Multi–Instantons and Exact Results I:

Conjectures, WKB Expansions, and Instanton Interactions

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Abstract We consider specific quantum mechanical model problems for which perturbation theory fails to explain physical properties like the eigenvalue spectrum even qualitatively, even if the asymptotic perturbation series is augmented by resummation prescriptions to "cure" the divergence in large orders of perturbation theory. Generalizations of perturbation theory are necessary which include instanton configurations, characterized by nonanalytic factors $\exp(-a/g)$ where a is a constant and g is the coupling. In the case of one-dimensional quantum mechanical potentials with two or more degenerate minima, the energy levels may be represented as an infinite sum of terms each of which involves a certain power of a nonanalytic factor and represents itself an infinite divergent series. We attempt to provide a unified representation of related derivations previously found scattered in the literature. For the considered quantum mechanical problems, we discuss the derivation of the instanton contributions from a semi-classical calculation of the corresponding partition function in the path integral formalism. We also explain the relation with the corresponding WKB expansion of the solutions of the Schrödinger equation, or alternatively of the Fredholm determinant $\det(H-E)$ (and some explicit calculations that verify this correspondence). We finally recall how these conjectures naturally emerge from a leading-order summation of multi-instanton contributions to the path integral representation of the partition function. The same strategy could result in new conjectures for problems where our present understanding is more limited.

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Chapter 1

Introduction

The divergence of perturbation theory in higher orders and the asymptotic character of the perturbation series have led to fairly extensive investigations on large-order perturbation theory [1]. Here, we are concerned with time-dependent, classically allowed field configurations (or classical particle trajectories that solve the Euclidean equations of motion) for which the contribution to the field energy (the classical Euclidean action) is finite. These configurations give dominant contributions the generating functionals (partition functions) in quantum field theory (quantum mechanics). The instantons manifest themselves in a particularly clear manner in the path integral representation from which they were originally derived. However, the analysis suffers, even in comparatively simple cases, from a number of mathematical subtleties, and confusion may easily arise with regard to a number of necessary analytic continuations that assign a well–defined meaning to the resulting infinite series. Here, we are concerned with a number of quantum mechanical model problems in which instantons play a crucial role: in the cases considered, perturbation theory fails to account for the eigenvalue spectrum even qualitatively; two or more distinct energy levels are characterized by one and the same perturbation series. The degeneracy which persists after the application of perturbation theory is lifted only when instanton configurations are additionally taken into account. The example to be considered is the quantum mechanical double-well oscillator in which the particle trajectory may describe an arbitrary number n of oscillations between the two minima (and we also consider generalizations of this problem with more than two minima). The Euclidean action of two oscillations between the minima is found to differ slightly from the sum of two single oscillations, the difference giving rise to a modification of the contribution to the path integral and the partition function: this is the origin of the instanton interaction and the multi-instantons. The result of the investigations is that the energy eigenvalue is given as an infinite sum over series each of which characterizes a particular configuration in which the particle oscillates n times between the minima, including the modifications to the resulting Euclidean action (the n-instanton configuration).

Let us consider a double-well oscillator with a coupling g whose inverse is proportional to the spatial separation of the two minima. An expansion in powers of g then corresponds to an expansion about the case of infinite separation of the two minima (i.e., about the case where the other minimum at $x = \infty$ can be ignored and a single minimum results). This cannot be assumed to be satisfactory because a situation with two degenerate minima is qualitatively different from a potential with a single minimum. Instanton configurations provide the necessary supplement to perturbation theory, which is a pure expansion in powers of g. The expansion of the eigenvalue in the instanton formalism is systematic and leads to a well-defined representation as a triple series in (i) the nonperturbative expression $\exp(-1/g)$, raised to the power n of the number of instanton oscillations, (ii) logarithms of the form $\ln(-g)$ which are caused by proportionality factors multiplying the instanton interaction, and (iii) powers of the coupling g. The logarithms $\ln(-g)$, for positive coupling $g > 0$, give rise to imaginary contributions which are compensated by imaginary parts of generalized Borel sums of lower-order instanton configurations, resulting in a real energy eigenvalue, as it should be. The necessary analytic continuations have given rise to some discussion and confusion in the past; today, we can verify the validity of this procedure by comparing the "predictions" of the multi-instanton expansion, including the inherent analytic continuations, with numerically determined energy eigenvalues of up to 180 decimal figures.

Let us briefly expand on the connection between the generalized expansions discussed here and the theory of differential equations as developed by Riemann. It is well known that the hypergeometric equation is a second-order

differential equation with three singularities at $z = 0, 1, \infty$. The solutions of this equation, the hypergeometric functions, can be expressed as power series in z. If one assumes further singularities, the solutions are no longer expressible in terms of simple power series. Instead, they may be expressed as series of the form $c\, z^a\, (\ln z)^p$ (c constant, $a \in C$, p integer, $p \geq 0$ confined). The Riemann–Hilbert theorem shows that they are essentially characterized by the way in which they reproduce themselves under analytic continuations along closed paths in the complex plane. An equation with essential singularities admits solutions which are expressible as a sum of terms of the form $c\, \exp[q(z)\, z^{-d}]\, z^a\, (\ln z)^p$ (c constant, q a polynomial, d positive and integer, $a \in C$, p integer, $p \geq 0$ confined). Inspired by the ideas expressed in the volume [2], we call expansions of this type "resurgent expansion."

Here, we discuss in detail a set of conjectures about the complete form of the perturbative expansion of the spectrum of a quantum Hamiltonian H, in situations where the potential has degenerate minima [2–6]. It will be shown that the coupling parameter g takes the formal role of the natural unit of action $\hbar$, and the systematic expansion about the classical problem (expansion in power of $\hbar$ in the form of a WKB expansion) will be used in order to derive the resurgent expansions in a systematic way. Perturbative expansions are obtained by first approximating the potential by a harmonic potential near its minimum. They are expansions for $\hbar \to 0$ valid for energy eigenvalues of order $\hbar$, in contrast with the WKB expansion where energies are non-vanishing in this limit (WKB approximation applies to large quantum numbers). When the potential has degenerate minima, perturbation series can be shown to be non-Borel summable. Moreover, quantum tunneling generates additional contributions to eigenvalues of order $\exp(-\text{const.}\ /\hbar)$, which have to be added to the perturbative expansion (for a review and more detail about barrier penetration in the semi-classical limit see for example [7]).

Therefore, the determination of eigenvalues starting from their expansion for $\hbar$ small is a non-trivial problem. The conjectures we describe here, give a systematic procedure to calculate eigenvalues, for $\hbar$ finite, from expansions which are shown to contain powers of $\hbar$, $\ln \hbar$ and $\exp(-\text{const.}\ /\hbar)$, i.e. resurgent expansions. Moreover, generalized Bohr–Sommerfeld formulae allow us to derive the many series which appear in such formal expansions from only two of them, which can be extracted by suitable transformations from the corresponding WKB expansions. Note that the relation to the WKB expansion is not completely trivial. Indeed, the perturbative expansion corresponds (from the point of view of a semi-classical approximation) to a situation with confluent singularities and thus, for example, the WKB expressions for barrier penetration are not uniform when the energy goes to zero.

These concepts will be applied to the following classes of potentials,

- the double-well potential,
- more general symmetric potentials with degenerate minima,
- a potential with two equal minima but asymmetric wells,
- a periodic-cosine potential,
- resonances of the $\mathcal{O}(\nu)$-symmetric anharmonic oscillator, for negative coupling,
- eigenvalues of the $\mathcal{O}(\nu)$-symmetric anharmonic oscillator, for negative coupling but with the Hamiltonian endowed with nonstandard boundary conditions,
- a special potential which has the property that the perturbative expansion of the ground-state energy vanishes to all orders of the coupling constant (Fokker–Planck Hamiltonians).

Based on the extensive mathematical work carried out on the subject [2], it is perhaps rather natural to remark that several of these conjectures have meanwhile found a natural explanation in the framework of Ecalle's theory of resurgent functions [8] and have now been proven by Pham and his collaborators [9–12]. In what follows, we always assume that the potential is an analytic entire function. This is also the framework in which the available mathematical proofs exist. We first explain the conjecture in the case of the so-called *double-well* potential. Note that, in what follows, the symbol g plays the role of $\hbar$ and the energy eigenvalues are measured in units of $\hbar$, a normalization adapted to perturbative expansions. Although several conjectures have now been proven, we believe that heuristic arguments based on instanton considerations are still useful because, suitably generalized, they could lead to new conjectures in more complicated situations.

Instantons have played a rather significant role in explaining unexpected behaviour in several aspects of quantum field theory, for example the nontrivial structure of the quantum chromodynamic vacuum or the absence of the "superfluous" η' meson. Instantons effectively eliminate the the $U(1)$ symmetry that would generates the η' particle, eliminating the problem. In the case of the one-dimensional problems studied in the current review, the instanton contributions can be subjected to a systematic study, including an investigation of the interaction among instantons which leads to a systematic expansion of the energy eigenvalues in $\hbar$, $\ln \hbar$ and $\exp(-\text{const.}\,/\hbar)$.

This review is organized as follows. In chapter 2, we describe the conjectures. In chapter 3, we discuss the connection with the WKB expansion as derived by different methods from Schrödinger equation. In chapter 4, we explain how these conjectures were suggested by a summation of the leading order *multi-instanton* contributions to the quantum partition function $\text{Tr}\,\exp(-\beta H)$ in the path integral representation. In chapter 6, we discuss in the same way the periodic cosine potential, and in chapter 5 more general potentials with degenerate minima. In chapter 7, related problems in the example of the $\mathcal{O}(\nu)$ quartic anharmonic oscillator are considered. Finally, the appendix contains additional technical details and explicit calculations verifying some implications of the conjectures at second WKB order.

Chapter 2

Generalized Bohr–Sommerfeld Quantization Formulae

2.1 Double–Well Potential

2.1.1 Resurgent Expansion (Double–Well)

Let us consider a quantal particle bound in a double-well potential which we write in the symmetric form

$$V_s(g,q) = \frac{g}{2}\left(\frac{1}{2\sqrt{g}}+q\right)^2\left(\frac{1}{2\sqrt{g}}-q\right)^2. \tag{2.1}$$

The minima are at $q = \pm 1/\sqrt{g}$. The potential is represented graphically in figure 2.1, with an indication of the ground state and the first excited state ($g = 0{,}08$). Further calculations profit from a translation of the coordinate

$$q \to q + \frac{1}{2\sqrt{g}}. \tag{2.2}$$

This translation preserves the spectrum of the Hamiltonian and leads to the quantum mechanical eigenvalue problem

$$H\psi(x) = E\,\psi(x) \tag{2.3}$$

in $L^2(R)$. The Hamiltonian after the translation is

$$H = -\frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}q}\right)^2 + V(g,q)\,, \qquad V(g,q) = \frac{1}{2}\,q^2\,(1-\sqrt{g}\,q)^2. \tag{2.4}$$

For $g \to 0$, we recover the unperturbed harmonic oscillator. Consequently, the unperturbed ground state in figure 2.1 has an energy of $E = 1/2$. When Rayleigh–Schrödinger perturbation theory is applied to the Nth harmonic oscillator state, the energy shift due to the terms of order g^3 and g^4 in $V(g,q)$ [see equation (2.4)] gives rise to a formal power expansion in g (not $\sqrt{g}$),

$$E_N \sim \sum_{l=0}^{\infty} E_{N,l}^{(0)}\, g^l\,. \tag{2.5}$$

For the ground state ($N = 0$), the first terms read

$$E_0 \sim \frac{1}{2} - g - \frac{9}{2}\,g^2 - \frac{89}{2}\,g^3 - \frac{5013}{8}g^4 - \ldots \tag{2.6}$$

The coefficients in this series grow factorially, and the series is not Borel summable (all coefficients except the leading term have negative sign (a complete list of the leading 300 perturbative coefficients for the ground state

can be found at [13]). In higher orders of perturbation theory, the numerators and denominators of the coefficients exhibit rather prime factors. For instance, we have

$$E_{0,17} = -\frac{3^2}{2^{17}}\,130\,116\,860\,668\,372\,133\,614\,952\,623. \tag{2.7}$$

Recently, connections between number theory and physical perturbation theory have attracted considerable attention. We will not pursue these questions any further in the current work.

We continue the discussion by observing that for negative g, the series (2.5) and in particular (2.6) are alternating and indeed Borel summable. One might now expect that a suitable analytic continuation of the Borel sum from negative to positive g gives the desired result for the energy levels of the double-well problem. That is not the case. Perturbation theory fails to account for the spectrum even qualitatively. For every one eigenstate of the unperturbed problem ($g = 0$), two eigenstates emerge in the case of nonvanishing coupling $g > 0$. For example, the unperturbed ground state with an energy $E = 1/2$ splits into two states with different energy for $g > 0$, as shown in figure 2.1. The new quantum number that differentiates the two states is the parity $\varepsilon = \pm 1$ [see (2.10) below]. Indeed, as is well known, the ground state with $N = 0$ "splits up" into two states each of which has opposite parity. The two levels that emerge from the ground state as the coupling g is "switched on" are separated by an energy interval of

$$\approx \frac{2}{\sqrt{\pi\, g}}\,\exp\left(-\frac{1}{6\,g}\right). \tag{2.8}$$

This term is nonperturbative in g, i.e. its formal power series in g vanishes to all orders.

For all further discussions, we scale the coordinate q in (2.4) as

$$q \to \frac{1}{\sqrt{g}}\,q. \tag{2.9}$$

This scale transformation again conserves all eigenvalues. The Hamiltonian corresponding to the double-well potential can therefore be written alternatively as

$$H = -\frac{g}{2}\left(\frac{\mathrm{d}}{\mathrm{d}q}\right)^2 + \frac{1}{g}\,V(q), \tag{2.10a}$$

$$V(q) = \frac{1}{2}\,q^2(1-q)^2\,. \tag{2.10b}$$

This representation shows that g takes over the formal role of $\hbar$. The Hamiltonian is symmetric in the exchange $q \leftrightarrow 1-q$ and thus commutes with the corresponding parity operator P, whose action on wave functions is

$$P\,\psi(q) = \psi(1-q) \;\Rightarrow [H, P] = 0\,. \tag{2.11}$$

The eigenfunctions of H satisfy

$$H\,\psi_{\varepsilon,N}(q) = E_{\varepsilon,N}(g)\psi_{\varepsilon,N}(q)\,, \quad P\,\psi_{\varepsilon,N}(q) = \varepsilon\,\psi_{\varepsilon,N}(q), \tag{2.12}$$

where $\varepsilon = \pm 1$ is the parity and the quantum number N can be uniquely assigned to a given state by the requirement $E_{\varepsilon,N}(g) = N + 1/2 + \mathcal{O}(g)$, i.e. by identifying the specific unperturbed harmonic oscillator eigenstate to whose energy eigenvalue the state energy converges in the limit $g \to 0$. We have conjectured [4, 5] that the eigenvalues $E_{\varepsilon,N}(g)$ of the Hamiltonian (2.10) have a complete semi-classical resurgent expansion of the form

$$E_{\varepsilon,N}(g) = \sum_{l=0}^{\infty} E_{N,l}^{(0)}\,g^l + \sum_{n=1}^{\infty}\left(\frac{2}{g}\right)^{Nn}\left(-\varepsilon\frac{\mathrm{e}^{-1/6g}}{\sqrt{\pi g}}\right)^n \sum_{k=0}^{n-1}\left\{\ln\left(-\frac{2}{g}\right)\right\}^k \sum_{l=0}^{\infty} e_{N,nkl}\,g^l\,. \tag{2.13}$$

The expansion (2.13) is the sum of the perturbative expansion which is independent of the parity,

$$E_N^{(0)}(g) = \sum_{l=0}^{\infty} E_{N,l}^{(0)}\,g^l \tag{2.14}$$

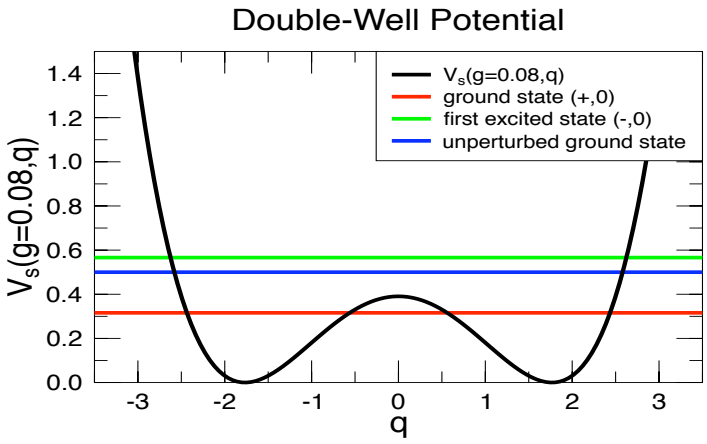

Figure 2.1: Double-well potential for the case $g = 0.08$ with the two lowest eigenvalues and the unperturbed eigenstate. The energy of the unperturbed ground state is the energy of the $(N = 0)$-state of the harmonic oscillator ground state with $E = 1/2$. The quantum numbers of the ground state in the potential $V_s(g = 0.08, q)$ are $(+, 0)$ (positive parity and unperturbed oscillator occupation quantum number $N = 0$). The potential V_s is defined in (2.1). The energy eigenvalue corresponding to the state $(+, 0)$ is $E_{+,0} = 0.317\,851\,364\,6\ldots$. The first excited state $(-, 0)$ has an energy of $E_{-,0} = 0.566\,114\,759\,4\ldots$. The arithmetic mean of the energies of the two states $(\pm, 0)$ is $0.441\,983\,062\,0\ldots$ and thus different from the value $1/2$. This is a consequence of the two-instanton (more general: even-instanton) shift of the energies.

and of the n-instanton contributions, each of which is given by

$$E^{(n)}_{\epsilon,N}(g) = \left(\frac{2}{g}\right)^{Nn} \left(-\varepsilon \frac{\mathrm{e}^{-1/6g}}{\sqrt{\pi g}}\right)^n \sum_{k=0}^{n-1} \left\{\ln\left(-\frac{2}{g}\right)\right\}^k \sum_{l=0}^{\infty} e_{N,nkl}\, g^l\,. \tag{2.15}$$

Here, $E^{(0)}_N(g)$ is the perturbation series whose coefficients $E^{(0)}_{N,l}$ only depend on the quantum number N (and the order of perturbation theory l), but not on the parity ε [see also (2.5)]. The index n gives the order of the "instanton expansion". One-instanton effects are characterized by a single power of the nonperturbative factor $\exp(-1/6g)$, two-instanton effects are multiplied by $\exp(-1/3g)$, etc. Actually, as shown below in chapters 4.3 and 4.4, the one-instanton effect $E^{(1)}_{\epsilon,N}(g)$ involves a summation over n-instanton configurations, however neglecting the instanton interaction. The two-instanton shift $E^{(2)}_{\epsilon,N}(g)$ and higher-order corrections involve the instanton interaction.

The logarithms of the form $\ln(-2/g)$ also enter into the formalism, their maximum power (for given n) is $n - 1$. Thus, the two-instanton effect carries one and only one logarithm etc. Each of the infinite series

$$\sum_{l=0}^{\infty} e_{N,nkl} g^l \tag{2.16}$$

is characterized by the state quantum number N, the instanton order n and the power of the logarithm k. The series $\sum e_{N,nkl} g^l$ in powers of g are not Borel summable for $g > 0$ and have to be summed for g negative. The values for

g positive are then obtained by analytic continuation, consistently with the determination of $\ln(-g)$. In the analytic continuation from g negative to g positive, the Borel sums become complex with imaginary parts exponentially smaller by about a factor $\exp(-1/3g)$ than the real parts. These imaginary contributions are canceled by the imaginary parts coming from the function $\ln(-2/g)$. For instance, the imaginary part incurred by analytic continuation of the perturbation series [equation (2.14) below] is canceled by the "explicit" imaginary part originating from the two-instanton effect [the term with $n = 2$ in (2.13)].

The instanton terms $E^{(n)}_{\epsilon,N}(g)$ are parity-dependent for odd n. In [14], a different notation was used for the coefficients that enter into the expansion (2.13). When comparing formulas, observe that in [14], ϵ denotes the coefficient, whereas here, the slightly different symbol $\varepsilon = \pm$ denotes the parity, and we have

$$\epsilon^{(N,\varepsilon)}_{nkl} \equiv (-\varepsilon)^n \, e_{N,nkl} \,. \tag{2.17}$$

The e-coefficients allow for a more compact notation. Their introduction is based on the observation that the odd-instanton coefficients have different sign for states with different parity, whereas the even-instanton contributions have the same sign for states with opposite parity. Thus, odd instantons contribute to the separation of energy levels with the same N, but opposite parity, whereas the energy shift due to even instantons is the same for both levels with the same N, irrespective of the parity. To give an example, we quote here from [14], without proof, several known coefficients for the one- and two-instanton contributions, from which the parity/sign pattern is apparent:

$$\epsilon^{(0,+)}_{100} = -\epsilon^{(0,-)}_{100} = -1\,, \quad \epsilon^{(0,+)}_{101} = -\epsilon^{(0,-)}_{101} = \frac{71}{12}\,, \tag{2.18a}$$

$$\epsilon^{(0,+)}_{101} = -\epsilon^{(0,-)}_{101} = \frac{6299}{288}\,, \quad \epsilon^{(0,+)}_{210} = \epsilon^{(0,-)}_{210} = 1\,, \tag{2.18b}$$

$$\epsilon^{(0,+)}_{211} = \epsilon^{(0,-)}_{211} = -\frac{53}{6}\,, \quad \epsilon^{(0,+)}_{212} = \epsilon^{(0,-)}_{212} = -\frac{1277}{72}\,, \tag{2.18c}$$

$$\epsilon^{(0,+)}_{200} = \epsilon^{(0,-)}_{200} = \gamma\,, \quad \epsilon^{(0,+)}_{201} = \epsilon^{(0,-)}_{201} = -\frac{23}{2} - \frac{53}{6}\,\gamma\,, \tag{2.18d}$$

$$\epsilon^{(0,+)}_{202} = \epsilon^{(0,-)}_{202} = \frac{13}{12} - \frac{1277}{72}\,\gamma\,. \tag{2.18e}$$

Here, $\gamma = 0.57221\ldots$ is Euler's constant. Utilizing the e-coefficients which enter into equation (2.13), these results can be summarized in a much more compact form as

$$e_{0,100} = 1\,, \quad e_{0,101} = -\frac{71}{12}\,, \quad e_{0,101} = -\frac{6299}{288}\,, \tag{2.19a}$$

$$e_{0,210} = 1\,, \quad e_{0,211} = -\frac{53}{6}\,, \quad e_{0,212} = -\frac{1277}{72}\,, \tag{2.19b}$$

$$e_{0,200} = \gamma\,, \quad e_{0,201} = -\frac{23}{2} - \frac{53}{6}\,\gamma\,, \quad e_{0,202} = \frac{13}{12} - \frac{1277}{72}\,\gamma\,. \tag{2.19c}$$

The coefficient $e_{0,100}$ gives the one-instanton separation of the levels with quantum numbers $(\pm, 0)$ which can be approximated as

$$E_{-,0} - E_{+,0} \approx -\frac{2}{\sqrt{\pi\, g}}\, \exp\left(-\frac{1}{6\, g}\right)\, e_{0,100}, \tag{2.20}$$

in agreement with (2.8). The well-known, classic treatment of the double-well problem is based on the "matched addition" or "matched subtraction" of the two solutions that characterize the two solutions in each single well. Only the leading term in the quantity $\exp(-1/6g)$ can be recovered in this way [15]. The advantage of the expansion (2.13) is that it generalizes the classic treatment to all orders in $\exp(-1/6g)$, thereby giving a clear interpretation of the way in which the many-instanton contributions manifest themselves in a generalized resurgent expansion in higher orders in $\exp(-1/6g)$. Also, the expansion (2.13) gives a systematic understanding of the error incurred upon terminating the instanton expansion at a given order.

