{M} + \text{ const.}\,. \tag{A37.22}$$

Taking into account the boundary conditions, we obtain Van Vleck's formula [382],

$$\langle \mathbf{x}\,| U(T,T')|\,\mathbf{x}'\rangle \sim \frac{1}{(2\pi i\hbar)^{n/2}}\left(-\det\frac{\partial^2 A}{\partial x_i \partial x_j}\right)^{1/2} \mathrm{e}^{iA(\mathbf{x},\mathbf{x}';t)/\hbar}\,. \tag{A37.23}$$

It is straightforward to derive from this equation the corresponding expression for imaginary time.