2.1.2 Quantization Condition (Double–Well)

We have conjectured [16] that all series that enter into the generalized resurgent expansion (2.13) can be obtained by a small-g expansion of a generalized Bohr–Sommerfeld quantization formula. In the case of the double-well

potential, this quantization condition reads

$$\frac{1}{\sqrt{2\pi}}\,\Gamma\left(\frac{1}{2}-B_{\rm dw}(E,g)\right)\,\left(-\frac{2}{g}\right)^{B_{\rm dw}(E,g)}\,\exp\left[-\frac{A_{\rm dw}(E,g)}{2}\right]=\varepsilon{\rm i}\,, \tag{2.21}$$

or alternatively

$$\left[\Gamma\left(\frac{1}{2}-B_{\rm dw}(E,g)\right)\right]^{-1}+\frac{\varepsilon{\rm i}}{\sqrt{2\pi}}\left(-\frac{2}{g}\right)^{B_{\rm dw}(E,g)}\,\exp\left[-\frac{A_{\rm dw}(E,g)}{2}\right]=0\,, \tag{2.22}$$

($\varepsilon=\pm1$) where the A and the B-functions enjoy symmetry properties and can be expressed as formal series in their arguments,

$$B_{\rm dw}(E,g) \;=\; -B_{\rm dw}(-E,-g)=E+\sum_{k=1}^{\infty}g^k\,b_{k+1}(E), \tag{2.23a}$$

$$A_{\rm dw}(E,g) \;=\; -A_{\rm dw}(-E,-g)=\frac{1}{3g}+\sum_{k=1}^{\infty}g^k\,a_{k+1}(E)\,. \tag{2.23b}$$

The coefficients $b_k(E)$ and $a_k(E)$ are odd or even polynomials in E of degree k, as necessitated by the symmetry properties. The three first orders, for example, are

$$B_{\rm dw}(E,g) \;=\; E+g\left(3\,E^2+\frac{1}{4}\right)+g^2\left(35\,E^3+\frac{25}{4}E\right)+\mathcal{O}\left(g^3\right), \tag{2.24a}$$

$$\begin{aligned}A_{\rm dw}(E,g) \;=\;& \frac{1}{3}\,g^{-1}+g\left(17\,E^2+\frac{19}{12}\right)\\ &+g^2\left(227\,E^3+\frac{187}{4}E\right)+\mathcal{O}\left(g^3\right).\end{aligned} \tag{2.24b}$$

The function $B_{\rm dw}(E,g)$ has been inferred from the perturbative expansion, and indeed, the perturbative quantization condition reads

$$B_{\rm dw}(E,g)=N+\tfrac{1}{2}\,. \tag{2.25}$$

Here, N is a nonnegative integer. The perturbative expansion for an energy level is obtained by solving this equation for E. The function $A_{\rm dw}(E,g)$ had initially been determined at this order by a combination of analytic and numerical calculations.

The formula (2.13) is an exact expansion for the energy eigenvalues of the double-well anharmonic oscillator at finite g, which can be inferred by a systematic expansion of the quantization condition (2.22) for small g. The generalized resurgent expansion (2.13) can be derived either by a systematic expansion of the path integral representing the partition function about nontrivial saddle points of the Euclidean action, or by a systematic investigation of the WKB expansion. Both of these methods will be discussed in the sequel.

We illustrate the statements made by considering some example calculations. Specifically, we start by investigating approximations to the energies of the states $(+,0)$ and $(-,0)$ which emerge from the unperturbed oscillator ground state. The resurgent expansion is explicitly given in (2.13), with the first perturbative terms provided in (2.6) and the leading instanton coefficients (2.19). Neglecting higher-order perturbative (in g) and higher-order instanton effects [in $\exp(-1/6g)$], the energies of the two lowest-lying states are given by

$$E_{\varepsilon,0}\approx\frac{1}{2}-\frac{\varepsilon}{\sqrt{\pi g}}\,\exp\left[-\frac{1}{6\,g}\right]. \tag{2.26}$$

Here, $\varepsilon=\pm$ is again the parity. We define the abbreviations

$$\xi(g)=\frac{1}{\sqrt{\pi g}}\,\exp\left[-\frac{1}{6\,g}\right] \tag{2.27}$$

and

$$\chi(g)=\ln\left(-\frac{2}{g}\right)\,. \tag{2.28}$$

An expansion of the quantization conditions (2.21) and (2.22) for small $\xi(g)$ [note that a small positive g implies a small $\xi(g)$] then involves an evaluation of the expression

$$\Gamma\left(\frac{1}{2} - B_{\rm dw}(E_{\varepsilon,0},g)\right) \approx \Gamma\left(\varepsilon\,\xi(g)\right) \approx \varepsilon\,\frac{1}{\xi(g)} = \varepsilon\,\frac{\sqrt{\pi g}}{\exp\left[-\frac{1}{6\,g}\right]}. \tag{2.29}$$

The quantization condition (2.21) then takes the form

$$\frac{1}{\sqrt{2\pi}}\,\left(\frac{\varepsilon\sqrt{\pi g}}{\exp\left[-\frac{1}{6\,g}\right]}\right)\,\left(-\frac{2}{g}\right)^{1/2}\,\exp\left[-\frac{1}{2}\,\frac{1}{3\,g}\right] \approx \varepsilon{\rm i}. \tag{2.30}$$

This equation is approximately fulfilled provided that the analytic continuation of the square root is carried out such that for $g > 0$

$$\left(-\frac{2}{g}\right)^{1/2} \to {\rm i}\,\left(\frac{2}{g}\right)^{1/2}. \tag{2.31}$$

A systematic expansion of the quantization conditions (2.21) or alternatively (2.22) in powers of $\chi(g)$, $\xi(g)$ and g then leads in a natural way to the generalized resurgent expansion (2.13). We recall that some of the known coefficients for the ground state have been given in the form of the $\epsilon_{nkl}^{(N,\pm)}$ (2.18) or in the form of the $e_{N,nkl}$-coefficients (2.19). We now turn to a discussion of states with general N. The treatment is simplified if we restrict the discussion to the dominant effects in each order of the instanton expansion, i.e. if we restrict the discussion to the terms with $l = 0$ in the resurgent expansion (2.13). We employ the approximation

$$B_{\rm dw}(E,g) \to E \tag{2.32}$$

in (2.23a) and obtain the following approximative quantization condition

$$\frac{{\rm e}^{-1/6g}}{\sqrt{2\pi}}\,\left(-\frac{2}{g}\right)^{E} = -\frac{\varepsilon{\rm i}}{\Gamma(\frac{1}{2}-E)} \;\Leftrightarrow\; \frac{\cos\pi E}{\pi} = \varepsilon{\rm i}\,\frac{{\rm e}^{-1/6g}}{\sqrt{2\pi}}\,\left(-\frac{2}{g}\right)^{E}\,\frac{1}{\Gamma(\frac{1}{2}+E)}\,. \tag{2.33}$$

We show in chapter 4 that, from the point of view of the path integral representation, the successive terms correspond to *multi-instanton* contributions, i.e. to contributions which are generated by the modification of the instanton action due to the overlap region which results when "gluing together" two (or more) instanton solutions to a multi-instanton configuration.

For example, the term $n = 1$ in (2.13), which is also the one-instanton contribution, is

$$E_N^{(1)}(g) = -\frac{\varepsilon}{N!}\,\left(\frac{2}{g}\right)^{N+1/2}\,\frac{{\rm e}^{-1/6g}}{\sqrt{2\pi}}(1+\mathcal{O}(g)). \tag{2.34}$$

This result generalizes the coefficient $e_{0,100} = 1$ (2.19) to the case of arbitrary N,

$$e_{N,100} = \frac{1}{N!}. \tag{2.35}$$

The term $n = 2$, which is the two-instanton contribution, is

$$E_N^{(2)}(g) = \frac{1}{(N!)^2}\,\left(\frac{2}{g}\right)^{2N+1}\,\frac{{\rm e}^{-1/3g}}{2\pi}\,\left[\ln(-2/g) - \psi(N+1) + \mathcal{O}\left(g\ln g\right)\right], \tag{2.36}$$

where ψ is the logarithmic derivative of the Γ-function. This result generalizes the coefficient $e_{\,0,210} = 1$ (2.19) to the case of arbitrary N,

$$e_{N,210} = \left(\frac{1}{N!}\right)^2. \tag{2.37}$$

and the result $e_{0,200} = \gamma$ to

$$e_{N,200} = -\left(\frac{1}{N!}\right)^2\,\psi(N+1). \tag{2.38}$$

More generally, it can be easily be verified upon inspection of (2.13) that the n-instanton contribution has at leading order the form

$$E_N^{(n)}(g) = \left(\frac{2}{g}\right)^{n(N+1/2)} \left(-\varepsilon \frac{\mathrm{e}^{-1/6g}}{\sqrt{2\pi}}\right)^n \left[P_n^N\big(\ln(-g/2)\big) + \mathcal{O}\left(g\,(\ln g)^{n-1}\right)\right], \tag{2.39}$$

in which $P_n^N(\sigma)$ is a polynomial of degree $n-1$ (not the Legendre polynomial). For example, for $N=0$ one finds

$$P_1^0(\sigma) = 1\,, \qquad P_2^0(\sigma) = \sigma + \gamma\,, \qquad P_3^0(\sigma) = \frac{3}{2}\,(\sigma+\gamma)^2 + \frac{\pi^2}{12}\,, \tag{2.40}$$

in which γ is Euler's constant: $\gamma = -\psi(1) = 0.577215....$

2.1.3 Large–Order Behaviour (Double–Well)

The perturbation series fails to describe the energy levels at the one-instanton level. However, the mean of the energies of the levels $(+,N)$ and $(-,N)$ may be described to greater accuracy by the perturbation series than each of the two opposite-parity energy levels, because the one-instanton effect has opposite sign for opposite-parity state. The perturbation series, which is nonalternating, may be resummed using standard techniques; the only difficulty which persists is the singularity along the integration axis in the Laplace–Borel integral. However, one may easily define a generalized Borel transform. The calculation of such a generalized transform is rather trivial and discussed for example in [17]. In particular, the Borel sum naturally develops an imaginary part for $g > 0$ which represents a fundamental ambiguity. In the case of the quantum electrodynamic effective action, the imaginary part which describes pair production emerges from an appropriate analytic continuation. In the case of the double-well potential, the energy values are real, and there are compensating imaginary contributions from higher-order instanton effects which compensate the imaginary part incurred by the Borel sum of the nonalternating perturbation series.

The mean of the energies of the levels $(+,N)$ and $(-,N)$ is described by the perturbation series up to a common shift received by both levels $(\pm,N)$ via the *two*-instanton effect. Thus, it is up to the *two*-instanton level that the perturbation series has a physical meaning: indeed, perturbation theory describes approximately the mean of the energies of the levels with the same N, but opposite parity. The mean of the energy of these levels, to better accuracy, is then given as the sum of the real part of the (complex) Borel sum of the perturbation series, and of the two-instanton effect. Thus, at the level of the two-instanton effect, we expect the asymptotic perturbation series to go through its minimal term which, for a factorially divergent series, is of the same order-of-magnitude as the imaginary part of its Borel sum and also of the same order-of-magnitude as the difference of the real part of the generalized Borel sum of the perturbation series and the result obtained by optimal truncation of that same series.

Thus, after an analytic continuation of the series $\sum_{l=0}^{\infty} e_{N,nkl}\, g^l$ in (2.13) from g negative to g positive, two things happen: the Borel sums become complex with an imaginary part exponentially smaller by about a factor $\exp(-1/3g)$ than the real part. Simultaneously, the function $\ln(-2/g)$ that enters into the two-instanton contribution in equation (2.13) also becomes complex and gets an imaginary part $\pm \mathrm{i}\,\pi$. Since the sum of all contributions is real, the imaginary parts must cancel. This property relates, for example, the non-perturbative imaginary part of the Borel sum of the perturbation series to the perturbative imaginary part of the two-instanton contribution. We have identified (in the sense of a formal power series) the quantity (2.14)

$$E_N^{(0)}(g) = \sum_{l=0}^{\infty} E_{N,l}^{(0)}\, g^l \tag{2.41}$$

as the perturbative expansion. We now specialize to the $(N=0)$-states with positive and negative parity. The relation to the two-instanton contribution as given by the polynomial P_2^N implicitly defined in (2.39) is

$$\mathrm{Im}\, E_0^{(0)}(g) \underset{g\to 0}{\sim} \frac{1}{\pi g}\, \mathrm{e}^{-1/3g}\, \mathrm{Im}\left[P_2^0\big(\ln(-g/2)\big)\right] = -\frac{1}{g}\mathrm{e}^{-1/3g}\,. \tag{2.42}$$

An introductory discussion of dispersion relations and imaginary parts generated by the summation of nonalternating factorially divergent series is given in appendix D, especially in chapter D.1. The coefficients $E_{N,k}^{(0)}$ are related

to the imaginary part by a Cauchy integral [see equation (D.5)]:

$$E_{0,k}^{(0)} = \frac{1}{\pi}\int_0^\infty \mathrm{Im}\left[E_0^{(0)}(g)\right]\frac{\mathrm{d}g}{g^{k+1}}. \tag{2.43}$$

For $k \to \infty$, the integral is dominated by small g values. From the asymptotic estimate (2.42) of $\mathrm{Im}\,E^{(0)}$ for $g \to 0$, one then derives the large order behaviour of the perturbative expansion [1]:

$$E_{0,k}^{(0)} \underset{k\to\infty}{\sim} -\frac{1}{\pi}3^{k+1}k!\,. \tag{2.44}$$

Let us us now consider the perturbative expansion about the one-instanton shift in the sense of equation (2.15), with the convention $E_{k,N}^{(1)} \equiv e_{N,10k}$:

$$E_{\varepsilon,N}^{(1)}(g) = -\frac{\varepsilon}{\sqrt{\pi g}}\mathrm{e}^{-1/6g}\left(1+\sum_{k=0}^{\infty}E_{k,N}^{(1)}\,g^k\right). \tag{2.45}$$

One may derive, from the imaginary part of P_3^N, the large-order behaviour of this expansion, by expressing that the imaginary part of $E_0^{(1)}(g)$ and $E_0^{(3)}(g)$ must cancel at leading order:

$$\mathrm{Im}\,E_0^{(1)}(g) \sim -\varepsilon\left(\frac{\mathrm{e}^{-1/6g}}{\sqrt{\pi g}}\right)^3 \mathrm{Im}\left[P_3\big(\ln(-g/2)\big)\right]. \tag{2.46}$$

The coefficients $E_{k,0}^{(1)}$ again are given by a dispersion integral:

$$\varepsilon\,E_{k,0}^{(1)} = \frac{1}{\pi}\int_0^\infty \left\{\mathrm{Im}\left[E_0^{(1)}(g)\right]\sqrt{\pi g}\,\mathrm{e}^{1/6g}\right\}\frac{\mathrm{d}g}{g^{k+1}}. \tag{2.47}$$

Using then equations (2.40) and (2.46), one finds

$$E_{k,0}^{(1)} \sim -\frac{1}{\pi}\int_0^\infty 3\left(\ln\frac{2}{g}+\gamma\right)\mathrm{e}^{-1/3g}\frac{\mathrm{d}g}{g^{k+2}}. \tag{2.48}$$

At leading order for k large, g can be replaced by its saddle point value $1/3k$ in $\ln g$ and, finally, one obtains

$$E_{k,0}^{(1)} = e_{0,10k} = -\frac{3^{k+2}}{\pi}k!\left[\ln(6\,k)+\gamma+\mathcal{O}\left(\frac{\ln k}{k}\right)\right]. \tag{2.49}$$

Both results (2.44) and (2.49) have been checked against the numerical behaviour of the corresponding series for which 300 terms can easily be calculated [13, 14].

2.1.4 The Function $\triangle$ (Double–Well)

A specific function Δ of the energy levels of the double-well potential, expressed as a function of the coupling g, has been the subject of rather intensive investigations in the past [5]. Here, we discuss the motivation for the definition of Δ, as well as its evaluation and the comparison to the instanton expansion.

We define the quantity $\mathcal{B}\left\{E_N^{(0)}(g)\right\}$ as the real part of the Borel sum of the the perturbation series (2.14),

$$\mathcal{B}\left\{E_N^{(0)}(g)\right\} = \mathrm{Re}\left[\text{Borel sum of } E_N^{(0)}(g) \equiv \sum_{l=0}^{\infty}E_{N,l}^{(0)}\,g^l\right]. \tag{2.50}$$

In [17], some explicit examples are given for the calculation of Borel sums in cases where the perturbation series is nonalternating (as in our case). In the same sense, we denote by $\mathcal{B}\left\{E_N^{(1)}(g)\right\}$ the real part of the Borel sum of

the the perturbation series about one instanton in the notation (2.15), evaluated for the state with negative parity (so that the result, for $g > 0$, is positive):

$$\mathcal{B}\left\{E_N^{(1)}(g)\right\} = \frac{\mathrm{e}^{-1/6g}}{\sqrt{\pi\, g}} \left\{ \mathrm{Re} \left[\text{Borel sum of } \sum_{l=0}^{\infty} e_{N,10l}\, g^l \right] \right\} . \tag{2.51}$$

An illustrative example is provided by equation (8.13) below, where the case $N = 0$ is considered and the first terms ($l = 0, \ldots, 8$) are given explicitly. The quantity $\mathcal{B}\left\{E_N^{(1)}(g)\right\}$ is of importance for the entire discussion in chapter 8.9 below.

We now consider the ratio

$$\Delta(g) = 4 \frac{\left\{ \frac{1}{2}\,(E_{+,0} + E_{-,0}) - \mathcal{B}\left\{E_0^{(0)}(g)\right\} \right\}}{(E_{+,0} - E_{-,0})^2\,[\ln(2g^{-1}) + \gamma]}. \tag{2.52}$$

In this expression $E_{+,0}$ and $E_{-,0}$ are the two lowest eigenvalues of H. In the sum $(E_{+,0} + E_{-,0})$ the contributions corresponding to an odd number of instantons cancel. Therefore, the numerator is dominated for g small by the real part of the two-instanton contribution proportional to $\mathrm{Re}\, P_2$. Note that, if the perturbation series were able to describe the mean of the energies $E_{+,0}$ and $E_{-,0}$ exactly, then the numerator would vanish. The difference $(E_+ - E_-)$, as we know, is dominated by the one-instanton contribution which in turn is characterized by a nonperturbative factor $\exp[-1/6g]$. Squaring the energy difference, we obtain an expression of the order of $\exp[-1/3g]$ which is characteristic of the two-instanton effect. Forming the ratio of the two-instanton effect, divided by the squared one-instanton, we obtain an expression of order one (the additional logarithm appears because of the nonvanishing $e_{0,210}$ coefficient). Using the expansion (2.13) together with the explicit results for the coefficients (2.19), one verifies easily that $\Delta(g)$ indeed tends to unity as $g \to 0$.

Moreover, performing an expansion in powers of g and inverse powers of $\ln(2/g)$ and keeping only the first few terms in $\{1/\ln(2/g)\}$ in each term in the g-expansion, one finds [14]

$$\begin{aligned} \Delta(g) \sim 1 + 3\,g - \frac{23}{2}\frac{g}{\ln(2/g)} \left[1 - \frac{\gamma}{\ln(2/g)} + \frac{\gamma^2}{\ln^2(2/g)} + \mathcal{O}\left(\frac{1}{\ln^3(2/g)}\right) \right] \\ + \frac{53}{2} g^2 - 135 \frac{g^2}{\ln(2/g)} \left[1 - \frac{\gamma}{\ln(2/g)} + \frac{\gamma^2}{\ln^2(2/g)} + \mathcal{O}\left(\frac{1}{\ln^3(2/g)}\right) \right] + \mathcal{O}\left(g^3\right) . \end{aligned} \tag{2.53}$$

The higher-order corrections, which are only logarithmically suppressed with respect to the leading terms $1 + 3\,g$, change the numerical values quite significantly, even for small g.

Table 2.1: The ratio $\Delta(g)$ as a function of g.

coupling g	0.005	0.006	0.007	0.008	0.009	0.010
$\Delta(g)$ num.	1.0063(5)	1.0075(5)	1.00832(5)	1.00919(5)	1.00998(5)	1.01078(5)
$\Delta(g)$ asymp.	1.00640	1.00739	1.00832	1.00919	1.01001	1.01078

Table 2.1 displays numerical results, obtained by solving the Schrödinger equation in a range of small values of g for which the evaluation is still reasonably precise; there are in agreement with the first few asymptotic terms up to numerical precision [14].

Of course, for larger values, significant deviations from the leading asymptotics must be expected due to higher-order effects; these are indeed observed as seen in figure 2.2. For example, at $g = 0.1$ the numerically determined value reads $\Delta(0.1) = 0.87684(1)$ whereas the first asymptotic terms sum up to a numerical value of 0.86029. Further calculations are described in chapter 8, where also reference values for $\Delta(g)$ are given.

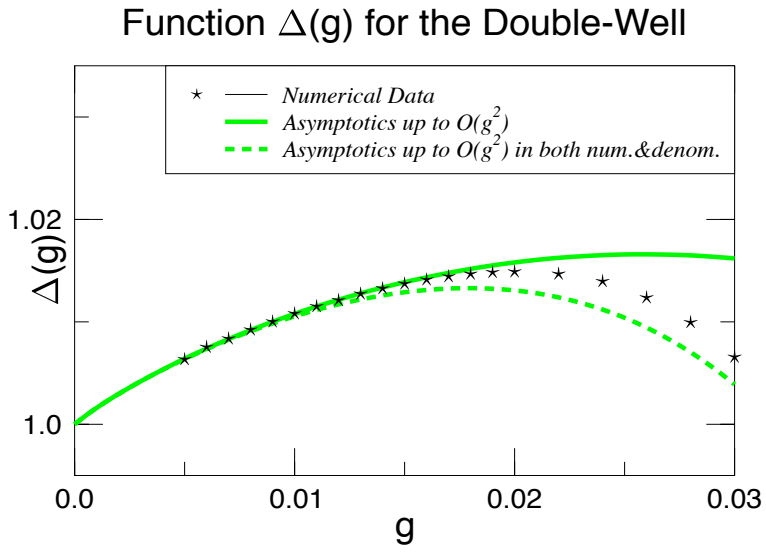

Figure 2.2: Double-well potential: Comparison of numerical data obtained for the function $\Delta(g)$ with the sum of the terms up to the order of g^2 of its asymptotic expansion for g small [see equation (2.53)], solid line. If we express both the numerator and the denominator of (2.52) as a power series in g [with the help of the instanton coefficients (2.18)] and keep all terms up to the order of g^2, the dashed curve results. This latter approach is also used for the curves in figures 8.1, 8.2, and 8.3 below.

2.2 Other Potentials

2.2.1 Symmetric Wells

We consider a slight generalization of (2.21), i.e. a potential with degenerate minima at $q = 0$ and $q = q_0$, and

$$V(q) = \tfrac{1}{2}\,\omega^2\,q^2 + \mathcal{O}(q^3)\,, \quad V(q) = \tfrac{1}{2}\,\omega^2\,(q-q_0)^2 + \mathcal{O}\left((q-q_0)^3\right)\,. \tag{2.54}$$

The potential V is supposed to fulfill the symmetry condition $V(q) = V(q_0 - q)$. Without loss of generality, one may set

$$\omega = 1 \tag{2.55}$$

in (2.54), by a simple scaling argument. Indeed, a Hamiltonian [see equation (2.10a)]

$$H(g,\omega) = -\frac{g}{2}\left(\frac{\mathrm{d}}{\mathrm{d}q}\right)^2 + \frac{1}{g}\left(\frac{1}{2}\,\omega^2\,q^2 + \frac{1}{2}\,\omega^2\,(q-q_0)^2\right) \tag{2.56}$$

satisfies

$$H(g,\omega) = \omega\,H\left(\frac{g}{\omega},1\right)\,, \tag{2.57}$$

which maps the spectrum of the general case with arbitrary ω onto a seemingly more special case, with $\omega = 1$ and a redefined coupling g. The constant C is given as [see also equation (E.10b) below],

$$C = q_0^2\,\exp\left[\int_0^{q_0}\left(\frac{1}{\sqrt{2V(q)}} - \frac{1}{q} - \frac{1}{q_0 - q}\right)\right]\,. \tag{2.58}$$

As in the case of the double-well potential, the function $A_{\rm sym}(E,g)$, which described the instanton-related effects, has no term of order g^0 [cf. equation (2.23b)]

$$A_{\rm sym}(E,g) = a/g + \mathcal{O}(g)\,. \tag{2.59}$$

The constant a is given by [see equation (E.10a) below]

$$a = 2\int_0^{q_0} {\rm d}q\,\sqrt{2V(q)}\,. \tag{2.60}$$

There is, just as in the case of the double-well problem, degeneracy on the level of perturbation theory which is lifted by instantons. The quantization condition is conjectured to be

$$\frac{1}{\sqrt{2\pi}}\,\Gamma\left(\frac{1}{2}-B_{\rm sym}(E,g)\right)\,\left(-\frac{2C}{g}\right)^{B_{\rm sym}(E,g)}\,\exp\left[-\frac{A_{\rm sym}(E,g)}{2}\right] = \varepsilon{\rm i}\,, \tag{2.61}$$

with ε denoting the parity. The function $B_{\rm sym}(E,g) = E + \mathcal{O}(g)$ is related to the perturbative expansion about each of the two symmetric wells, as given in (3.31) below and explained in detail in chapter 3.2.5. The perturbative quantization condition reads

$$B_{\rm sym}(E,g) = N + \tfrac{1}{2} \tag{2.62}$$

with integer positive N. Explicit calculations of the first few terms in the expansion of $B_{\rm sym}(E,g)$ in g are carried out in appendix B.1, and relevant formulas can be found in equation (B.11). For $A_{\rm sym}(E,g)$, see appendix F.5.

It is important to remark that the A and B-functions (2.89a) and (2.89b) are determined by the formal properties of the potential alone. Specifically, these functions may be inferred, for a given potential, via an evaluation of the contour integrals of the WKB expansion [left-hand side of equation (3.57)]. We distinguish here several different A and B functions by assigning indices to these symbols, depending on the potential in question. However, it is necessary to remember that the potential alone determine the instanton-related A-function and the perturbative B-function are determined by the potential alone [which we always use in the convention (2.10a)].

2.2.2 Asymmetric Wells

In the case of a potential with two asymmetric wells, we have to modify the *quantization condition* (2.21). Specifically, we will discuss the case of a potential with two asymmetric wells about which one may expand

$$V(q) = \tfrac{1}{2}\,\omega_1^2\,q^2 + \mathcal{O}(q^3)\,,\quad V(q) = \tfrac{1}{2}\,\omega_2^2\,(q-q_0)^2 + \mathcal{O}\left((q-q_0)^3\right)\,. \tag{2.63}$$

Of course, the asymmetry manifests itself in the relation $V(q) \neq V(q_0-q)$. The generalized Bohr–Sommerfeld quantization formula takes the form [see also equations (3.57), (5.1), (5.3), (5.8), (5.16), (7.20b), and (F.35) below]

$$\begin{aligned}&\frac{1}{\Gamma(\frac{1}{2}-B_1(E,g))\,\Gamma(\frac{1}{2}-B_2(E,g))}\\ &\quad+\frac{1}{2\pi}\,\left(-\frac{2C_1}{g}\right)^{B_1(E,g)}\,\left(-\frac{2C_2}{g}\right)^{B_2(E,g)}\,{\rm e}^{-A(g,E)} = 0\,,\end{aligned} \tag{2.64}$$

where $B_1(E,g)$ and $B_2(E,g)$ are determined by the perturbative expansions (see chapter 3.2.5) around each of the two minima of the potential

$$B_1(E,g) = E/\omega_1 + \mathcal{O}(g),\quad B_2(E,g) = E/\omega_2 + \mathcal{O}(g)\,, \tag{2.65}$$

The perturbative quantization conditions are

$$B_1(E,g) = N_1 + \tfrac{1}{2}\,,\quad B_2(E,g) = N_2 + \tfrac{1}{2}\,, \tag{2.66}$$

with nonnegative integer N_1 and N_2. In equation (2.64), the quantities C_1 and C_2 are numerical constants, adjusted in such a way that $A(E,g)$ has no term of order g^0:

$$A(E,g) = a/g + \mathcal{O}(g)\,. \tag{2.67}$$

Again, a is given by

$$a = 2 \int_0^{q_0} \mathrm{d}q \, \sqrt{2V(q)} \, . \tag{2.68}$$

Equation (2.64) has two series of energy eigenvalues,

$$E_N = \left(N + \tfrac{1}{2}\right) \omega_1 + \mathcal{O}(g) \, , \quad E_N = \left(N + \tfrac{1}{2}\right) \omega_2 + \mathcal{O}(g) \tag{2.69}$$

close for $g \to 0$ to the poles of the two Γ-functions. The same expression contains the instanton contributions to the two different sets of eigenvalues.

The quantization condition (2.64) is qualitatively different from (2.21) and (2.61) because parity is explicity broken in the asymmetric case. One verifies that multi-instanton contributions are singular for $\omega = 1$. But, if one takes the symmetric limit, one obtains a form consistent with the product of the two equations (2.61).

Without loss of generality, one may set

$$\omega_1 = 1 \, , \qquad \omega_2 = \omega \tag{2.70}$$

in (2.63), by a simple scaling argument. Indeed, a Hamiltonian [see equation (2.10a)]

$$H(g, \omega_1, \omega_2) = -\frac{g}{2} \left(\frac{\mathrm{d}}{\mathrm{d}q} \right)^2 + \frac{1}{g} \left(\frac{1}{2} \omega_1^2 \, q^2 + \frac{1}{2} \omega_2^2 \, (q - q_0)^2 \right) \tag{2.71}$$

satisfies

$$H(g, \omega_1, \omega_2) = \omega_1 \, H \left(\frac{g}{\omega_1}, 1, \frac{\omega_2}{\omega_1} \right) = H(\tilde{g}, 1, \tilde{\omega}) \, , \tag{2.72}$$

a relation that maps the spectrum of the general case with arbitrary g, ω_1, and ω_2 onto the more special case $\tilde{g}$, $\omega_1 = 1, \omega_2 = \tilde{\omega}$. One may than redefine $\tilde{g} \to g$ and $\tilde{\omega} \to \omega$. The constant C, defined as [see equation (5.3) below],

$$C_\omega = q_0^2 \, \omega^{2/(1+\omega)} \, \exp\left\{ \frac{2\omega}{1+\omega} \left[\int_0^{q_0} \mathrm{d}q \, \left(\frac{1}{\sqrt{2V(q)}} - \frac{1}{q} - \frac{1}{\omega(q_0 - q)} \right) \right] \right\} \, , \tag{2.73}$$

tends to (2.58) in the limit $\omega \to 1$. The constants C_1 and C_2 are then given by [see equation (5.8) below]:

$$C_1 = C_\omega \, , \qquad C_2 = C_\omega / \omega \, . \tag{2.74}$$

These enter into the quantization condition (2.64). We note also that the quantization condition (2.64) may be derived, to leading order in g, by an exact evaluation of the multi-instanton contribution to the path integral [see (5.16)].

We now consider the imaginary part of the leading-instanton contribution and large-order estimates. The expression (2.64) can be used to determine the large order behaviour of perturbation theory by calculating the imaginary part of the leading instanton contribution and writing a dispersion integral. Setting $\omega_1 = 1$, $\omega_2 = \omega$, for the energy $E_N(g) = N + \frac{1}{2} + \mathcal{O}(g)$ one finds the imaginary part

$$\mathrm{Im} \, E_N(g) \underset{g \to 0}{\sim} K_N \, g^{-(N+1/2)(1+1/\omega)} \, \mathrm{e}^{-a/g} \tag{2.75}$$

with [equation (2.73)]

$$K_N = \frac{(-1)^{N+1}}{2\pi \, N!} \, \omega^{-(N+1/2)/\omega} \, \left(2 \, C_\omega\right)^{(N+1/2)(1+1/\omega)} \tag{2.76}$$

$$\times \sin\left[\pi(N + \tfrac{1}{2})(1 + 1/\omega)\right] \, \Gamma\left[\tfrac{1}{2} - (N + \tfrac{1}{2})/\omega\right] \, . \tag{2.77}$$

From $\mathrm{Im} \, E_N(g)$, one infers that the coefficients $E^{(0)}_{N,k}$ of the perturbative expansion of $E_N(g)$ behave, for order $k \to \infty$, like

$$E^{(0)}_{N,k} \underset{k \to \infty}{=} K_N \, \frac{\Gamma[k + (N + 1/2)(1 + 1/\omega)]}{a^{k + (N+1/2)(1+1/\omega)}} \left[1 + \mathcal{O}\left(k^{-1}\right)\right] . \tag{2.78}$$

Note that this expression, in contrast to the instanton contribution to the real part, is uniform in the limit $\omega = 1$ in which the result (2.44) is recovered.

2.2.3 Periodic Cosine Potential

We first consider the *periodic cosine potential*. This example differs from the preceding ones because the potential is still an entire function but no longer a polynomial. On the other hand the periodicity of the potential simplifies the analysis, because it allows classifying eigenfunctions according to their behaviour under a translation of one period:

$$\psi_\varphi(q+T) = \mathrm{e}^{i\varphi}\psi_\varphi(q), \tag{2.79}$$

where T is the period. For the cosine potential $\frac{1}{16}(1-\cos 4q)$ (and thus $T=\pi/2$), the conjecture then takes the form

$$\left(\frac{2}{g}\right)^{-B_{\mathrm{pc}}(E,g)} \frac{\mathrm{e}^{A_{\mathrm{pc}}(E,g)/2}}{\Gamma[\frac{1}{2}-B_{\mathrm{pc}}(E,g)]} + \left(\frac{-2}{g}\right)^{B_{\mathrm{pc}}(E,g)} \frac{\mathrm{e}^{-A_{\mathrm{pc}}(E,g)/2}}{\Gamma[\frac{1}{2}+B_{\mathrm{pc}}(E,g)]} = \frac{2\cos\varphi}{\sqrt{2\pi}}. \tag{2.80}$$

The first few terms of the perturbative expansions of the functions A_{pc} and B_{pc} for the periodic potential are

$$B_{\mathrm{pc}}(E,g) = E + g\left(E^2+\frac{1}{4}\right) + g^2\left(3\,E^3+\frac{5}{4}\,E\right) + \mathcal{O}\left(g^3\right), \tag{2.81a}$$

$$A_{\mathrm{pc}}(E,g) = g^{-1} + g\left(3\,E^2+\frac{3}{4}\right) + g^2\left(11\,E^3+\frac{23}{4}\,E\right) + \mathcal{O}\left(g^3\right), \tag{2.81b}$$

where again A has been initially obtained by a combination of analytic and numerical techniques. The perturbative quantization condition is

$$B_{\mathrm{pc}}(E,g) = N + \tfrac{1}{2}\,. \tag{2.82}$$

The conjecture has been verified numerically up to four-instanton order with decreasing precision. The theory of resurgence has allowed to also investigate this potential, as well as general trigonometric potentials [12].

2.2.4 $\mathcal{O}(\nu)$–Anharmonic Oscillator and Fokker–Planck Equation

We consider now the $\mathcal{O}(\nu)$-*symmetric anharmonic oscillator* with the Hamiltonian

$$H = -\tfrac{1}{2}\,\boldsymbol{\nabla}^2 + \tfrac{1}{2}\,\mathbf{q}^2 + g\left(\mathbf{q}^2\right)^2, \tag{2.83}$$

where $\mathbf{q}$ belongs to $\mathbb{R}^\nu$. The analytic continuations of the eigenvalues to $g<0$ are complex, the imaginary part determining the decay rate by barrier penetration of states concentrated initially in the well at $\mathbf{q}=0$. Moreover, the behaviour of the imaginary part for $g\to 0_-$ is directly related to the large-order behaviour of the perturbative expansion.

The eigenfunctions of H can be classified according to the irreducible representations of the orthogonal $\mathcal{O}(\nu)$ group. We work in $\mathbb{R}^\nu$; at fixed angular momentum l, the Hamiltonian (2.83), expressed in terms of the radial variable $r=|\mathbf{q}|$, takes the form

$$H_l \equiv H_l(g) = -\frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2 - \frac{1}{2}\,\frac{\nu-1}{r}\,\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{2}\,\frac{l\,(l+\nu-2)}{r^2} + \frac{1}{2}\,r^2 + g\,r^4. \tag{2.84}$$

After the change of variables

$$H_l \mapsto \tilde{H}_l = r^{(\nu-1)/2}\,H_l\,r^{(1-\nu)/2}\,, \tag{2.85}$$

one finds

$$\tilde{H}_l = -\frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2 + \frac{1}{2}\,\frac{j^2-1/4}{r^2} + \frac{1}{2}\,r^2 + g\,r^4 \tag{2.86}$$

with

$$j = l + \nu/2 - 1\,. \tag{2.87}$$

The Hamiltonian H_l is one-dimensional with a non-polynomial potential. Eigenvalues depend on the parameter $j\equiv j(l)$ (but with the constraint $j(l)\geq \nu/2-1$). Note also the formal symmetry $j\mapsto -j$.

Writing the perturbative quantization condition as

$$B_\nu(E,g,j) = 1 + j + 2N\,, \quad N \geq 0\,, \tag{2.88}$$

one finds [see also equations (2.24a), (7.16), and (7.48)]

$$B_\nu(E,g,j) = E - \frac{1}{2}\left[3\,E^2 - j^2 + 1\right] g + \frac{5}{4}\left[7\,E^3 + (5 - 3\,j^2)\,E\right] g^2 + \mathcal{O}\left(g^3\right)\,. \tag{2.89a}$$

The first few terms of the expansion of the function A_ν are [see also (7.49)]:

$$\begin{aligned} A_\nu(E,g,j) &= -\frac{1}{3}\,g^{-1} + \left(\frac{3}{4}\,j^2 - \frac{19}{12} - \frac{17}{4}\,E^2\right) g \\ &\quad + \frac{1}{8}\left(227\,E^2 - 77\,j^2 + 187\right) E\,g^2 + \mathcal{O}\left(g^3\right). \end{aligned} \tag{2.89b}$$

The A and B functions are determined exclusively by the semi-classical expansion of the solutions of the spectral equation of the Hamiltonian (2.84).

In order to write down a quantization condition, it is necessary to specify boundary conditions for the Hamiltonian. In the current chapter, we will take advantage of a well-known connection between the $\mathcal{O}(\nu)$-anharmonic oscillator at negative (!) coupling on the one hand to the double-well potential at positive coupling with a symmetry-breaking term on the other hand [18, 19]. (This result, initially conjectured on the basis of numerical evidence, was first proven later by path integral manipulations [20] or recursion formulae [21], and later generalized to arbitrary j [19].)

We briefly recall here the central statement regarding the connection between "broken-double-well and the $\mathcal{O}(\nu)$–symmetric quartic potential. Indeed, as shown below in chapter 7.2.1, the spectral equation implied by the Hamiltonian

$$H_l(-g) = -\frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2 - \frac{1}{2}\,\frac{\nu-1}{r}\,\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{2}\,\frac{l\,(l+\nu-2)}{r^2} + \frac{1}{2}\,r^2 - g\,r^4\,. \tag{2.90a}$$

may be reformulated under appropriate substitutions into

$$-\frac{g}{2}\,\varphi''(p) + \frac{1}{2g}\left(p^2 - \frac{1}{4}\right)^2 \varphi(p) - j\,p\,\varphi(p) = \frac{E}{2}\,\varphi(p)\,. \tag{2.90b}$$

The spectrum of this equation is bound from below and leads naturally to a self-adjoint extension of the $\mathcal{O}(\nu)$ anharmonic oscillator at negative coupling. This spectrum is not the same as the resonances implied for negative coupling if the Hamiltonian is endowed with boundary conditions that imply a vanishing of the wave function in complex directions of the parameters, which would lead to resonances discussed below in chapter 2.2.5. As is evident from (2.90a) and (2.90b), the Hamiltonian H_l for $g < 0$, with proper boundary conditions, thus has a self-adjoint extension, which in turn is (almost) equivalent to the double-well potential, but with a linear symmetry-breaking term.

In the case $j = 0$ the linear symmetry-breaking term in (2.90b) vanishes. Setting $q = p + 1/2$, equation (2.90b) becomes identical to the spectral equation of the double-well potential. This consideration leads immediately to the following correspondence

$$B_\nu(E,-g,j=0) = 2\,B_{\mathrm{dw}}(E/2,g)\,, \tag{2.91a}$$

$$A_\nu(E,-g,j=0) = A_{\mathrm{dw}}(E/2,g)\,. \tag{2.91b}$$

The correspondence between the $j = 0$-component of the $\mathcal{O}(\nu)$-anharmonic oscillator and the (symmetric) double-well potential [18, 19], thus finds a natural extension to instanton effects described by the function $A_\nu(E,-g,j=0) = A_{\mathrm{dw}}(E/2,g)$. The perturbation series implied by the condition $B_{\mathrm{dw}}(E/2,g) = N + \frac{1}{2}$ leads to a non-Borel summable series for E as a function of g; the imaginary parts are compensated by instantons.

In view of (2.89a), (2.89b) and (2.90b), we conjecture for the self-adjoint extension of the Hamiltonian (2.84) at negative coupling $-g$ (with $g > 0$) the quantization condition

$$\begin{aligned} &\frac{1}{\Gamma\left[\frac{1}{2}(1+j-B_\nu(E,-g,j))\right]\,\Gamma\left[\frac{1}{2}(1-j-B_\nu(E,-g,j))\right]} \\ &\qquad + \left(-\frac{2}{g}\right)^{B_\nu(E,-g,j)}\,\frac{\exp\left(-A_\nu(E,-g)\right)}{2\pi} = 0\,. \end{aligned} \tag{2.92}$$

In leading order in g, this equation may be derived via instanton calculus [see equation (7.46)]:

$$\frac{1}{\Gamma\left(\frac{1}{2}(1+j-E)\right)\Gamma\left(\frac{1}{2}(1-j-E)\right)} + \left(-\frac{2}{g}\right)^{E} \frac{\mathrm{e}^{-1/3g}}{2\pi} \approx 0\,. \tag{2.93}$$

We now turn our attention to an important special case. Setting $j=-1$ in (2.90b) and shifting $E \to 2E$, we obtain the Fokker–Planck Hamiltonian

$$H_{\mathrm{FP}} = -\frac{g}{2}\frac{\mathrm{d}^2}{\mathrm{d}p^2} + \frac{1}{2g}\left(p^2-\frac{1}{4}\right)^2 + p\,, \tag{2.94a}$$

with the associated eigenvalue problem

$$H_{\mathrm{FP}}\,\varphi(p) = E\,\varphi(p)\,, \tag{2.94b}$$

which is known to have a peculiar property: the perturbative expansion of the ground-state energy vanishes to all orders in the coupling. Of course, the symmetry $j \to -j$, which is present in (2.86), implies that the the spectrum of (2.94) is invariant under a change of the sign of the linear symmetry-breaking term.

(*Remark.*) With the shift $p = q - 1/2$ in (2.94), we may rewrite the Fokker–Planck Hamiltonian as

$$H_{\mathrm{FP}} = -\frac{g}{2}\frac{\mathrm{d}^2}{\mathrm{d}q^2} + \frac{1}{g}\left[\frac{1}{2}\,q^2\,(1-q)^2 + g\,q\right] - \frac{1}{2}\,. \tag{2.95}$$

We may thus identify the Fokker–Planck Hamiltonian as originating from the double-well Hamiltonian (2.10b), with an additional linear symmetry-breaking term of relative order g, and an additional global shift of $-1/2$ which compensates the ground-state energy of the harmonic oscillator.

In view of the correspondence implied by (2.90) and the necessary shift $E \to 2E$ in going from (2.90b) to (2.94), we conjecture the following secular equation for the Fokker–Planck Hamiltonian as a special case of the anharmonic oscillator (2.92),

$$\frac{1}{\Gamma\left(-B_{\mathrm{FP}}(E,g)\right)\,\Gamma\left(1-B_{\mathrm{FP}}(E,g)\right)} + \left(-\frac{2}{g}\right)^{2B_{\mathrm{FP}}(E,g)} \frac{\exp\left(-A_{\mathrm{FP}}(E,g)\right)}{2\pi} = 0\,. \tag{2.96}$$

The perturbative quantization condition is

$$B_{\mathrm{FP}}(E,g) = N \tag{2.97}$$

where N is a nonnegative integer. The functions $B_{\mathrm{FP}}(E,g)$ and $A_{\mathrm{FP}}(E,g)$ are given by

$$B_\nu(E,-g,j=\pm 1) \;=\; 2B_{\mathrm{FP}}\left(\frac{E}{2},g\right)\,, \tag{2.98a}$$

$$A_\nu(E,-g,j=\pm 1) \;=\; A_{\mathrm{FP}}\left(\frac{E}{2},g\right)\,, \tag{2.98b}$$

where either sign of j leads to the same result. The first terms read

$$B_{\mathrm{FP}}\,(E,g) \;=\; E + 3\,E^2\,g + \left(35\,E^3+\frac{5}{2}\,E\right)\,g^2 + \mathcal{O}(g^3)\,, \tag{2.99a}$$

$$A_{\mathrm{FP}}\,(E,g) \;=\; \frac{1}{3g} + \left(17\,E^2+\frac{5}{6}\right)\,g + \left(227\,E^3+\frac{55}{2}\,E\right)\,g^2 + \mathcal{O}(g^3)\,. \tag{2.99b}$$

Indeed, the quantization condition (2.96) may be derived, at leading order in g, using instanton calculus [see equation (7.29) with $C=1$]:

$$\Delta(E) = \frac{1}{\Gamma(-E)\,\Gamma(1-E)} + \left(-\frac{2}{g}\right)^{2E} \frac{\mathrm{e}^{-a/g}}{2\pi}\,. \tag{2.100}$$

2.2.5 $\mathcal{O}(\nu)$–Anharmonic Oscillator: Resonances

In the current chapter, we investigate the quantization condition for the resonances of the $\mathcal{O}(\nu)$-anharmonic oscillator at negative coupling. These may be found by analytic continuation of the eigenvalues to negative coupling. The notation is the same as in chapter 2.2.4.

First, we briefly investigate the special case $j = 0$ at $g > 0$. The correspondence (2.91) implies the perturbative condition $B_\nu(E, g, j = 0) = 2\, B_{\rm dw}(E/2, -g) = 2N + 1$ for eigenvalues of the $\mathcal{O}(\nu)$-anharmonic oscillator at positive coupling.

The generalization to arbitrary j at $g > 0$ implies a Borel-summable, alternating series for E as a function of g. Indeed, the perturbative quantization condition (2.88) becomes exact in this case,

$$B_\nu(E, g, j) = 1 + j + 2N\,, \qquad N \geq 0\,. \tag{2.101}$$

We now turn to the resonances for arbitrary j at $g < 0$. We recall that the A_ν and B_ν-functions (2.89a) and (2.89b) are determined by the formal properties of the potential alone. However, the actual quantization condition may also depend on the boundary conditions. The secular equation for resonances at $g < 0$ is conjectured to be

$$\begin{aligned} &\mathrm{i}\,\mathrm{e}^{-A_\nu(E,g)} \left(-\frac{2}{g}\right)^{B_\nu(E,g)} \exp\left[\mathrm{i}\,\pi\,\frac{j+1+B_\nu(E,g)}{2}\right] \\ &\quad\times \frac{\Gamma\left[\frac{1}{2}\,(j+1-B_\nu(E,g))\right]}{\Gamma\left[\frac{1}{2}\,(j+1+B_\nu(E,g))\right]} = 1\,. \end{aligned} \tag{2.102}$$

In leading order in g, the corresponding relation may be derived on the basis of instanton calculus [see equations (7.66) and (7.70)].

2.3 Summary of the Quantization Conditions

We summarize the conjectured quantization conditions. The general convention for the potential is indicated in equation (2.10a). The A and B-functions are determined by equation (3.57), once the potential is fixed. All quantization conditions discussed here have been derived, in leading order in g, by instanton calculus.

(*Double-well potential*.) For the double-well potential (2.10b),

$$H = -\frac{g}{2}\left(\frac{\mathrm{d}}{\mathrm{d}q}\right)^2 + \frac{1}{g}\left[\frac{1}{2}\,q^2(1-q)^2\right]\,, \tag{2.103}$$

we have (2.21),

$$\frac{1}{\sqrt{2\pi}}\,\Gamma\left(\frac{1}{2} - B_{\rm dw}(E,g)\right)\left(-\frac{2}{g}\right)^{B_{\rm dw}(E,g)} \exp\left[-\frac{A_{\rm dw}(E,g)}{2}\right] = \varepsilon\mathrm{i}\,. \tag{2.104}$$

The functions $A_{\rm dw}$ and $B_{\rm dw}$ are defined in (2.23), and the perturbative quantization condition, from which the perturbative expansion of an eigenvalue may be obtained, is given in (2.25).

(*General symmetric potential*.) We now consider a general symmetric potential with degenerate minima of the form (2.54),

$$V(q) = \tfrac{1}{2}\,q^2 + \mathcal{O}(q^3)\,, \quad V(q) = \tfrac{1}{2}\,(q-q_0)^2 + \mathcal{O}\left((q-q_0)^3\right)\,, \tag{2.105}$$

where we have used (2.70). The quantization condition is (2.61),

$$\frac{1}{\sqrt{2\pi}}\,\Gamma\left(\frac{1}{2} - B_{\rm sym}(E,g)\right)\left(-\frac{2C}{g}\right)^{B_{\rm sym}(E,g)} \exp\left[-\frac{A_{\rm sym}(E,g)}{2}\right] = \varepsilon\mathrm{i}\,. \tag{2.106}$$

By contrast, the purely perturbative quantization condition is (2.62). The constant C is given in (2.58),

$$C = q_0^2\,\exp\left[\int_0^{q_0}\left(\frac{1}{\sqrt{2V(q)}} - \frac{1}{q} - \frac{1}{q_0 - q}\right)\right]\,. \tag{2.107}$$

(*Asymmetric wells, degenerate minima.*) For general asymmetric wells with degenerate minima [see equation (2.63)], we have

$$V(q) = \tfrac{1}{2}\,q^2 + \mathcal{O}(q^3)\,, \quad V(q) = \tfrac{1}{2}\,\omega^2\,(q-q_0)^2 + \mathcal{O}\left((q-q_0)^3\right)\,. \tag{2.108}$$

The generalized Bohr–Sommerfeld quantization formula takes the form (2.64),

$$\begin{aligned}&\frac{1}{\Gamma(\frac{1}{2}-B_1(E,g))\,\Gamma(\frac{1}{2}-B_2(E,g))}\\ &\quad+\frac{1}{2\pi}\,\left(-\frac{2\,C_\omega}{g}\right)^{B_1(E,g)}\,\left(-\frac{2\,C_\omega}{\omega\,g}\right)^{B_2(E,g)}\,\mathrm{e}^{-A(g,E)} = 0\,,\end{aligned} \tag{2.109}$$

The perturbative quantization condition is (2.66). Here, we have [see equation (5.3)]

$$C_\omega = q_0^2\,\omega^{2/(1+\omega)}\,\exp\left\{\frac{2\omega}{1+\omega}\,\left[\int_0^{q_0}\mathrm{d}q\,\left(\frac{1}{\sqrt{2V(q)}}-\frac{1}{q}-\frac{1}{\omega(q_0-q)}\right)\right]\right\}\,. \tag{2.110}$$

(*Periodic cosine potential.*) For the periodic cosine potential $V(q) = \frac{1}{16}\,(1-\cos 4q)$, the conjecture then takes the form

$$\left(\frac{2}{g}\right)^{-B_{\mathrm{pc}}(E,g)}\,\frac{\mathrm{e}^{A_{\mathrm{pc}}(E,g)/2}}{\Gamma[\frac{1}{2}-B_{\mathrm{pc}}(E,g)]}+\left(\frac{-2}{g}\right)^{B_{\mathrm{pc}}(E,g)}\,\frac{\mathrm{e}^{-A_{\mathrm{pc}}(E,g)/2}}{\Gamma[\frac{1}{2}+B_{\mathrm{pc}}(E,g)]}=\frac{2\cos\varphi}{\sqrt{2\pi}}. \tag{2.111}$$

The functions A_{pc} and B_{pc} are defined in (2.81), and the perturbative quantization condition can be found in (2.82).

(*Self-adjoint extension of the anharmonic oscillator with $\mathcal{O}(\nu)$-symmetry, at negative coupling.*) For the $\mathcal{O}(\nu)$-anharmonic oscillator with the radial Hamiltonian (2.84),

$$H_l \equiv H_l(g) = -\frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2-\frac{1}{2}\,\frac{\nu-1}{r}\,\frac{\mathrm{d}}{\mathrm{d}r}+\frac{1}{2}\,\frac{l\,(l+\nu-2)}{r^2}+\frac{1}{2}\,r^2+g\,r^4. \tag{2.112}$$

For $g<0$, the radial Hamiltonian being endowed with a self-adjoint extension, the quantization condition is (2.92)

$$\begin{aligned}&\frac{1}{\Gamma\left[\frac{1}{2}(1+j-B_\nu(E,g,j))\right]\,\Gamma\left[\frac{1}{2}(1-j-B_\nu(E,g,j))\right]}\\ &\quad+\left(-\frac{2}{g}\right)^{B_\nu(E,g,j)}\,\frac{\exp\left(A_\nu(E,g)\right)}{2\pi}=0\,.\end{aligned} \tag{2.113}$$

The functions A_ν and B_ν are defined in (2.89).

(*Resonances of the anharmonic oscillator with $\mathcal{O}(\nu)$-symmetry, at negative coupling.*) For $g<0$, the resonances of the radial Hamiltonian are conjectured to follow the quantization condition (2.102),

$$\begin{aligned}&\mathrm{i}\,\mathrm{e}^{-A_\nu(E,g)}\,\left(-\frac{2}{g}\right)^{B_\nu(E,g)}\,\exp\left[\mathrm{i}\,\pi\,\frac{j+1+B_\nu(E,g)}{2}\right]\\ &\quad\times\frac{\Gamma\left[\frac{1}{2}\,(j+1-B_\nu(E,g))\right]}{\Gamma\left[\frac{1}{2}\,(j+1+B_\nu(E,g))\right]}=1\,,\end{aligned} \tag{2.114}$$

(*Fokker–Planck Hamiltonian.*) An important special case of (2.92) is the Fokker–Planck Hamiltonian (2.94)

$$H_{\mathrm{FP}} = -\frac{g}{2}\,\frac{\mathrm{d}^2}{\mathrm{d}p^2}+\frac{1}{2g}\,\left(p^2-\frac{1}{4}\right)^2+p\,, \tag{2.115}$$

The corresponding conjecture for the quantization condition is given by the equation (2.96),

$$\frac{1}{\Gamma\left(-\frac{1}{2}B_{\mathrm{FP}}(E,g)\right)\,\Gamma\left(1-\frac{1}{2}B_{\mathrm{FP}}(E,g)\right)}+\left(-\frac{2}{g}\right)^{B_{\mathrm{FP}}(E,g)}\,\frac{\exp\left(-A_{\mathrm{FP}}(E,g)\right)}{2\pi}=0\,. \tag{2.116}$$

The functions A_{FP} and B_{FP} are defined in (2.99).

Chapter 3

Perturbative and WKB Expansions from Schrödinger Equations

3.1 Orientation

In the simplest examples these conjectures, based on the semi-classical evaluation of path integrals and instanton calculus, have obtained independent heuristic confirmations by considerations based on the Schrödinger equations, as we now explain.

We write the Schrödinger equation as

$$H\,\psi(q) \equiv -\frac{g}{2}\,\psi''(q) + \frac{1}{g}\,V(q)\,\psi(q) = E\,\psi(q). \tag{3.1}$$

We consider only potentials V that are entire functions. This allows extending the Schrödinger equation and thus its solutions to the q complex plane.

Moreover, we assume that $V(q)$ has an absolute minimum, for convenience located at $q = 0$, where $V(q) = \frac{1}{2}\,q^2 + \mathcal{O}(q^3)$.

3.2 General Considerations

3.2.1 The Transition to Quantum Mechanics

We recall in this chapter how the transition from classical to quantum mechanics can be understood in terms of matter waves whose wave fronts are given approximately by the 2-dimensional manifolds of constant classical action. The classical action A_0 for a particle whose Lagrangian is not explicitly time-dependent, reads

$$A_0(t, \boldsymbol{r}) = \int_0^t \mathrm{d}t'\, L(\boldsymbol{r}(t'), \dot{\boldsymbol{r}}(t'))\,. \tag{3.2}$$

One immediately verifies the relations

$$\frac{\mathrm{d}A_0}{\mathrm{d}t} = L\,, \quad \frac{\mathrm{d}A_0}{\mathrm{d}t} = \frac{\partial A_0}{\partial t} + \dot{\boldsymbol{r}}\,\boldsymbol{p}\,, \quad \boldsymbol{\nabla} A_0 = \boldsymbol{p}\,, \tag{3.3}$$

where $\boldsymbol{p}$ is the momentum of the classical particle. This can be rewritten as

$$\frac{\partial A_0}{\partial t} = -(\boldsymbol{p}\,\dot{\boldsymbol{r}} - L) = -H\,, \tag{3.4}$$

where H is the Hamiltonian. Using $H = \boldsymbol{p}^2/(2m) + V$, where V is the potential and m is the mass of the particle, the Hamilton–Jacobi equation is recovered,

$$-\frac{\partial A_0}{\partial t} = \frac{(\boldsymbol{\nabla} A_0)^2}{2m} + V(r)\,. \tag{3.5}$$

The momentum $\boldsymbol{p} = \boldsymbol{\nabla} A_0$ is thus perpendicular to the manifolds of constant classical action $A_0 = \text{constant}$. That is to say, the classically allowed trajectories are perpendicular to the surfaces of constant action. On the other hand, the wave fronts of a traveling wave are characterized by a constant phase, and the wave moves perpendicular to the surfaces of constant phase. Therefore, choosing the ansatz

$$\psi_0(t, \boldsymbol{r}) = \exp(\mathrm{i}\,\xi_0(t, \boldsymbol{r})) \tag{3.6}$$

for the wave function, we are led to the conclusion that A_0 should be constant on the surfaces of constant ξ. Because ξ has to have dimension one, but A_0 has the dimension of an action, the identification

$$\xi_0(t, \boldsymbol{r}) = \frac{A_0(t, \boldsymbol{r})}{\hbar} \tag{3.7}$$

is suggested. If the dynamics of the matter wave were purely governed by the laws of classical mechanics, generalized to matter waves, then the equation (3.5) would adequately describe the time evolution of the wave packet described by the matter wave function ψ_0, and the transition from classical to quantum mechanics would be completely equivalent to the transition from ray to wave optics. In order to verify how well (3.5) is applicable to the description of a quantal wave packet, we choose the ansatz

$$\psi(t, \boldsymbol{r}) = \exp\left(\frac{\mathrm{i}}{\hbar}\, A(t, \boldsymbol{r})\right) \tag{3.8}$$

for the quantum mechanical wave function and insert this into the Schrödinger equation. The result is

$$-\frac{\partial A}{\partial t} = \frac{(\boldsymbol{\nabla} A)^2}{2m} + V(r) - \frac{\mathrm{i}\,\hbar}{2m}\,\boldsymbol{\nabla}^2 A\,. \tag{3.9}$$

This is *not* identical to (3.5). The third term on the right-hand side characterizes a diffusive process in the context of the Brownian motion of the quantal particle [22] and is responsible for the spreading of quantum mechanical wave packets. It may be interpreted as a quantum mechanical correction to the classical equations of motion of matter waves. The correction is of order $\hbar$. An expansion in powers of $\hbar$ is a semiclassical expansion, or WKB expansion [23].

For a stationary state, the ansatz

$$A(t, \boldsymbol{r}) = a(\boldsymbol{r}) - E\,t \tag{3.10}$$

leads to

$$E = \frac{(\boldsymbol{\nabla} a)^2}{2m} + V(r) - \frac{\mathrm{i}\,\hbar}{2m}\,\boldsymbol{\nabla}^2 a\,. \tag{3.11}$$

We now specialize this equation to the one-dimensional Hamiltonian given by equation (2.10) where, upon multiplication by a overall factor g, the coupling g takes the formal role of $\hbar$ with $m = 1$. We therefore have to replace $E \to g\,E$, as well as $\hbar \to g$, and we also set $a(q) = \mathrm{i} \int S(q')\,\mathrm{d}q'$. Then,

$$gE = -\frac{1}{2}\,S^2(q) + V(q) + \frac{g}{2}\,S'(q)\,. \tag{3.12}$$

3.2.2 Riccati Equation

According to the previous chapter, a convenient way to generate semiclassical expansions is to use the Riccati equation derived from the Schrödinger equation (3.1) by setting

$$S(q) = -g\,\psi'/\psi\,. \tag{3.13}$$

The function S then satisfies (3.12)

$$g\,S'(q) - S^2(q) + 2V(q) - 2gE = 0\,. \tag{3.14}$$

Following the discussion of the appendix A, we also introduce two independent solutions $\psi_{1,2}$ of equation (3.1) such that

$$\psi_2(q) \underset{q\to+\infty}{\to} 0\,, \quad \psi_1(q) \underset{q\to-\infty}{\to} 0\,, \tag{3.15}$$

and the decomposition (A.13) with

$$S_\pm(q) = \frac{g}{2}\left(\frac{\psi_1'}{\psi_1} \mp \frac{\psi_2'}{\psi_2}\right). \tag{3.16}$$

[The derivations of a few simple identities needed in this chapter are recalled in appendix A, but with different normalizations.]

In the leading WKB expansion, the two wave functions ψ_1 and ψ_2, for large q, i.e. in regions where $V(q) > gE$, may be expressed as $\exp(-1/g\int \mathrm{d}q\,\sqrt{2\,V(q)-2gE})$ and $\exp(1/g\int \mathrm{d}q\,\sqrt{2\,V(q)-2gE})$, respectively (the positive square root being implied).

Then, equation (3.14) translates into [see (A.15)]

$$g\,S_-' - S_+^2 - S_-^2 + 2\,V(q) - 2\,gE = 0\,, \tag{3.17a}$$

$$g\,S_+' - 2S_+S_- = 0\,. \tag{3.17b}$$

We note that in equations (3.17) a change $(g,E) \mapsto (-g,-E)$ can be formally compensated by the change $(S_+,S_-) \mapsto (S_+,-S_-)$. That is to say, S_+ is even under $(g,E)\mapsto(-g,-E)$, whereas S_- is odd.

It follows that in the sense of a series expansion

$$S_\pm(q,-g,-E) = \pm\,S_\pm(q,g,E)\,. \tag{3.18}$$

The relations (3.17) allow to write the wave function in terms of S_+ only,

$$\psi(q) = (S_+)^{-1/2}\,\exp\left[-\frac{1}{g}\int^q \mathrm{d}q'\,S_+(q')\right]. \tag{3.19}$$

3.2.3 Spectral Equation and Fredholm Determinant

We now consider the *resolvent operator*

$$R(E) = [H-E]^{-1}\,. \tag{3.20}$$

The poles in E of its trace

$$G(E) = \mathrm{Tr}\,R(E) = \mathrm{Tr}\,[H-E]^{-1}\,, \tag{3.21}$$

give the complete spectrum of the Hamiltonian H. Note that this expression may require some regularization to deal with the divergence of the sum over eigenvalues. The resulting ambiguity corresponds to adding a polynomial in E and does not affect poles and residues, i.e. it leaves the spectrum invariant.

The trace of the resolvent $G(E)$ is equal to the negative logarithmic derivative of the Fredholm determinant $\mathcal{D}(E) = \det(H-E)$,

$$G(E) = -\frac{\partial \ln \mathcal{D}(E)}{\partial E}\,, \tag{3.22}$$

in terms of which the spectral equation reads

$$\mathcal{D}(E) = \det(H-E) = 0\,. \tag{3.23}$$

This can be seen as follows,

$$\begin{aligned}\frac{\partial}{\partial E}\ln\mathcal{D}(E) &= \frac{\partial}{\partial E}\ln\det(H-E)\\ &= \frac{\partial}{\partial E}\mathrm{Tr}\,\ln(H-E)\\ &= -\mathrm{Tr}\,\frac{1}{H-E} \;=\; -G(E)\,.\end{aligned} \tag{3.24}$$

3.2.4 Spectral Equation and Logarithmic Derivative of the Wave Function

In the normalization 3.1, the Schrödinger equation can be written as,

$$\left(-\mathrm{d}_q^2 + 2\,V(q)/g^2 - 2E/g\right)\psi(q) = 0\,, \tag{3.25}$$

which, in the notation of appendix A, implies $L = 2\,(H-E)/g$, $u(q) = 2\,V(q)/g^{\,2}$, $z = 2\,E/g$ and thus a different normalization for the resolvent (3.20). The corresponding diagonal elements $r(q)$ of the resolvent $[H-E]^{\,-1}$ satisfy

$$\frac{1}{2}\,g^2\,r\,r'' - \frac{1}{4}\,g^2\,r'^2 = 2\left(V(q) - Eg\right)r^2 - 1\,. \tag{3.26}$$

The equation defines $r(q)$ up to a sign that is fixed by the behaviour for $E \to -\infty$. The trace of $R(E)$ is then given by

$$G(E) = \mathrm{Tr}\,\frac{1}{H-E} = \int \mathrm{d}q\,r(q), \tag{3.27}$$

an expression that requires some regularization to deal with the large q divergences.

Returning to the formalism of appendix A, one finds $r(q) \propto 1/S_+(q)$. A comparison between the different normalizations leads to

$$r(q) = 1/S_+(q). \tag{3.28}$$

We then conclude that

$$G(E) = \int \mathrm{d}q\,\frac{1}{S_+(q)}\,, \quad \ln \mathcal{D}(E) = \frac{1}{g}\int \mathrm{d}q\,S_+(q). \tag{3.29}$$

The integral may diverge for $|q| \to \infty$ and has then to be regularized.

One way of writing the *spectral equation*, or quantization condition, is then [see equation (A.24)]

$$\frac{1}{2\mathrm{i}\pi g}\lim_{\varepsilon\to 0_+}\int \mathrm{d}q\,[S_+(q,g,E_N - i\varepsilon) - S_+(q,g,E_N + i\varepsilon)] = N + \tfrac{1}{2}\,, \tag{3.30}$$

for $N \geq 0$. In the case of analytic potentials, the contour of integration can be locally deformed in the q complex plane, and the limit $\varepsilon \to$ can then be taken. The spectral equation in terms of the logarithmic derivative of the wave function (3.13) becomes

$$B(E,g) \equiv -\frac{1}{2\mathrm{i}\pi g}\oint_C \mathrm{d}z\,S_+(z,g,E) = N + \tfrac{1}{2}\,, \tag{3.31}$$

where N has also the interpretation of the number of real zeros of the eigenfunction, and C is a contour that encloses them.

3.2.5 Perturbative Expansion

The purpose of the current chapter is to investigate the condition (3.31) in detail. Before embarking on this endeavour, we remark that the rather elegant formulation discussed here is restricted, however, to one dimension and analytic potentials, which represents integrable systems from the point of view of classical mechanics. Our treatment bypasses the difficulties generally associated with turning points. This is the form that is useful here in the context of perturbative and WKB expansions. Recently, it has been pointed out by Rosenfelder [24] that non-analytic energy shifts of the form $\exp(-a/g)$ also occur in potentials which cannot be represented as polynomials.

In general, canonical considerations which lead to the Bohr–Sommerfeld quantization conditions (see, e.g., chapter III of [23]), are replaced here by a simpler rigorous approach, based on the Riccati equation, that uses only the uniqueness of the wave function at $q = 0$. We thus assume that the potential has a unique minimum at $q = 0$. In order to see the connection with the uniformity of the wave function, we note that the condition (3.31) may be rewritten as

$$\frac{1}{2\mathrm{i}\pi}\oint \mathrm{d}z\,\frac{\psi'(z)}{\psi(z)} = N\,. \tag{3.32}$$

At $q \to 0$, this implies that the coefficient of q^{-1} in the Laurent expansion of $S_+(q)$ is of the form $-gN/q$ where N is an integer. *Idem est*, we have $\ln \psi(q) \sim N \ln q$ for $q \to 0$, a relation which is uniform under a sign change of q only if N is an integer.

The expansion for $g \to 0$ at E fixed of the equations (3.17), or (3.26), leads to the expansion in powers of g of the function $B(E, g)$ that enters the left-hand side of (3.31). This function enters in expressions like (2.22) and other quantization conditions. We first indicate how the function $B(E, g)$ can be calculated *(i)* as a series expansion in powers of g at E fixed, which leads to the perturbative expansion, and *(ii)* at Eg fixed, which leads to the WKB expansion. We also discuss the relation between the two expansions.

In view of (3.17), (3.18) and (3.19), we conclude that

$$B(E, g) = -B(-E, -g)\,. \tag{3.33}$$

The latter reflection symmetry is purely formal — it is valid in the sense of power series — since it corresponds to change the quantum number N in $-1-N$, which is unphysical.

The *perturbative expansion* is obtained by expanding the solution of Riccati's equation (3.14) in powers of g (at E fixed):

$$S(q) = \sum_{k \geq 0} g^k\, s_k(q)\,. \tag{3.34}$$

Setting

$$U(q) = \sqrt{2\,V(q)}, \quad U(q) = q + \mathcal{O}(q^2)\,, \tag{3.35}$$

we first find

$$s_0(q) = U(q), \quad s_1(q) = \frac{1}{2U(q)}\big(U'(q) - 2E\big). \tag{3.36}$$

The square root in (3.35) is to be understood such that the resulting function is uniform at the two minima of V, and positive in the region between the minima. For example, in the case of the double-well potential $V(q) = q^2\,(1-q)^2/2$, we have $U(q) = q\,(1-q)$.

Higher orders are obtained from the recursion relation

$$s_k(q) = \frac{1}{2U(q)} \left(s'_{k-1}(q) - \sum_{l=1}^{k-1} s_{k-l}(q) s_l(q) \right)\,. \tag{3.37}$$

For example,

$$s_2(q) = \frac{U''}{4U^2} - \frac{3U'^2}{8U^3} + \frac{EU'}{2U^3} - \frac{E^2}{2U^3}\,. \tag{3.38}$$

Thus

$$S_+ = U(q) - g\frac{E}{U(q)} + g^2 \left(\frac{U''}{4U^2} - \frac{3U'^2}{8U^3} - \frac{E^2}{2U^3} \right) + \mathcal{O}(g^3). \tag{3.39}$$

The contour integral (3.31) reduces to the residue at $q = 0$ (where the potential has its unique absolute minimum). Thus, it depends only on the expansion of $U(q)$ at $q = 0$. To find the perturbative spectrum, it is sufficient to expand the recursion relation (3.37) in powers of q. For two (or more) degenerate minima, this procedure gives rise to perturbative functions $B_1, B_2, \ldots$ in the sense of chapter 2 [see also equation (3.57) below].

For instance, at order g, one finds $B(E, g) = E$. The next orders, for a general polynomial potential, are given in equation (B.11). The condition (3.31) then implies that the eigenfunctions are uniform at $q = 0$, as they should be.

There is an interesting connection to *Borel summability*. Note that even in situations where the perturbative expansion of eigenvalues is Borel summable, it is not clear whether the function $B(E, g)$ is Borel summable in g at E fixed. Indeed, the wave function $\psi(q)$ is unambiguously defined only when the quantization condition is satisfied with N a non-negative integer. When E is not an eigenvalue, the solution of the Schrödinger equation is an undefined linear combination of two particular solutions.

3.2.6 WKB Expansion

As explained in chapter 3.2.1, the WKB expansion [25] is an expansion for $g \to 0$ at Eg fixed, in contrast to the perturbative expansion where E is fixed. In [26, chapter 6], it has been stressed that the loop expansion in quantum field theory is actually an expansion in powers of $\hbar \sim g$, i.e. a generalized WKB expansion. We thus expand equation (3.14) in the complex q-plane in powers of g, at Eg fixed, starting from

$$S(q) = S_0(q)\,, \qquad S_0^2(q) = 2\,V(q) - 2\,gE\,. \tag{3.40}$$

For $E > 0$, the function S_0 has two branch points $q_- < q_+$ on the real axis. We put the cut between q_- and q_+ and choose the determination of S_0 to be positive for $q > q_+$. This ensures the decrease of wave functions on the real axis for $|q| \to \infty$, at least in the WKB approximation.

Then [see equation (B.13)],

$$S(q) = \sum_{k\geq 0} g^k S_k(q). \tag{3.41a}$$

One first obtains

$$S_1 = \frac{S_0'}{2S_0}\,. \tag{3.41b}$$

For $k > 1$, one finds the recursion relation

$$S_k(q) = \frac{1}{2S_0(q)} \left(S_{k-1}'(q) - \sum_{l=1}^{k-1} S_{k-l}(q) S_l(q) \right). \tag{3.41c}$$

At order g^2, for example,

$$S_2 = \frac{S_0''}{4S_0^2} - \frac{3S_0'^2}{8S_0^3}. \tag{3.42}$$

In the semi-classical limit, the contour C in the expression (3.31) encloses the cut of $S_0(q)$ which joins the two solutions of $S_0(q) = 0$ (classical turning points).

Note that equation (3.31) can also be written as

$$\exp\left[-\frac{1}{g}\oint_C \mathrm{d}z\, S_+(z)\right] + 1 = 0\,. \tag{3.43}$$

The contribution of S_1 as well as that of all S_j with odd j to the symmetric component S_+ vanishes. This is evident as we inspect the symmetry condition (3.18), the properties of the leading approximation (3.40) and take into account the additional odd-power-of-g prefactor that prevails in all S_j with odd j. Therefore, we may safely ignore all odd-order WKB approximants in the sequel; this simplifies the analysis carried out in appendix F.

We now consider the *WKB expansion* of the *resolvent*. In the WKB limit $Eg = \mathcal{O}(1)$, the solution of equation (3.26) at leading order, in the notation (3.14), is

$$r(q) = \frac{1}{S_0(q)} = \frac{1}{\sqrt{2\,V(q) - 2\,Eg}} \;\Rightarrow\; G(E) = \int \frac{\mathrm{d}q}{\sqrt{2\,V(q) - 2\,Eg}}. \tag{3.44}$$

Formally,

$$\ln \mathcal{D}(E) = \frac{1}{g}\int \mathrm{d}q\, S_0(q) = \frac{1}{g}\int \mathrm{d}q\, \sqrt{2\,V(q) - 2\,Eg}\,, \tag{3.45}$$

but the divergence of the integral for $|q| \to \infty$ has to be eliminated by subtracting a E-independent infinite constant.

At order g^2, one finds [see equation (B.16)]

$$S_+(q) = S_0(q) + g^2 \left(\frac{S_0''}{4S_0^2} - \frac{3S_0'^2}{8S_0^3} \right) + \mathcal{O}(g^4), \tag{3.46}$$

and thus, after an integration by parts,

$$\ln \mathcal{D}(E) = \frac{1}{g}\int \mathrm{d}q\, S_0(q) + \frac{g}{8}\int \mathrm{d}q\, S_0'^{\,2}(q)\, S_0^{-3}(q) + \mathcal{O}(g^3). \tag{3.47}$$

In the present formulation, it is easy to *relate the WKB and the perturbative expansions*. The terms in the WKB expansion of the quantization condition (3.31) are contour integrals that, clearly, are regular functions of E at $E = 0$. To obtain the perturbative expansion from the WKB expansion, one thus expands the functions $S_{2k}(q)$ in powers of E and calculates the residues.

For example, at leading WKB order [see also appendix B.2 and equation (B.18)],

$$S_0 = U \sum_{n=0} \left(2gE\, U^{-2}\right)^n \frac{\Gamma(n-\frac{1}{2})}{\Gamma(n+1)\Gamma(-\frac{1}{2})}. \tag{3.48}$$

One has then to evaluate the residue at the origin of

$$-\frac{1}{2\mathrm{i}\pi}\oint_C \mathrm{d}q\, U^{1-2n}\,. \tag{3.49}$$

More generally, replacing S_+ by its WKB expansion and expanding each term in a power series of Eg, one obtains the perturbative expansion of the function $B(E,g)$. The WKB expansion corresponds to successive summations, to all orders in g, of the terms of highest degree in E of the perturbative expansion. A few terms are calculated in appendix B.

3.3 Resolvent and Degenerate Minima in Specific Cases

3.3.1 Potentials with Degenerate Minima

We now consider potentials of double-well type, with two (not necessarily symmetric) degenerate minima. The symmetric case is displayed in figure 3.1, whereas the discussion here is actually applicable also to the case of minima with unequal curvatures [see equation (2.63)]. For E small enough, the function $S_0(q)$ has four branch points $q_1, \ldots, q_4$ on the real axis.

One expects, on intuitive grounds, to find two perturbative functions $B_1(E,g)$ and $B_2(E,g)$ obtained by integrating S_+ around the two cuts $[q_1, q_2]$ and $[q_3, q_4]$ of figure 3.1.

However, if one thinks in global terms, an obvious difficulty arises: a function $S_0(q)$ with the corresponding two cuts is no longer an appropriate solution because it increases both for $q \pm \infty$, and thus the wave function cannot decrease both for $q \pm \infty$. Moreover, the contour integral of S_0 cannot give the correct answer. For example, if the potential is symmetric, the integral vanishes.

For symmetric potentials, the correct perturbative answer is obtained from the difference between the two integrals when the additional zero at the symmetry point for odd eigenfunctions is taken into account. One then finds

$$2B(E,g) = 1 + 2[N/2], \tag{3.50}$$

where $[N/2]$ is the integer part of $N/2$, and this is the correct perturbative answer.

Moreover, quite generally the WKB expansion of the spectral condition has a singularity when $2E$ reaches the relative maximum of the potential between the degenerate minima, where two complex singularities of the $S_0(q)$ pinch the real axis and the number of real singularities passes from two to four.

Therefore, let us examine what happens if one starts from E large enough, where S_0 has only two branch points on the real axis and no special difficulty arises, and proceeds by analytic continuation of the spectral condition. At leading order, before continuation, the function $B(E,g)$ can be written as

$$B(E,g) = \mathcal{B}(E,g) \equiv \frac{1}{\pi g}\int_{q_-(E)}^{q_+(E)} \mathrm{d}q\, \sqrt{2\,Eg - 2\,V(q)} + \mathcal{O}(g)\,, \tag{3.51}$$

where $q_\pm$ are the two real zeros of $Eg - V$. To avoid the singularity when E reaches the local maximum of the potential, we take g, and thus Eg slightly complex. Eventually, the initial contour is deformed into a sum C' of three contours around the cuts:

$$\mathcal{B}(E,g) = B_1(E,g) + B_2(E,g) + B_{12}(E,g) \tag{3.52}$$

with

$$B_{12}(E,g) = \frac{1}{\pi g}\int_{q_2}^{q_3} \mathrm{d}q\,\sqrt{2\,Eg - 2\,V(q)} + \mathcal{O}(g)\,, \tag{3.53}$$

where the cuts now are $[q_1,q_2]$ and $[q_3,q_4]$. The function B_{12} is imaginary and the determination of the square root in the integral depends on the continuation. The integral can also be written as

$$B_{12}(E,g) = \frac{1}{2\pi g}\oint_{C'} \mathrm{d}q\,\sqrt{2\,Eg - 2\,V(q)} + \mathcal{O}(g)\,, \tag{3.54}$$

where C' surround the function cut along $[q_2,q_3]$. Note that $B_{12}(E,g)$ as a function of E has a branch point at $E=0$. In a rotation about an angle 2π around $E=0$, B_{12} becomes $B_{12} \pm (B_1 + B_2)$.

The quantization condition (3.31) or alternatively (3.43),

$$-\frac{1}{2\mathrm{i}\pi g}\oint_{C'} \mathrm{d}z\,S_+(z,g,E) = N + \tfrac{1}{2}\,, \qquad\qquad \exp\left[-\frac{1}{g}\oint_{C'}\mathrm{d}z\,S_+(z)\right] + 1 = 0\,, \tag{3.55}$$

then becomes

$$\exp\left[2\mathrm{i}\pi\,\left(B_1(E,g) + B_2(E,g) + B_{12}(E,g)\right)\right] + 1 = 0\,. \tag{3.56}$$

The contribution B_{12} contains the effect of barrier penetration and we choose the sign in front of it, which depends on the analytic continuation, to obtain decreasing corrections to perturbation theory. Finally, the contribution $B_1 + B_2$ can be absorbed into in a redefinition of B_{12} by going to the proper sheet in the E Riemann surface.

Comparing with the instanton result, one infers the decomposition [in the notation of equation (2.64)]

$$\begin{aligned}\frac{1}{g}\oint_{C'}\mathrm{d}z\,S_+(z) &= A(E,g) + \ln(2\pi) \\ &\quad - \sum_{i=1}^{2}\left\{\ln\Gamma\left(\frac{1}{2} - B_i(E,g)\right) + B_i(E,g)\ln\left(-\frac{g}{2C_i}\right)\right\}\,,\end{aligned} \tag{3.57}$$

where the constants C_i are adjusted in such a way that $A(E,g)$ has no term of order g^0 and the coefficient of g^0 is proportional to the expansion of $B_1 + B_2$. This equation, adapted to specific cases, almost directly leads to the conjectures discussed in chapter 2 and summarized in chapter 2.3 when combined with the quantization condition (3.55).

The expansion for Eg small of its WKB expansion yields the function $A(E,g)$. To identify with the WKB expansion, the function $\Gamma(\frac{1}{2} - B)$ has to be replaced by its asymptotic expansion for B large:

$$-\ln\Gamma(\tfrac{1}{2} - B) \underset{E\to\infty}{\sim} B\ln(-B) - B \underset{g\to 0}{\sim} B\ln(-E) + \cdots \tag{3.58}$$

Therefore, at leading order,

$$\frac{1}{g}\,\mathrm{Re}\oint_{C'}\mathrm{d}z\,S_+(z) = A(E,g) + \ln(2\pi) + \sum_{i=1}^{2} B_i(E,g)\left[\ln\left(\frac{gE}{2C_i}\right) - 1\right]\,. \tag{3.59}$$

Here, we have assumed that the determinations of all functions of E are such that $A(E,g)$ is real in perturbation theory, something that is possible since the ambiguities are proportional to $2\mathrm{i}\pi(B_1 + B_2)$: in the WKB expansion, the discontinuity comes from the asymptotic expansion (3.58) of the sum of the Γ functions, which also has a discontinuity $-2\mathrm{i}\pi(B_1 + B_2)$, showing the consistency of the whole scheme. Moreover, the contribution proportional to $\ln(-g)$ leads to the combination $\ln(gB_i)$, which is globally even in E, g as it should be [because it results from an integral over S_+ with the symmetry property (3.18)].

A calculation of $A(E,g)$ at a finite order in g requires the WKB expansion and the asymptotic expansion of the Γ-function only to a finite order. For example, the expansions up to order g^2 (2.24b) and (2.81b) of the function $A(E,g)$ for the double-well and cosine potentials, which have initially been determined in part by numerical calculations, are reproduced by the expansion of the two first WKB orders (the calculations for the double-well potential are given in appendix B).

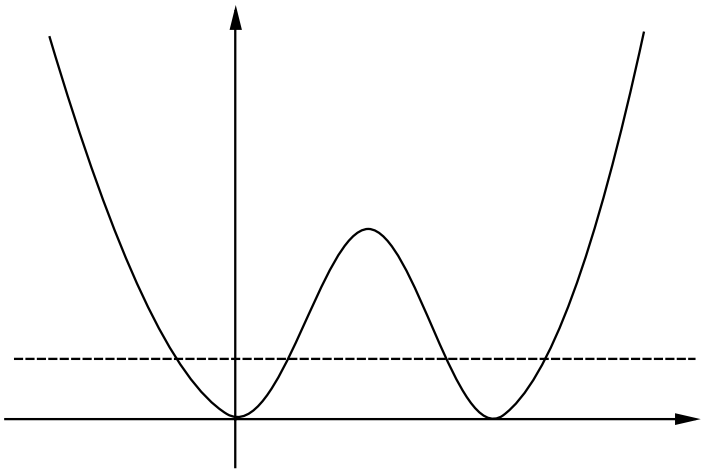

Figure 3.1: The four turning points.

3.3.2 General Symmetric Potentials

We first consider general symmetric potentials: $V(-q) = V(q)$. As is evident from the discussion in chapter 2.1 above and chapter 4.2.1 below, it is necessary to introduce a further quantum number in this particular case, which is the parity. States are classified according to the principal quantum number N and the parity ε. We again combine the formalism of chapter 3.2.6 and appendix A. Using equation (A.28), and taking care of the different normalization, one infers

$$G_a(E) \equiv \mathrm{Tr}\, P\,[H-E]^{-1} = 2\int_0^\infty \frac{\mathrm{d}q}{S_+(q)} \exp\left[-\frac{2}{g}\int_0^q \mathrm{d}y\, S_+(y)\right], \tag{3.60}$$

where P is the reflection operator that acts here according to $P\,\psi(q) = \psi(-q)$ [cf. equation (4.11) where the reflection symmetry is about $q = 1/2$ in contrast to the case of a center of symmetry at $q = 0$ discussed here].

An alternative integrated form is [equation (A.30)]

$$\mathcal{D}_a(E) = \exp\left[-\mathrm{Tr}\, P \ln(H-E)\right] \approx -\frac{1}{S_+(0)}\,\frac{\partial}{\partial E} S_+(0) = -\frac{g}{[S_+(0)]^2}\,. \tag{3.61}$$

At leading order in the WKB limit, one finds $-(2E)^{-1}$, the harmonic oscillator result for $E \to -\infty$ [equation (A.39)].

In the case of the *symmetric double-well potentials,* this situation again is more subtle, because one has to consider two different WKB approximations near the two wells. number in this case A strategy consists in calculating [27]

$$G_a\big(\tfrac{1}{2}(E_{+,N} + E_{-,N})\big) \sim -\frac{4}{E_{-,N} - E_{+,N}}. \tag{3.62}$$

We thus consider the Schrödinger equation in the normalization (3.1) with $E = N + \frac{1}{2}$ and call $q_0 > 0$ the position of one of the minima of the potential: $V(q) \sim \frac{1}{2}(q-q_0)^2$.

For $q \geq 0$, at leading order in the semi-classical limit,

$$S_+(q) = \sqrt{U^2(q) - 2Eg} = U(q) - \frac{Eg}{U(q)} + \mathcal{O}(g^2)\,, \tag{3.63}$$

where $U(q)$ is defined as [see equation (3.35)]

$$U(q) = \sqrt{2\,V(q)}, \quad U(q) = q + \mathcal{O}(q^2)\,. \tag{3.64}$$

We choose the branch cut of the square-root function such that $U(q)$ becomes a function regular at $q = q_0$ and positive for $q > q_0$. The approximation (3.63) is valid for $|q - q_0|$ large.

The solution $\psi_N(q)$ can be written as

$$\begin{aligned}\psi_N(q) &\sim q_0^{-N-1/2}(q_0-q)^N\sqrt{\frac{q-q_0}{U(q)}}\exp\left[-\frac{1}{g}\int_0^q \mathrm{d}q'\,U(q')\right]\\ &\quad\times\exp\left[(N+\tfrac{1}{2})\int_0^q \mathrm{d}q'\left(\frac{1}{U(q')}-\frac{1}{q'-q_0}\right)\right].\end{aligned} \tag{3.65}$$

We introduce the definitions

$$a = -4\int_0^{q_0}\mathrm{d}q\,U(q)\,, \tag{3.66}$$

$$C = q_0^2\exp\left[-2\int_0^{q_0}\mathrm{d}q\left(\frac{1}{U(q)}+\frac{1}{q+q_0}-\frac{1}{q-q_0}\right)\right]. \tag{3.67}$$

When comparing to (5.6), it is necessary to remember that we are dealing with a symmetric potential $V(-q) = V(q)$ in the current section, and we integrate from the center of symmetry at $q = 0$ to one of the minima of the potential. By contrast, in (2.60) and in (5.6), the integration extends from one of the minima to the other. Also, the convention for the square root is the opposite $\tilde{U} = -U$ for q inside the region between the two minima.

Based on (A.27a), we can write $r_a(q)$ as

$$r_a(q) = C^{-N-1/2}\,\mathrm{e}^{a/2g}\,\eta_N^2(q) \tag{3.68}$$

with

$$\eta_N(q) \sim (q_0-q)^N\,\mathrm{e}^{-(q-q_0)^2/2g}\,, \tag{3.69}$$

an expression valid for $1 \ll |q-q_0| \ll \sqrt{g}$.

The leading contribution to the integral comes from the neighbourhood of $q = q_0$, where the harmonic oscillator approximation is relevant. The corresponding eigenfunction with norm $\sqrt{\pi}$ is

$$\varphi_N(q) = \frac{1}{2^{N/2}\sqrt{N!}}\,(q-\mathrm{d}_q)^N\,\mathrm{e}^{-q^2/2} \underset{q\to\infty}{\sim} \frac{2^{N/2}}{\sqrt{N!}}q^N\mathrm{e}^{-q^2/2}\,. \tag{3.70}$$

Therefore, $\eta_N(q)$ has to be approximated by

$$\eta_N(q) \sim \sqrt{N!}(g/2)^{N/2}\varphi_N\big((q-q_0)/\sqrt{g}\big). \tag{3.71}$$

We conclude

$$\begin{aligned}G_a\big(\tfrac{1}{2}(E_{N+}+E_{N-})\big) &\sim 2\,C^{-N-1/2}\,N!\,(2/g)^N\,\mathrm{e}^{a/2g}\int\mathrm{d}q\,\varphi_N^2\left((q-q_0)/\sqrt{g}\right)\\ &\sim 2\sqrt{\pi g}\,C^{-N-1/2}\,N!\,(g/2)^N\,\mathrm{e}^{a/2g}\,.\end{aligned} \tag{3.72}$$

Using equation (3.62), one obtains the one-instanton contribution to the energy difference

$$\delta E_N(g) \sim \frac{2}{\sqrt{2\pi}}\frac{1}{N!}\left(\frac{2C}{g}\right)^{N+1/2}\mathrm{e}^{-a/2g}, \tag{3.73}$$

a result consistent with the expansion of the zeros of expression (5.18).

Note that to go beyond leading order by this method is simple for N fixed, but not for generic N because the WKB expansion yields the perturbative eigenfunction under the form of an expansion only valid for large arguments.

To compare with instanton calculations, we calculate the *contribution of the twisted resolvent at leading order*,

$$\mathrm{Tr}\,P\ln(H-E) = \sum_N \ln\left(\frac{E_N-\delta E_N/2-E}{E_N+\delta E_N/2-E}\right) \sim -\sum_N\frac{\delta E_N}{E_N-E}\,, \tag{3.74}$$

where E has been assumed to be not too close to an eigenvalue. At leading we can replace E_N by $N+\frac{1}{2}$. Thus,

$$\begin{aligned}
&\operatorname{Tr} P\ln(H-E)\\
\sim\ & -\frac{2}{\sqrt{2\pi}}\,\mathrm{e}^{-a/2g}\sum_N \frac{1}{N!}\left(\frac{2C}{g}\right)^{N+1/2}\int_0^\infty \mathrm{d}\beta\,\mathrm{e}^{\beta(E-N-1/2)}\\
\sim\ & -2\left(\frac{C}{\pi g}\right)^{1/2}\mathrm{e}^{-a/2g}\int_0^\infty \mathrm{d}\beta\,\exp\left[\beta(E-\tfrac{1}{2})+2\,C\mathrm{e}^{-\beta}/g\right].
\end{aligned} \tag{3.75}$$

We note that if we evaluate the integral in the limit $g\to 0_-$, we obtain

$$\operatorname{Tr} P\ln(H-E)\sim -2\,\frac{\mathrm{e}^{-a/2g}}{\sqrt{2\pi}}\,\exp\left[\mathrm{i}\,\pi(E-\tfrac{1}{2})\right]\left(\frac{2C}{g}\right)^E\Gamma(\tfrac{1}{2}-E), \tag{3.76}$$

an expression that appears in equation (4.60) and has the correct poles and residues. Of course, the real part,

$$\operatorname{Tr} P\ln(H-E)\sim -2\frac{\mathrm{e}^{-a/2g}}{\sqrt{2\pi}}\,\cos\bigl(\pi(E-1/2)\bigr)\left(\frac{2C}{g}\right)^E\Gamma(\tfrac{1}{2}-E), \tag{3.77}$$

has the same poles with the same residues, but has zeros for $E<0$.

3.3.3 $\mathcal{O}(\nu)$–Symmetric Hamiltonians in the Radial Coordinate

A general $\mathcal{O}(\nu)$-symmetric Hamiltonian, after diagonalization of the angular momentum, decomposes into a set of Hamiltonians H_l, where l is the angular momentum, of the form

$$H_l=\frac{g}{2}\left[-\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2-\frac{\nu-1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{l(l+\nu-2)}{r^2}\right]+\frac{1}{g}V(r). \tag{3.78}$$

We assume that $V(r)$ is an analytic function of r^2, in such a way that the Schrödinger equation can be continued to the complete real axis. Eigenfunctions are then odd or even, and they behave like r^l for $r\to 0$. The eigenfunction $\psi_{l,N}$ corresponding to angular momentum l and quantum number N thus has $l+2N$ zeros on the real axis. The quantization condition (3.31) is replaced by

$$\frac{1}{2\mathrm{i}\pi}\oint_C \mathrm{d}z\,\frac{\psi'_{l,N}(z)}{\psi_{l,N}(z)}=l+2N\,, \tag{3.79}$$

where the contour C now encloses all zeros of the eigenfunction $\psi(r)$ on the real axis (this includes $r\le 0$).

The transformation

$$\frac{\psi'(r)}{\psi(r)}=-\frac{1}{g}S(r)-\frac{\nu-1}{2r}, \tag{3.80}$$

leads to the Riccati equation

$$gS'(r)-S^2(r)+2V(r)-2Eg+g^2\,\frac{j^2-1/4}{r^2}=0 \tag{3.81}$$

with $j=\nu/2+l-1$.

Introducing the two functions $S_\pm$, we can write the quantization condition as

$$-\frac{1}{2\mathrm{i}\pi\,g}\oint_C \mathrm{d}z\,S_+(z)=j+2N+1\,. \tag{3.82}$$

In the *perturbative expansion of the $\mathcal{O}(\nu)$-symmetric Hamiltonian*, the effect of angular momentum appears only at order g. In the parameterization (B.6) [see also equations (7.48), (B.11) and (B.12)], this implies the following relation between $B_\nu(E,g,j)$ and $B_{\mathrm{dw}}(E,g)$:

$$B_\nu(E,g,j)=2\,B_{\mathrm{dw}}\left(\frac{E}{2},-g\right)+\frac{1}{12}\,\alpha_2\,\left(j^2-1\right)\,g+\mathcal{O}(g^2)\,. \tag{3.83}$$

The *WKB expansion of the $\mathcal{O}(\nu)$-symmetric Hamiltonian* is now an expansion at $E\,g$ and $g^{\,2}\,(j^2-1/4)$ fixed. The leading order is

$$S(r) = \sqrt{U^2(r) - 2E\,g + \frac{g^2}{r^2}\,\left(j^2 - \frac{1}{4}\right)}\,. \tag{3.84}$$

Again, the perturbation series is recovered by simply expanding in powers of g.

Chapter 4

Instantons in the Double–Well Problem

4.1 Orientation

The conjectures presented in chapter 2 have been initially motivated by semi-classical evaluations of path integrals, more precisely by summation of leading order multi-instanton contributions.

Therefore, we now explain, first in the example of the double-well potential, how multi-instanton contributions can be summed explicitly, yielding results consistent with the conjectured form (2.22) of the secular equations. The reason for still emphasizing instanton calculus in situations now rather well understood by other methods, is that the arguments can be generalized to other examples where our understanding is more limited.

4.2 General Considerations

4.2.1 Partition Function and Resolvent

The path integral formalism allows calculating directly the quantum partition function, which for Hamiltonians with discrete spectrum has the expansion

$$\mathcal{Z}(\beta) \equiv \operatorname{Tr} \mathrm{e}^{-\beta H} = \sum_{N=0}^{\infty} \mathrm{e}^{-\beta E_N} \,. \tag{4.1}$$

Eigenvalues are labeled E_N ($N \in \mathbb{N}_0$), with E_0 being the ground-state energy and $E_N \leq E_{N+1}$. The trace $G(E)$ of the resolvent of H is related to the partition function by Laplace transformation:

$$G(E) = \operatorname{Tr} \frac{1}{H-E} = \int_0^\infty \mathrm{d}\beta \, \mathrm{e}^{\beta E} \, \mathcal{Z}(\beta) \,, \tag{4.2}$$

where we have to assume initially that $E < E_0$ (with E_0 being the ground state energy), to ensure the convergence of the integral for $\beta \to \infty$.

The poles of $G(E)$ then yield the spectrum of the Hamiltonian H. From $G(E)$ one can also derive the Fredholm determinant $\mathcal{D}(E) = \det(H-E)$, which vanishes on the spectrum (chapter 3.2.3).

Note that the integral (4.2) does not necessarily converge at $\beta = 0$ because the eigenvalues may not increase fast enough, as the example of the harmonic oscillator shows:

$$G_{\text{osc.}}(E) = \int_0^\infty \mathrm{d}\beta \, \frac{\mathrm{e}^{\beta E}}{2\sinh(\beta/2)}, \tag{4.3}$$

which diverges. However, $G(E) - G(0)$ is defined, and fixing the irrelevant constant term we can set [see equation (A.32)]

$$G_{\text{osc.}}(E) = -\psi\left(\tfrac{1}{2} - E\right) = \frac{\partial}{\partial E} \ln \Gamma\left(\tfrac{1}{2} - E\right) \,. \tag{4.4}$$

Note that for the double-well potential, one can separate eigenvalues corresponding to symmetric and antisymmetric eigenfunctions by considering the two functions

$$\mathcal{Z}_{\pm}(\beta) = \mathrm{Tr}\,\left[\tfrac{1}{2}\,(1 \pm P)\,\mathrm{e}^{-\beta H}\right] = \sum_{N=0}^{\infty} \mathrm{e}^{-\beta E_{\pm,N}}\,, \tag{4.5}$$

where P is the parity operator (2.11). The eigenvalues are then poles of the Laplace transforms ($\varepsilon = \pm$):

$$G_{\varepsilon}(E) = \int_0^{\infty} \mathrm{d}\beta\, \mathrm{e}^{\beta E}\, \mathcal{Z}_{\varepsilon}(\beta)\,. \tag{4.6}$$

4.2.2 Path Integrals and Spectra of Hamiltonians

In the path integral formulation of quantum mechanics, the partition function is given by

$$\mathcal{Z}(\beta) \propto \int_{q(-\beta/2)=q(\beta/2)} [\mathrm{d}q(t)] \exp\left[-\frac{1}{g}\,\mathcal{S}\big(q(t)\big)\right], \tag{4.7}$$

where the symbol $\int [\mathrm{d}q(t)]$ means summation over all paths which satisfy the boundary conditions, that is closed paths, and $\mathcal{S}(q)$ is the Euclidean action:

$$\mathcal{S}(q) = \int_{-\beta/2}^{\beta/2} \left[\tfrac{1}{2}\,\dot{q}^2(t) + V\big(q(t)\big)\right] \mathrm{d}t\,. \tag{4.8}$$

In [28], it has been stressed that the formulation in terms of the Euclidean action follows naturally from an analytic continuation of the usual definition of the path integral to imaginary time.

In the case of the symmetric potential (2.10) which has degenerate minima, it is actually necessary to also consider the quantity

$$\mathcal{Z}_{\mathrm{a}}(\beta) \equiv \mathrm{Tr}\,\left(P\mathrm{e}^{-\beta H}\right) \propto \int_{q(-\beta/2)+q(\beta/2)=1} [\mathrm{d}q(t)] \exp\left[-\frac{1}{g}\mathcal{S}\big(q(t)\big)\right], \tag{4.9}$$

where P is the parity operator (2.11). Then, eigenvalues corresponding to symmetric and antisymmetric eigenfunctions can be derived from the combinations

$$\mathcal{Z}_{\pm}(\beta) = \mathrm{Tr}\,\left[\tfrac{1}{2}\,(1 \pm P)\,\mathrm{e}^{-\beta H}\right] = \tfrac{1}{2}\big(\mathcal{Z}(\beta) \pm \mathcal{Z}_{\mathrm{a}}(\beta)\big). \tag{4.10}$$

This construction is not necessary (even impossible) in the case of asymmetric wells discussed below in chapter 5. Because there is no parity in the asymmetric case, the quantity $\mathcal{Z}_{\mathrm{a}}(\beta)$ does not find a natural representation in terms of eigenfunctions in contrast to the equations (4.13) and (4.11) below, and it is only the quantity $\mathcal{Z}(\beta)$ as defined in (4.7) which contributes to the partition function. Of course, $\mathcal{Z}(\beta)$ is composed exclusively of paths in which the starting and the endpoints are identical, and one-instanton effects therefore do not contribute to $\mathcal{Z}(\beta)$.

We adopt here a convention, in which the proportionality sign in the notation (4.7) implies that the final integration over $Q = q(\beta/2)$ is understood.

Because the only irreducible representations of the parity operator are one-dimensional, the nondegenerate eigenfunctions have definite parity,

$$P\phi_{\epsilon,N}(1-q) = \epsilon\,\phi_{\epsilon,N}(q)\,. \tag{4.11}$$

Here, $\varepsilon = \pm 1$ is the eigenvalue of the parity operator defined according to (2.11). It is instructive to consider the eigenfunction decomposition of the spectral partition function $\mathcal{Z}(\beta)$,

$$\mathcal{Z}(\beta) = \int \mathrm{d}q \sum_{\varepsilon,N} \phi_{\varepsilon,N}(q)\,\phi^*_{\varepsilon,N}(q)\,\exp(-\beta\,E_{\varepsilon,N})\,. \tag{4.12}$$

Here, we assume a Hamiltonian whose spectrum is discrete (no continuous spectrum). The quantity $\mathcal{Z}_a(\beta)$ then finds a representation as

$$\mathcal{Z}_a(\beta) = \sum_{\varepsilon,N} \int \mathrm{d}q\,\phi_{\varepsilon,N}(q)\,\phi^*_{\varepsilon,N}(1-q)\,\exp(-\beta\,E_{\varepsilon,N})\,. \tag{4.13}$$

Now, $\mathcal{Z}_+(\beta)$ is determined by the even eigenfunctions alone,

$$\begin{aligned}\mathcal{Z}_+(\beta) &= \sum_{N=0}^{\infty} \int \mathrm{d}q\, \phi_{+,N}(q)\, \phi^*_{+,N}(q) \exp(-\beta\, E_{+,N}) \\ &= \frac{\mathcal{Z}(\beta) + \mathcal{Z}_a(\beta)}{2}\,. \end{aligned} \tag{4.14}$$

whereas $\mathcal{Z}_-(\beta)$ is determined by the odd eigenfunctions,

$$\begin{aligned}\mathcal{Z}_-(\beta) &= \sum_{N=0}^{\infty} \int \mathrm{d}q\, \phi_{-,N}(q)\, \phi^*_{-,N}(q) \exp(-\beta\, E_{-,N}) \\ &= \frac{\mathcal{Z}(\beta) - \mathcal{Z}_a(\beta)}{2}\,. \end{aligned} \tag{4.15}$$

4.2.3 Perturbation Theory

Perturbative expansions, that is expansions in powers of g for $g \to 0$, can be obtained by applying the steepest descent method to the path integral. Saddle points are solutions $q_{\mathrm{c}}(t)$ to the Euclidean equations of motion (Euclidean equations differ from the normal equations of classical mechanics by the sign in front of the potential). When the potential has a unique minimum, located for example at $q = 0$, the leading saddle point is $q_{\mathrm{c}}(t) = 0$. A systematic expansion around the saddle point then leads to a purely perturbative expansion of the eigenvalues of the Hamiltonian of the form

$$E(g) = \sum_{l=0}^{\infty} E_l\, g^l\,. \tag{4.16}$$

In the case of a potential with degenerate minima, one must sum over several saddle points: to each saddle point corresponds an eigenvalue and thus several eigenvalues are degenerate at leading order. Because the potential (2.10) is symmetric, the lowest eigenvalue, and more generally all eigenvalues which remain finite when g goes to zero, are twice degenerate to all orders in perturbation theory [see equation (2.5)]:

$$E_{\pm,N}(g) \approx E^{(0)}_N(g) \equiv \sum_{l=0}^{\infty} E^{(0)}_{N,l}\, g^l\,. \tag{4.17}$$

4.2.4 Instanton Configurations

Eigenvalues which remain finite when g goes to zero can be extracted from the large β expansion. In the infinite β limit, leading contributions to the path integral come from paths which are solutions of the Euclidean equations of motion that have a finite action. In the case of the path integral representation of $\mathcal{Z}_{\mathrm{a}}(\beta)$, constant solutions of the equation of motion do not satisfy the boundary conditions. Finite action solutions necessarily correspond to paths which connect the two minima of the potential (see figure 4.1).

In the example of the double-well potential (2.10), such solutions are

$$q_{\mathrm{c}}(t) = \left(1 + \mathrm{e}^{\pm(t - t_0)}\right)^{-1}, \qquad \mathcal{S}(q_{\mathrm{c}}) = 1/6\,. \tag{4.18}$$

Since the two solutions depend on an integration constant t_0, one finds two one-parameter families of degenerate saddle points.

Non-constant (in time) solutions with finite action are called *instanton* solutions. Since the main contribution to the action comes from the region around $t = t_0$, one calls t_0 the *position* of the instanton.

The corresponding contribution to the path integral is proportional, at leading order in g and for $\beta \to \infty$, to $\mathrm{e}^{-1/(6g)}$ and thus is non-perturbative. It is also proportional to β because one has to sum over all degenerate saddle points and the integration constant t_0 varies in $[0, \beta]$ for β large but finite. The complete calculation involves taking

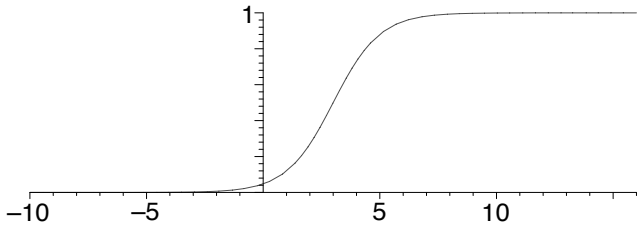

Figure 4.1: The instanton configuration.

the time t_0 as a collective coordinate, and integrating over the remaining fluctuations in the Gaussian limit. One finds that the two lowest eigenvalues are given by ($\varepsilon = \pm$)

$$\begin{aligned} E_{\varepsilon,0}(g) &= \lim_{\beta\to\infty} -\frac{1}{\beta}\ln \mathcal{Z}_\varepsilon(\beta) \underset{g\to 0,\beta\to\infty}{=} E_0^{(0)}(g) - \varepsilon E_0^{(1)}(g), \\ E_0^{(1)}(g) &= \frac{1}{\sqrt{\pi g}} \mathrm{e}^{-1/6g}\big(1+\mathcal{O}(g)\big). \end{aligned} \tag{4.19}$$

4.3 Multi–Instantons

Taking into account $E^{(0)}(g)$ and $E^{(1)}(g)$, one obtains for the functions (4.5) an expansion of the form

$$\mathcal{Z}_\varepsilon(\beta) \underset{\beta\to\infty}{\sim} \mathrm{e}^{-\beta(E_0^{(0)}-\varepsilon E_0^{(1)})} \sim \mathrm{e}^{-\beta E_0^{(0)}} \sum_{n=0}^{\infty} \frac{(\varepsilon\beta)^n}{n!} \left(E_0^{(1)}\right)^n. \tag{4.20}$$

Thus, the existence of a one-instanton contribution to eigenvalues implies the existence of n-instanton contributions to the functions (4.5), proportional to β^n.

For β finite, the path integrals indeed have other saddle points which correspond to oscillations in the well of the potential $-V(q)$. In the infinite β limit, the solutions with n oscillations have an action $n \times 1/6$ and thus give contributions to the path integral of the expected form.

However, there is a subtlety: naively one would expect these configurations to give a contribution of order β (for β large) because a given classical trajectory depends only on one time integration constant. This has to be contrasted with the expansion (4.20) where the n^{th} term is of order β^n.

Indeed, one discovers that the Gaussian integration near the saddle point involves the determinant of an operator that has eigenvalues which vanish exponentially in the large-β limit. The divergence has the following origin: in the large-β limit, the classical solution decomposes into a succession of largely separated instantons and fluctuations which tend to change the distances between instantons induce an infinitesimal variation of the action. It follows that, to properly study the limit, one has to introduce additional *collective coordinates* that parameterize all configurations close to solutions of the Euclidean equation of motion, even though they have a sightly different action. It is then easy to understand where in the expansion (4.20) the factor β^n originates from: Although a given classical trajectory can only generate a factor β, these new configurations depend on n independent collective coordinates over which one has to integrate.

To summarize: we know that n-instanton contributions do exist. However, these contributions do not correspond, in general, to solutions of the classical equation of motion. They correspond to configurations of largely separated instantons connected in a way which we shall discuss, which become solutions of the equation of motion only asymptotically, in the limit of infinite separation. These configurations depend on n times more collective coordinates than the one-instanton configuration.

4.4 Specific Calculations

4.4.1 Instanton Interaction

We now briefly explain, still with the example of the double-well potential, how multi-instanton contributions to the path integral can be evaluated at leading order for $g \to 0$.

In the infinite β limit, the instanton solutions can be written as

$$q_{\pm}(t) = f\big(\mp(t-t_0)\big)\,, \tag{4.21a}$$
$$f(t) = 1/\left(1+\mathrm{e}^{t}\right) = 1 - f(-t), \tag{4.21b}$$

where the integration constant t_0 characterizes the instanton position.

We first construct the *two-instanton configuration*. Actually it is convenient to now call instanton a solution which goes from 0 to 1 and anti-instanton a solution which goes from 1 to 0. Then, the relevant configurations are instanton-anti-instanton pairs. These configurations depend on one additional time parameter, the separation between instantons, decompose in the limit of infinite separation into two instantons and for large separation must minimize the variation of the action [29, 30]. For this purpose, we could introduce a constraint in the path integral fixing the separation between instantons (see chapter C.3), and solve the equation of motion with a Lagrange multiplier for the constraint. Instead, we use a method which, at least at leading order, is simpler and more intuitive.

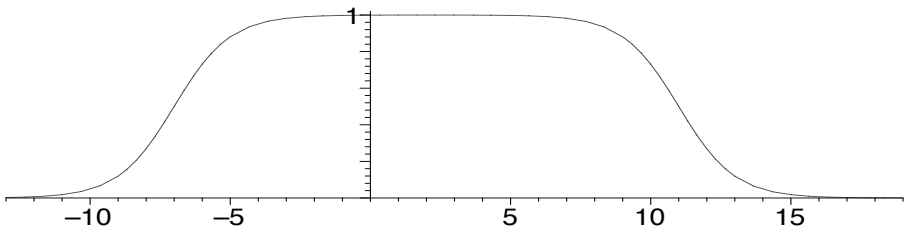

Figure 4.2: The two-instanton configuration.

We consider a configuration $q_{\mathrm{c}}(t)$ that is the sum of instantons separated by a distance θ, up to an additive constant adjusted in such a way as to satisfy the boundary conditions (figure 4.2):

$$q_{\mathrm{c}}(t) = f(t-\theta/2) + f(-t-\theta/2) - 1 = f(t-\theta/2) - f(t+\theta/2)\,, \tag{4.22}$$

where $f(t)$ is the function (4.21) (and of course all configurations deduced by time translation). This path has the following properties: it is continuous and differentiable and when θ is large it differs, near each instanton, from the instanton solution only by exponentially small terms of order $\mathrm{e}^{-\theta}$. Although the calculation of the corresponding action is straightforward, we give here some details to show that the ansatz (4.22) applies to more general symmetric potentials.

It is convenient to introduce some additional notation:

$$u(t) = f(t-\theta/2)\,,$$
$$v(t) = u(t+\theta)\,, \tag{4.23}$$

and thus $q_c = u - v$. The action corresponding to the path (4.22) can be written as

$$\mathcal{S}(q_c) = \int \mathrm{d}t\ \left[\tfrac{1}{2}\,\dot{q}_c^2 + V(q_c)\right]$$
$$= 2\times\frac{1}{6} + \int \mathrm{d}t\ \left[-\dot{u}\,\dot{v} + V(u-v) - V(u) - V(v)\right]\,. \tag{4.24}$$

The parity of q_c allows us to restrict the integration to the region $t > 0$, where v is at least of order $\mathrm{e}^{-\theta/2}$. After an integration by parts of the term $\dot{v}\dot{u}$, one finds

$$\mathcal{S}(q_c) = \frac{1}{3} + 2\left\{ v(0)\,\dot{u}(0) + \int_0^{+\infty} \mathrm{d}t\ \left[v\,\ddot{u} + V(u-v) - V(u) - V(v) \right] \right\}. \tag{4.25}$$

One then expands the integrand in powers of v. Since the leading correction to $\mathcal{S}$ is of order $\mathrm{e}^{-\theta}$, one needs the expansion only up to order v^2. The term linear in v vanishes as a consequence of the u-equation of motion. One obtains

$$\mathcal{S}(q_c) - \frac{1}{3} \sim 2\,v(0)\,\dot{u}(0) + 2\left\{ \int_0^{+\infty} \mathrm{d}t\ \left[\tfrac{1}{2}\,v^2\,V''(u) - \tfrac{1}{2}\,V''(0)\,v^2 \right] \right\}. \tag{4.26}$$

The function v decreases exponentially away from the origin so the main contributions to the integral come from the neighbourhood of $t = 0$, where $u = 1 + \mathcal{O}(\mathrm{e}^{-\theta/2}$ and thus $V''(u) \sim V''(1) = V''(0)$. Therefore, at leading order the two terms in the integral cancel. At leading order,

$$v(0)\,\dot{u}(0) \sim -\mathrm{e}^{-\theta} \tag{4.27}$$

and thus

$$\mathcal{S}(q_c) = \frac{1}{3} - 2\mathrm{e}^{-\theta} + \mathcal{O}\left(\mathrm{e}^{-2\theta}\right). \tag{4.28}$$

It will become clearer later why the classical action is needed only up to order $\mathrm{e}^{-\theta}$. In analogy with the partition function of a classical gas (instantons being identified with particles), one calls the quantity $-2\mathrm{e}^{-\theta}$ the interaction potential between instantons.

Actually, it is simple to extend the result to β large but finite. Symmetry between θ and $\beta - \theta$ then implies

$$\mathcal{S}(q_c) = \frac{1}{3} - 2\mathrm{e}^{-\theta} - 2\mathrm{e}^{-(\beta-\theta)} + \text{ negligible contributions.} \tag{4.29}$$

This expression can be verified by calculating its extremum as a function of θ. One obtains

$$\theta_c = \beta/2,\ \Rightarrow\ \mathcal{S}(q_c) = \frac{1}{3} - 4\mathrm{e}^{-\beta/2} + \mathcal{O}\left(\mathrm{e}^{-\beta}\right). \tag{4.30}$$

For the same Hamiltonian, one can calculate for β finite the action corresponding to a solution of the equation of motion with one oscillation. One finds

$$\mathcal{S}(q_c) = \frac{1}{6} - 2\,\mathrm{e}^{-\beta} + \mathcal{O}\left(\mathrm{e}^{-2\beta}\right). \tag{4.31}$$

Both results are consistent. Indeed, to compare them one has to replace β by $\beta/2$ in equation (4.31) and multiply the action by a factor 2, since the action corresponds to a trajectory described twice in the total time β.

We now examine the *variation of the action* due to the multi-instanton configuration. Specifically, we show that if we modify infinitesimally (for θ large) the configuration to further decrease the variation of the action, the change $r(t)$ of the path is of order $\mathrm{e}^{-\theta}$ and the variation of the action of order $\mathrm{e}^{-2\theta}$ at least. Setting

$$q(t) = q_c(t) + r(t) \tag{4.32}$$

and expanding the action up to second order in $r(t)$, one finds

$$\begin{aligned} \mathcal{S}(q_c + r) \quad &= \quad \mathcal{S}(q_c) + \int \left[\dot{q}_c(t)\,\dot{r}(t) + V'\big(q_c(t)\big)\,r(t) \right] \mathrm{d}t \\ &\quad + \frac{1}{2}\int \mathrm{d}t\,\left[\dot{r}^2(t) + V''(q_c)\,r^2(t) \right] + \mathcal{O}\left(\big[r(t)\big]^3 \right). \end{aligned} \tag{4.33}$$

In the term linear in $r(t)$, one integrates by parts $\dot{r}(t)$, in order to use the property that $q_c(t)$ approximately satisfies the equation of motion. In the term quadratic in $r(t)$, one replaces V'' by 1, since $r(t)$ is expected to be large only far from the instantons. One then verifies that the term linear in r is of order $\mathrm{e}^{-\theta}$ while the quadratic term is of order 1. A shift of r to eliminate the linear term would then give a negligible contribution, of order $\mathrm{e}^{-2\theta}$.

We now consider an *n-instanton configuration*, i.e. a succession of n instantons (more precisely, alternatively instantons and anti-instantons) separated by times θ_i with

$$\sum_{i=1}^{n}\theta_i = \beta. \tag{4.34}$$

At leading order, we need only consider "interactions" between nearest neighbour instantons. Other interactions are negligible because they are of higher order in $\mathrm{e}^{-\theta}$. This is an essential simplifying feature of quantum mechanics compared to quantum field theory. The classical action $\mathcal{S}_{\mathrm{c}}(\theta_i)$ can then be directly inferred from expression (4.29):

$$\mathcal{S}_{\mathrm{c}}(\theta_i) = \frac{n}{6} - 2\sum_{i=1}^{n}\mathrm{e}^{-\theta_i} + \mathcal{O}\left(\mathrm{e}^{-(\theta_i+\theta_j)}\right). \tag{4.35}$$

Note that for n even, the n-instanton configurations contribute to $\mathrm{Tr}\,\mathrm{e}^{-\beta H}$, while for n odd they contribute to $\mathrm{Tr}\,\left(P\mathrm{e}^{-\beta H}\right)$ (P is the parity operator). But all contributes to the combination (4.5).

(*Remark.*) Since we keep in the action all terms of order $\mathrm{e}^{-\beta}$, we expect to find the contributions not only to the two lowest energies but also to all energies which remain finite when g goes to zero.

4.4.2 The n–Instanton Contribution

We have calculated the n-instanton action. We now evaluate, at leading order, the contribution to the path integral of the neighbourhood of the n-instanton configuration [7, 31]. We expand the action up to second order in the deviation from the classical path. Although the path is not a solution of the equation of motion, it has been chosen it in such a way that the linear terms in the expansion can be neglected. The Gaussian integration involves then the determinant of the second derivative of the action at the classical path

$$M(t',t) = \left[-\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + V''\big(q_{\mathrm{c}}(t)\big)\right]\delta(t-t'). \tag{4.36}$$

The operator M has the form of a Hamiltonian with a potential that consists of n wells asymptotically identical to the well arising in the one-instanton problem, and which are largely separated. At leading order the corresponding spectrum is, therefore, the spectrum arising in the one-instanton problem n-times degenerate. Corrections are exponentially small in the separation. Simultaneously, by introducing n collective time variables, we have suppressed n times the zero eigenvalue and generated the Jacobian of the one-instanton case to the power n. Therefore, the n-instanton contribution to the combination (4.5)

$$\mathcal{Z}_\varepsilon(\beta) = \tfrac{1}{2}\,\mathrm{Tr}\,\left[(1+\varepsilon P)\,\mathrm{e}^{-\beta H}\right], \tag{4.37}$$

($\varepsilon = \pm 1$), can be written as

$$\mathcal{Z}_\varepsilon^{(n)}(\beta) = \mathrm{e}^{-\beta/2}\,\frac{\beta}{n}\,\left(\varepsilon\frac{\mathrm{e}^{-1/6g}}{\sqrt{\pi g}}\right)^n \int_{\theta_i\geq 0}\delta\left(\sum\theta_i - \beta\right)\prod_i \mathrm{d}\theta_i \exp\left[\frac{2}{g}\sum_{i=1}^{n}\mathrm{e}^{-\theta_i}\right]. \tag{4.38}$$

All factors have already been explained, except the factor β, which comes from the integration over a global time translation, and the factor $1/n$, which arises because the configuration is invariant under a cyclic permutation of the θ_i. Finally, the normalization factor $\mathrm{e}^{-\beta/2}$ corresponds to the partition function of the harmonic oscillator. Odd-n instanton effects contribute positively to $\mathcal{Z}_+^{(n)}(\beta)$, and negatively to $\mathcal{Z}_-^{(n)}(\beta)$.

If the instanton interactions are neglected (but instanton configuration with an arbitrarily large number of tunnelings are allowed), the integration over the θ_i's is straightforward and the sum of the leading order n-instanton contributions

$$\mathcal{Z}_\varepsilon(\beta,g) \approx \Sigma_\varepsilon(\beta,g) = \mathrm{e}^{-\beta/2} + \sum_{n=1}^{\infty}\mathcal{Z}_\varepsilon^{(n)}(\beta,g) \tag{4.39}$$

can be calculated:

$$\mathcal{Z}_\varepsilon(\beta,g) \approx \Sigma_\varepsilon(\beta,g) = \mathrm{e}^{-\beta/2}\left[1 + \frac{\beta}{n}\sum_{n=1}^{\infty}\left(\varepsilon\frac{\mathrm{e}^{-1/6g}}{\sqrt{\pi g}}\right)^n \frac{\beta^{n-1}}{(n-1)!}\right] = \mathrm{e}^{-\beta E_{\varepsilon,0}(g)} \tag{4.40}$$

with

$$E_{\varepsilon,0}(g) = \frac{1}{2} + \mathcal{O}(g) - \frac{\varepsilon}{\sqrt{\pi g}} \mathrm{e}^{-1/6g} \left(1 + \mathcal{O}(g)\right). \tag{4.41}$$

We recognize the perturbative and one-instanton contribution, at leading order, to $E_{\varepsilon,0}(g)$, the ground state and the first excited state energies.

In view of problematic issues related to the instanton interaction, the summation of these effects and necessary analytic continuations which have to be performed in order to calculate eigenvalues, we add here a small discussion. To go beyond the one-instanton approximation, it is necessary to take into account the interaction between instantons (see chapters 4.4.1 and 4.4.2). Unfortunately, if one examines expression (4.38), one discovers that the interaction between instantons is *attractive*. Therefore, for g small, the dominant contributions to the integral come from configurations in which the instantons are close. For such configurations, the concept of instanton is no longer meaningful, since the configurations cannot be distinguished from fluctuations around the constant or the one-instanton solution.

We should have expected such a difficulty. Indeed, the large-order behaviour analysis has shown that the perturbative expansion in the case of potentials with degenerate minima is not Borel summable. An ambiguity is expected at the two-instanton order. But if the perturbative expansion is ambiguous at the two-instanton order, contributions of the same order or even smaller are ill-defined. To proceed any further, we must first give a meaning to the sum of the perturbative expansion.

In the example of the double-well potential, it is possible to show that the perturbation series is Borel summable for g negative, by relating it to the perturbative expansion of the $\mathcal{O}(2)$ anharmonic oscillator. Therefore, we *define* the sum of the perturbation series as the analytic continuation of this Borel sum from g negative to $g = |g| \pm i0$. This corresponds in the Borel transformation to an integration above or below the real positive axis. We then note that, for g *negative*, the interaction between instantons is *repulsive* and, simultaneously, the expression (4.38) becomes meaningful. Therefore, we first calculate, for g small and negative, both the sum of the perturbation series and the instanton contributions, and perform an analytic continuation to g positive of all quantities consistently. In the same way, the perturbative expansion around each multi-instanton configuration is also non-Borel summable and the sum is defined by the same procedure.

At the same time, it should be remembered that the various analytic continuations and cancellations of imaginary parts, while illustrating the internal consistency of the approach, are not really necessary in order to obtain the energy eigenvalue via generalized resummation of the resurgent expansion: it would suffice to say that the energy eigenvalue is obtained by assigning to every divergent series in g, i.e. to every perturbative expansion about the n-instanton contributions, the real part of the Borel sum associated with that (factorially divergent) series. The real part of the Borel sum is also obtained by evaluating the Laplace–Borel integral using the principal-value prescription. Although intuitively clear, we would like to remark that this principal-value prescription —of course— corresponds to the integration contour C_0 as outlined in [17].

While, on the one hand, the necessity for an analytic continuation may seem a little obscure at first sight (see for example remarks on p. 241 of[32]), this procedure is, on the other hand, a mathematically well defined concept. In the context of the double-well problem it gives a defined meaning to each of the factorially divergent, nonalternating power series occurring in equation (2.13). In the end, given the fact that even mathematical proof [10, 11] may be questioned by inquisitive minds, the soundness of the concept must be judged by its predictive power. *Exempli gratia*, one may ask the question whether the energy levels predicted by the analytically continued instanton expansion are able to accurately reproduce numerically determined levels. This is indeed the case, as shown in chapter 8 below.

4.4.3 The Sum of the Leading–Order Instanton Contributions

Let us now introduce two useful parameters [cf. equations (2.27) and (2.28)]

$$\mu \equiv -\frac{2}{g} = \exp\left(\chi(g)\right), \quad \lambda \equiv \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-1/6g}, \tag{4.42}$$

in such a way that the "fugacity" $\xi(g)$ of the instanton gas, which is half the one-instanton contribution at leading order, can be written as [see (2.27)]

$$\xi(g) = \frac{1}{\sqrt{\pi g}}\,\mathrm{e}^{-1/6g} = \lambda\sqrt{-\mu} = -\mathrm{i}\,\lambda\sqrt{\mu}\,, \tag{4.43}$$

where the quantity $\xi(g)$ also occurs in a form multiplied by the parity ε, and a sign change in the determination of $\sqrt{-\mu}$ is therefore equivalent to a change $\varepsilon \mapsto -\varepsilon$ [see also equation (4.55) below].

As discussed before, we now assume that initially g is negative. The Laplace transform

$$G_\varepsilon^{(n)}(E) = \int_0^\infty \mathrm{d}\beta\,\mathrm{e}^{\beta E}\,\mathcal{Z}_\varepsilon^{(n)}(\beta) \tag{4.44}$$

of the n-instanton contribution (4.38):

$$\mathcal{Z}_\varepsilon^{(n)}(\beta) \sim \frac{\beta\,\mathrm{e}^{-\beta/2}\,\left(-\mathrm{i}\,\varepsilon\lambda\sqrt{\mu}\right)^n}{n} \int_{\theta_i\geq 0} \delta\left(\sum\theta_i - \beta\right) \prod_{i=1}^n \mathrm{d}\theta_i \exp\left[\frac{2}{g}\sum_{i=1}^n \mathrm{e}^{-\theta_i}\right], \tag{4.45}$$

yields the leading contribution $G_\varepsilon^{(n)}(E)$ to the trace $G_\varepsilon(E)$ of the resolvent [equation (4.6)]. In order to factorize the integral over the θ_i, we introduce a complex contour integral representation for the δ-function,

$$\delta\left(\sum_{i=1}^n \theta_i - \beta\right) = \frac{1}{2\pi\mathrm{i}} \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \mathrm{d}s \exp\left[-s\left(\beta - \sum_{i=1}^n \theta_i\right)\right]. \tag{4.46}$$

In terms of the function

$$\mathcal{I}(s,\mu) = \sqrt{\mu}\int_0^{+\infty} \exp\left(s\,\theta - \mu\,\mathrm{e}^{-\theta}\right)\,\mathrm{d}\theta\,, \tag{4.47}$$

$\mathcal{Z}_\varepsilon^{(n)}(\beta)$ can be rewritten as

$$\mathcal{Z}_\varepsilon^{(n)}(\beta) \sim \frac{\beta\,\mathrm{e}^{-\beta/2}\,(-\mathrm{i}\,\varepsilon\lambda)^n}{2\pi\mathrm{i}n} \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \mathrm{d}s\,\mathrm{e}^{-\beta\,s}\,\left[\mathcal{I}(s,\mu)\right]^n\,. \tag{4.48}$$

In view of (4.44), we have

$$\begin{aligned}
G_\varepsilon^{(n)}(E) &= \int_0^\infty \mathrm{d}\beta\,\mathrm{e}^{\beta E}\,\mathcal{Z}_\varepsilon^{(n)}(\beta) \\
&= \int_0^\infty \mathrm{d}\beta\,\frac{\beta\,\mathrm{e}^{\beta(E-1/2)}\,(-\mathrm{i}\,\varepsilon\lambda)^n}{2\pi\mathrm{i}n} \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \mathrm{d}s\,\mathrm{e}^{-\beta\,s}\,\left[\mathcal{I}(s,\mu)\right]^n \\
&= \frac{\partial}{\partial E}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \mathrm{d}s\,\frac{(-\mathrm{i}\,\varepsilon\lambda)^n}{2\pi\mathrm{i}n}\,\left[\mathcal{I}(s,\mu)\right]^n \int_0^\infty \mathrm{d}\beta\,\mathrm{e}^{\beta(E-s-1/2)} \\
&= \frac{\partial}{\partial E}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \mathrm{d}s\,\frac{(-\mathrm{i}\,\varepsilon\lambda)^n}{2\pi\mathrm{i}n}\,\left[\mathcal{I}(s,\mu)\right]^n\,\frac{1}{s+1/2-E} \\
&= \frac{\partial}{\partial E}\,\frac{(-\mathrm{i}\,\varepsilon\lambda)^n}{n}\,\left[\mathcal{I}(E-\tfrac{1}{2},\mu)\right]^n\,.
\end{aligned} \tag{4.49}$$

Alternatively, one may observe that in (4.44), the integral over β is immediate and the integrals over the θ_i then factorize. One obtains

$$G_\varepsilon^{(n)}(E) \sim \frac{(-\mathrm{i}\,\varepsilon\lambda)^n}{n}\,\frac{\partial}{\partial E}\,\left[\mathcal{I}(E-\tfrac{1}{2},\mu)\right]^n\,. \tag{4.50}$$

The function $\mathcal{I}(s,\mu)$ is the only function needed for these leading-order calculations in one dimension. A first way to calculate it, is to expand

$$\mathcal{I}(s,\mu) = \int_0^{+\infty} \sum_{N=0}^{\infty} \frac{(-1)^N}{N!} \mu^{N+1/2}\, \mathrm{e}^{(s-N)\theta} \mathrm{d}\theta = \sum_{N=0}^{\infty} \frac{(-1)^N}{N!}\, \frac{\mu^{N+1/2}}{N-s}\,. \tag{4.51}$$

The expansion defines a real meromorphic function of s with poles at non-negative integers. The poles and residues can be trusted because they depend only on the large θ behaviour. However, after analytic continuation to $g > 0$, the function grows as $\mathrm{e}^{-\mu} = \mathrm{e}^{2/g}$, a behaviour due to the integration near $\theta = 0$ that cannot be trusted and cannot be correct.

Let us now evaluate the integral (4.47) in the limit $\mu \to +\infty$, and thus $g \to 0_-$. We change variables, setting $\mu\, \mathrm{e}^{-\theta} = t$, and the integral becomes

$$\mathcal{I}(s,\mu) = \mu^{s+1/2} \int_0^{\mu} \mathrm{d}t\, t^{-1-s}\, \mathrm{e}^{-t} = \mu^{s+1/2} \int_0^{+\infty} \mathrm{d}t\, t^{-1-s}\, \mathrm{e}^{-t} + \mathcal{O}\left(\mathrm{e}^{-\mu}/\sqrt{\mu}\right). \tag{4.52}$$

We thus obtain ($s = E - 1/2$)

$$\mathcal{I}(s,\mu) \approx \mu^{s+1/2}\, \Gamma(-s) = \left(-\frac{2}{g}\right)^E \Gamma\left(\frac{1}{2} - E\right), \tag{4.53}$$

a meromorphic function with the same poles and residues as the initial expression. For $\mu \to +\infty$, the difference is exponentially small and both expressions are equivalent, but after analytic continuation to $g > 0$, the asymptotic form (4.53) has now an acceptable behaviour. Therefore, our ansatz is that the estimate (4.53) gives the correct leading behaviour of the true function.

In view of (4.50), the generating function $\mathcal{G}_\varepsilon(E,g)$ of the leading-order multi-instanton contributions (4.39) then is given by [we use $\sum_n (-x)^n/n = -\ln(1+x)$]

$$\mathcal{G}_\varepsilon(E,g) = \sum_{n=1}^{\infty} G_\varepsilon^{(n)}(E) = -\frac{\partial}{\partial E} \ln \Delta_\varepsilon(E) \tag{4.54}$$

with

$$\Delta_\varepsilon(E) \;=\; 1 + \varepsilon\, \mathrm{i}\, \lambda\, \mathcal{I}\left(E - \frac{1}{2}, \mu\right) \;\approx\; 1 + \varepsilon\, \mathrm{i}\, \frac{e^{-1/6g}}{\sqrt{2\pi}} \left(-\frac{2}{g}\right)^E \Gamma\left(\frac{1}{2} - E\right), \tag{4.55}$$

where we now explicitly see that a change in the determination of $\sqrt{-\mu}$ is equivalent to a change $\varepsilon \mapsto -\varepsilon$. Because $\mathcal{G}_\varepsilon(E,g)$ approximates the trace of the resolvent,

$$\mathcal{G}_\varepsilon(E,g) \approx \mathrm{Tr}\left(\frac{1}{H_\epsilon - E}\right), \tag{4.56}$$

we have

$$\begin{aligned} \mathcal{G}_\varepsilon(E,g) &\approx -\frac{\partial}{\partial E}\, \mathrm{Tr}[\ln(H_\epsilon - E)] \\ &= -\frac{\partial}{\partial E}\, \ln[\det(H_\epsilon - E)] \\ &\approx -\frac{\partial}{\partial E}\, \ln \Delta_\varepsilon(E)\,. \end{aligned} \tag{4.57}$$

Here, H_ϵ denotes the Hamiltonian restricted on the Hilbert space spanned by the eigenvectors of H with parity ϵ. Therefore, the functions $\Delta_\varepsilon(E) \approx \det(H_\epsilon - E)$ are directly the sums of the leading order multi-instanton contributions to the products $\mathcal{D}_\varepsilon(E)$ of even or odd eigenvalues,

$$\mathcal{D}_\varepsilon(E) \propto \prod_N \left(1 - \frac{E}{E_{\varepsilon,N}}\right), \tag{4.58}$$

but, unlike $\mathcal{D}_\varepsilon(E)$, they are meromorphic functions in E because the zero-instanton contribution has not yet been included at all; an expansion of (4.55) in powers of λ starts with a term of order $\mathcal{O}(\lambda)$. Correcting for this effect, we add to $\mathcal{G}_\varepsilon(E,g)$ the trace of the resolvent of the harmonic oscillator, and we thus divide $\Delta_\varepsilon(E)$ by $\Gamma(\frac{1}{2}-E)$. This amounts to the replacement

$$\begin{aligned}\mathcal{G}_\varepsilon(E,g) &\to \mathcal{G}_\varepsilon(E,g)+G_{\text{osc.}}(E)\\ &\approx -\frac{\partial}{\partial E}\ln\Delta_\varepsilon(E)+\frac{\partial}{\partial E}\ln\Gamma\left(\frac{1}{2}-E\right)\\ &\approx -\frac{\partial}{\partial E}\ln\frac{\Delta_\varepsilon(E)}{\Gamma\left(\frac{1}{2}-E\right)}\,.\end{aligned} \tag{4.59}$$

This cancels the poles, and $\Delta_\varepsilon(E)$ becomes an entire function:

$$\Delta_\varepsilon(E)=\frac{1}{\Gamma(\frac{1}{2}-E)}+\varepsilon\mathrm{i}\left(-\frac{2}{g}\right)^E\frac{\mathrm{e}^{-1/6g}}{\sqrt{2\pi}}. \tag{4.60}$$

The first term is simply the Fredholm determinant (A.33) corresponding to the harmonic oscillator. We note here that the sum of all instanton contributions, in the leading approximation, i.e. neglecting subleading terms in the instanton interaction, simply yields some sort of one-instanton (but E-dependent) correction to the spectral equation.

Since λ is small, zeros of the equation $\Delta_\varepsilon(E)=0$ are close to eigenvalues of the harmonic oscillator:

$$E_{\varepsilon,N}=N+\frac{1}{2}+\mathcal{O}(\lambda)\,,\qquad N\geq 0\,. \tag{4.61}$$

The zeros of the function (4.60) can then be expanded in a power series in λ:

$$E_{\varepsilon,N}(g)=\sum_n E_N^{(n)}(g)\,(-\varepsilon\lambda)^n. \tag{4.62}$$

One obtains from a unique equation the multi-instanton contributions to all energy eigenvalues $E_{\varepsilon,N}(g)$ of the double-well potential at leading order in g, that is to say all the coefficients $e_{N,nk0}$ in the notation of the equations (2.13) and (2.15). Concrete results for the double-well potential are presented in chapter 8.7.

The appearance of a factor $\ln g$ in equation (2.39) can now be simply understood by noting that the interaction terms are only relevant for $g^{-1}\,\mathrm{e}^{-\theta}$ of order 1, that is θ of order $-\ln g$.

Assuming that an equation of the form (4.60) holds beyond leading order, we conclude that the argument of the Γ-function must be such that the equation reproduces at zero instanton order the perturbative expansion: E has to be replaced by the function $B(E,g)$. If we further assume that for B large there is some connection with the WKB expansion, we infer that $(-2/g)^E$ must also be replaced by $(-2/g)^B$ to reconstruct a term of the form $B\ln(Eg)$. This is the origin of the conjecture (2.21).

This concludes the first part of the treatise of multi-instanton effects in quantum mechanics. In the second part [33], we intend to generalize the instanton calculations to a wider family of potentials.

Appendix A

Schrödinger and Riccati Equations: Some Useful Results

A.1 Inverse Schrödinger Operator: Matrix Elements

In this appendix, we recall here the derivation of a few classical results that we have used throughout this article. We first consider the hermitian positive differential operator

$$L = -\mathrm{d}_x^2 + u(x), \tag{A.1}$$

where $u(x)$ has the form of a potential, which remains strictly positive for $|x| \to \infty$.

We recall the derivation of the differential equation satisfied by the diagonal matrix elements of its inverse $R = L^{-1}$.

Matrix elements $R(x,y)$ of R satisfy the Schrödinger equation

$$\big(-\mathrm{d}_x^2 + u(x)\big) R(x,y) = \delta(x-y)\,. \tag{A.2}$$

We recall that $R(x,y)$ can be expressed in terms of two independent solutions of the homogeneous equation

$$\big(-\mathrm{d}_x^2 + u(x)\big)\varphi(x) = 0\,. \tag{A.3}$$

We denote by φ_1, φ_2 two solutions, partially normalized by

$$\varphi_1'\,\varphi_2 - \varphi_1\,\varphi_2' = 1\,, \tag{A.4}$$

and, moreover, satisfying the boundary conditions

$$\varphi_1(x) \to 0 \text{ for } x \to -\infty, \quad \varphi_2(x) \to 0 \text{ for } x \to +\infty\,. \tag{A.5}$$

Then, it is easily verified that $R(x,y)$ is given by

$$R(x,y) = \varphi_1(y)\,\varphi_2(x)\,\theta(x-y) + \varphi_1(x)\,\varphi_2(y)\,\theta(y-x)\,, \tag{A.6}$$

where $\theta(x)$ is the usual Heaviside step function. The diagonal matrix elements

$$r(x) \equiv R(x,x) = \varphi_1(x)\,\varphi_2(x) \tag{A.7}$$

satisfy

$$\begin{aligned} r'(x) &= \varphi_1'(x)\,\varphi_2(x) + \varphi_1(x)\,\varphi_2'(x)\,, \\ r''(x) &= 2\,\big(\varphi_1'(x)\,\varphi_2'(x) + u(x)\,r(x)\big)\,, \end{aligned} \tag{A.8a}$$

where we have used the equation (A.3).

One then verifies that, as the consequence of equation (A.4), $r(x)$ satisfies the non-linear differential equation

$$2r(x)\,r''(x) - r'^2(x) - 4\,u(x)\,r^2(x) + 1 = 0\,. \tag{A.9}$$

A quantity of special interest is the trace G of the R:

$$G = \int \mathrm{d}x\, r(x). \tag{A.10}$$

A.2 Riccati's Equation

We now set

$$\sigma(x) = -\frac{\varphi'(x)}{\varphi(x)}, \tag{A.11}$$

in equation (A.3). We find

$$\sigma'(x) - \sigma^2(x) + u(x) = 0\,. \tag{A.12}$$

To the two solutions $\varphi_{1,2}$ correspond two functions $\sigma_{1,2}$. We introduce

$$\sigma_+ = \tfrac{1}{2}\,(\sigma_2 - \sigma_1), \quad \sigma_- = \tfrac{1}{2}(\sigma_2 + \sigma_1). \tag{A.13}$$

The Wronskian condition (A.4) implies

$$\sigma_+(x) = \frac{1}{2\,\varphi_1(x)\,\varphi_2(x)} = \frac{1}{2r(x)}\,. \tag{A.14}$$

The equation satisfied by $\sigma_{1,2}$ implies

$$\sigma_-' - \sigma_+^2 - \sigma_-^2 + u(x) = 0\,, \tag{A.15a}$$

$$\sigma_+' - 2\,\sigma_+\,\sigma_- = 0\,. \tag{A.15b}$$

The second allows expressing σ_- in terms of σ_+ and, thus,

$$\varphi_2 = \frac{1}{\sqrt{2\sigma_+}} \exp\left[-\int_{x_0}^{x} \mathrm{d}y\,\sigma_+(y)\right], \tag{A.16a}$$

$$\varphi_1 = \frac{1}{\sqrt{2\sigma_+}} \exp\left[\int_{x_0}^{x} \mathrm{d}y\,\sigma_+(y)\right]. \tag{A.16b}$$

A.3 Resolvent and Spectrum

We now substitute $u(x) \mapsto u(x) - z$, set $L = H - z$ and apply these results. The operator $R(z) = L^{-1}(z)$ becomes the resolvent of the Hamiltonian H. Riccati's equation becomes

$$\sigma'(x) - \sigma^2(x) + u(x) - z = 0\,. \tag{A.17}$$

Then,

$$\frac{\partial \sigma'}{\partial z} - 2\sigma\frac{\partial \sigma}{\partial z} = 1\,. \tag{A.18}$$

One first useful consequence is the identity

$$\frac{\partial \sigma_+(x)}{\partial z} + \varphi_1(x)\varphi_2(x) = \frac{\partial}{\partial x}\left[\frac{1}{2\sigma_+(x)}\frac{\partial \sigma_-(x)}{\partial z}\right]. \tag{A.19}$$

Then,

$$G(z) = \mathrm{Tr}\, L^{-1}(z) = \int \mathrm{d}x\, r(x) = -\int \mathrm{d}x\, \frac{\partial \sigma_+(x)}{\partial z}\,. \tag{A.20}$$

Integrating, one infers

$$\ln \mathcal{D}(z) \equiv \ln \det L(z) = \int \mathrm{d}x\, \sigma_+(x) = \frac{1}{2} \ln\left(\frac{\varphi_1(x)}{\varphi_2(x)}\right)\Big|_{-\infty}^{+\infty}\,. \tag{A.21}$$

The function $\mathcal{D}(z)$ is the Fredholm determinant of the operator $H - z$: Assuming a discrete spectrum, we have

$$\mathcal{D}(z) \propto \prod_{N=0} (1 - z/z_N). \tag{A.22}$$

Note that the infinite product may require some convergence factor, and the expressions in equation (A.21), in general, require some large-x regularization.

The spectrum of H is given by the solutions of the equation $\mathcal{D}(z) = 0$. An alternative and useful way of writing this spectral equation is

$$\lim_{\varepsilon \to 0_+} \ln \mathcal{D}(z_N - i\varepsilon) - \ln \mathcal{D}(z_N + i\varepsilon) = i\pi(2N+1)\,, \tag{A.23}$$

and, therefore,

$$\frac{1}{2i\pi} \lim_{\varepsilon \to 0_+} \int \mathrm{d}x\, [\sigma(x, z_N - i\varepsilon) - \sigma_+(x, z_N + i\varepsilon)] = N + \tfrac{1}{2}. \tag{A.24}$$

Finally , the large x behaviour then determines the solutions completely and one finds

$$\frac{\partial \sigma_2(x)}{\partial z} = -\frac{1}{\varphi_2^2(x)} \int_x^{+\infty} \mathrm{d}y\, \varphi_2^2(y), \tag{A.25a}$$

$$\frac{\partial \sigma_1(x)}{\partial z} = \frac{1}{\varphi_1^2(x)} \int_{-\infty}^{x} \mathrm{d}y\, \varphi_1^2(y) \tag{A.25b}$$

(*General symmetric potentials*.) We now assume $u(x) = u(-x)$. We then choose

$$\varphi_1(-x) = \varphi_2(x) \equiv \varphi(x). \tag{A.26}$$

Instanton calculus suggests that it is then also interesting to consider the quantities

$$r_a(x) = R(x, -x) = \varphi^2(x)\, \theta(x) + \varphi^2(-x)\theta(-x)\,, \tag{A.27a}$$

$$G_a(z) = \mathrm{Tr}\, PL^{-1}(z) = \int \mathrm{d}x\, r_a(x) = 2\int_0^{\infty} \mathrm{d}x\, \varphi^2(x)\,, \tag{A.27b}$$

where P is the $x \mapsto -x$ reflection operator.

Using equations (A.16a) and (A.4) taken at $x = 0$ to normalize, we obtain a first expression

$$G_a(z) = \int_0^{\infty} \frac{\mathrm{d}x}{\sigma_+(x)} \exp\left[-2\int_0^x \mathrm{d}y\, \sigma_+(y)\right]. \tag{A.28}$$

We then combine with equation (A.25) to obtain

$$G_a(z) = \frac{\partial}{\partial z} \ln\left(\frac{\varphi(0)}{\varphi'(0)}\right)\,. \tag{A.29}$$

In particular, integrating over z, one finds an expression for the generalization of the Fredholm determinant:

$$\exp\left[-\mathrm{Tr}\, P \ln(H - z)\right] = \prod_{N=0} \left(\frac{z - z_{2N}}{z - z_{2N+1}}\right) \propto \frac{\varphi'(0, z)}{\varphi(0, z)} = \frac{\sigma_+'(0)}{\sigma_+(0)} = -\frac{1}{[\sigma_+(0)]^2}, \tag{A.30}$$

an expression that can be easily understood since for even eigenfunctions $\varphi'(0)$ vanishes, while $\varphi(0)$ vanishes for odd eigenfunctions.

A.4 Example: Harmonic Oscillator

As an illustration, let us apply this formalism to the harmonic oscillator with $u(x) = x^{\,2}$ and $z = 2E$.

The trace of the resolvent for the harmonic oscillator formally reads

$$G_{\text{osc.}}(E) = \sum_{N=0} \frac{1}{N + 1/2 - E}\,, \tag{A.31}$$

which diverges. However, the first derivative of $G(E)$ is defined. Integrating one can choose

$$G_{\text{osc.}}(E) = -\psi(\tfrac{1}{2} - E), \tag{A.32}$$

where $\psi(z)$ is the logarithmic derivative of the Γ-function. Finally, from $G_{\text{osc.}}(E)$ one derives the Fredholm determinant

$$\mathcal{D}_{\text{osc.}}(E) = 1/\Gamma(\tfrac{1}{2} - E), \tag{A.33}$$

which vanishes on the poles of the Γ-function.

The solution of the Schrödinger equation that decreases for $x \to +\infty$ is proportional to

$$\varphi(x, E) = \frac{1}{2i\pi} \oint_C \frac{\mathrm{d}p}{p^{E+1/2}}\, \mathrm{e}^{-x^2/2 + px - p^2/4}\,, \tag{A.34}$$

where the contour encloses the real negative axis. The asymptotic form for $x \to -\infty$ is given by steepest descent:

$$\varphi(x, E) \underset{x\to-\infty}{\sim} \frac{2}{\sqrt{\pi}}\, (-2x)^{-E-1/2}\, \sin \pi(E + \tfrac{1}{2}) \mathrm{e}^{x^2/2}\,. \tag{A.35}$$

For $x \to +\infty$, the integral is dominated by the neighbourhood of the origin:

$$\varphi(x, E) \underset{x\to+\infty}{\sim} x^{E-1/2}\, \frac{1}{\Gamma(E + \frac{1}{2})}\, \mathrm{e}^{-x^2/2}\,. \tag{A.36}$$

Then,

$$\mathcal{D}(E) \propto \frac{\sin \pi(E + \frac{1}{2})}{\Gamma(E + \frac{1}{2})} \propto \frac{1}{\Gamma(\frac{1}{2} - E)}\,. \tag{A.37}$$

Moreover,

$$\varphi(0, E) \;=\; \frac{1}{\pi}\, 2^{-E-1/2}\, \sin[\pi(E + \tfrac{1}{2})]\, \Gamma\left(\frac{1}{4} - \tfrac{1}{2}E\right)\,, \tag{A.38a}$$

$$\varphi'(0, E) \;=\; -\frac{1}{\pi}\, 2^{1/2-E}\, \sin[\pi(E + \tfrac{1}{2})]\, \Gamma\left(\frac{3}{4} - \tfrac{1}{2}E\right)\,, \tag{A.38b}$$

and thus the expected result is obtained.

For example, in the case of the harmonic oscillator,

$$G_a(E) = \psi\left(\frac{1}{4} - \frac{1}{2}\,E\right) - \psi\left(\frac{3}{4} - \frac{1}{2}\,E\right) = -\frac{1}{2E} + \frac{1}{8E^3} + \mathcal{O}(1/E^5), \tag{A.39}$$

an expansion that is reproduced by the WKB approximation.

Appendix B

Spectral Equation: A Few Terms of Perturbative and WKB Expansions

B.1 Perturbative Expansion

For illustration purpose, we first calculate a few terms of the perturbative expansion of the function $B(E,g)$, using the expansion (3.37). We then verify the relation between perturbative and WKB expansions.

We expand the Riccati equation (3.14) in powers of g,

$$S(q) = \sum_{k\geq 0} g^k s_k(q)\,. \tag{B.1}$$

Setting

$$U(q) = \sqrt{2V(q)}\,, \tag{B.2}$$

we first find

$$s_0(q) = U(q), \quad s_1(q) = \frac{1}{2U(q)}\big(U'(q) - 2E\big)\,. \tag{B.3}$$

Higher orders are given by solving the recursion relation

$$s_k(q) = \frac{1}{2U(q)}\left(s'_{k-1}(q) - \sum_{l=1}^{k-1} s_{k-l}(q)s_l(q)\right). \tag{B.4}$$

At order g^2, one finds

$$s_2(q) = \frac{1}{8U^3(q)}\left(2U''U - 3U'^2 + 4EU' - 4E^2\right)\,. \tag{B.5}$$

We then simply need the residues at $q=0$.

As we show later, it is often convenient to parameterize the potential as the solution of the equation

$$U'^2 = \rho(U) = 1 + \alpha_1 U + \alpha_2 U^2 + \alpha_3 U^3 + \alpha_4 U^4 + \mathcal{O}\left(U^5\right). \tag{B.6}$$

Beyond perturbation theory, this implies simple well or symmetric double well potentials. For example, the quartic double-well potential corresponds to $\rho = 1 - 4u$ and the cosine potential to $\rho = 1 - 4u^{\,2}$.

Up to the order of g^6, the solution has the expansion

$$\begin{aligned} V(q) \;=\; & \frac{1}{2}q^2 + \frac{1}{4}\,\alpha_1\,q^3 + \left(\frac{1}{6}\,\alpha_2 + \frac{1}{32}\alpha_1^2\right)\,q^4 + \left(\frac{1}{16}\,\alpha_1\,\alpha_2 + \frac{1}{8}\,\alpha_3\right)q^5 \\ & + \left[\frac{3}{80}\,\alpha_1\,\alpha_3 + \frac{1}{45}\,\alpha_2^2 + \frac{1}{10}\,\alpha_4 + \frac{1}{4}\,\alpha_1\,\left(\frac{1}{48}\,\alpha_1\,\alpha_2 + \frac{1}{8}\,\alpha_3\right)\right]\,q^6\,. \end{aligned} \tag{B.7}$$

This suggests an alternative method of calculation. Introducing the parameterization

$$S = \sigma_+(U) + gU'\sigma_-(U) = U + \mathcal{O}(g)\,, \tag{B.8}$$

one obtains another form of Riccati's equation:

$$\sigma'_+(u) - 2\sigma_+(u)\sigma_-(u) = 0\,, \tag{B.9a}$$
$$g^2\left[\rho(u)\big(\sigma'_-(u) - \sigma^2_-(u)\big) + \tfrac{1}{2}\rho'(u)\,\sigma_-(u)\right] - \sigma^2_+(u) + u^2 - 2gE = 0\,. \tag{B.9b}$$

(One may first calculate σ^2_+.) Then

$$B(E,g) = -\frac{1}{2i\pi g}\oint \mathrm{d}u \frac{\sigma_+(u)}{\sqrt{\rho(u)}}, \tag{B.10}$$

and the residue at $q = 0$ becomes the residue at $u = 0$.

In terms of the parameters (B.6), one obtains up to the order g^2,

$$\begin{aligned} B(E,g) = E &+ \left[\left(-\frac{1}{4}\alpha_2 + \frac{3}{16}\alpha_1^2\right)E^2 - \frac{1}{16}\alpha_2 + \frac{1}{64}\alpha_1^2\right] g \\ &+ \left[\left(-\frac{1}{4}\,\alpha_4 + \frac{3}{8}\,\alpha_1\,\alpha_3 + \frac{3}{16}\,\alpha_2^2 - \frac{15}{32}\,\alpha_1^2\,\alpha_2 + \frac{35}{256}\,\alpha_1^4\right)E^3\right. \\ &\left. + \left(-\frac{5}{16}\,\alpha_4 + \frac{5}{32}\,\alpha_1\,\alpha_3 + \frac{5}{64}\,\alpha_2^2 - \frac{15}{128}\,\alpha_1^2\,\alpha_2 + \frac{25}{1024}\,\alpha_1^4\right)E\right] g^2\,. \end{aligned} \tag{B.11}$$

One immediately verifies that it agrees with the results obtained for various special potentials. In the case of an even potential ($\alpha_1 = \alpha_3 = 0$) and finite angular momentum, the expression at the same order becomes [see also equation (3.83)]

$$\begin{aligned} B(E,g) = E &+ \alpha_2\left[-\frac{1}{4}E^2 + \frac{1}{12}\,\left(j^2-1\right)\right] g + \left[\left(-\frac{1}{4}\alpha_4 + \frac{3}{16}\alpha_2^2\right)E^3\right. \\ &\left. + \left(\left\{j^2-1\right\}\left(-\frac{17}{240}\,\alpha_2^2 + \frac{3}{20}\,\alpha_4\right) - \frac{1}{5}\,\alpha_4 + \frac{1}{40}\,\alpha_2^2\right)E\right] g^2\,. \end{aligned} \tag{B.12}$$

B.2 WKB Expansion: Second–Order Calculation

(*General considerations.*) The WKB expansion of $B(E,g)$ is an expansion in powers of g at gE fixed. Therefore, we expand $S(q)$ in powers of g at gE fixed (or alternatively equation (3.26)):

$$S(q) = \sum_{k=0}^{\infty} g^k S_k(q). \tag{B.13}$$

Then,

$$S_1 = \frac{S'_0}{2S_0}\,, \tag{B.14}$$

and the recursion relation becomes

$$S_k(q) = \frac{1}{2S_0(q)}\left(S'_{k-1}(q) - \sum_{l=1}^{k-1} S_{k-l}(q)\,S_l(q)\right)\,. \tag{B.15}$$

At order g^2, one finds

$$S_2 = \frac{S''_0}{4S_0^2} - \frac{3S_0'^2}{8S_0^3}\,. \tag{B.16}$$

For the order g^2 contribution to the functions $A(E,g)$ and $B(E,g)$, we need only the integral of S_2. Integrating by parts, one finds

$$\int \mathrm{d}q\, S_2(q) = \int \mathrm{d}q\, \frac{S_0'^2(q)}{8S_0^3(q)}\,. \tag{B.17}$$

(*Perturbative and WKB expansions*.) One recovers the contributions to the perturbative expansion by expanding $S_k(q)$ in powers of Eg and calculating the residues at this minimum of the potential.

We expand the first WKB term in powers of gE:

$$S_0 = U \sum_{n=0}^{\infty} \left(2gEU^{-2}\right)^n \frac{\Gamma(n-\frac{1}{2})}{\Gamma(n+1)\Gamma(-\frac{1}{2})}. \tag{B.18}$$

One has thus to evaluate [see also the equations (F.9) and (F.38)]:

$$-\frac{1}{2\,\mathrm{i}\,\pi}\oint_C \mathrm{d}q\, U^{1-2n} = -\frac{1}{2\,\mathrm{i}\,\pi}\oint \mathrm{d}u\, \frac{u^{1-2n}}{\sqrt{\rho(u)}}\,, \tag{B.19}$$

where the parameterization (B.6) has been introduced.

For the next WKB order, we calculate the integrand of (B.17) more explicitly

$$\frac{S_0'^2(q)}{8S_0^3(q)} = \frac{U'^2\,U^2}{8S_0^5}\,. \tag{B.20}$$

Expanding S_0, one finds [see also the equations (F.10) and (F.39)]:

$$\int \mathrm{d}q\, S_2 = \frac{1}{8}\sum_{n=-1}^{\infty} \frac{(2gE)^n}{\Gamma(n+1)}\,\frac{\Gamma(n+5/2)}{\Gamma(5/2)}\,\int \mathrm{d}q\, U'^2\, U^{-2n-3}\,. \tag{B.21}$$

One thus has to evaluate

$$-\frac{1}{2\,\mathrm{i}\,\pi}\oint_C \mathrm{d}q\, U'^2 U^{-2n-3} = -\frac{1}{2\,\mathrm{i}\,\pi}\oint \mathrm{d}u\, \sqrt{\rho(u)}u^{-2n-3}. \tag{B.22}$$

(*A special class of potentials*.) We follow [6]. It is possible to calculate many terms of the WKB expansion for the class of potentials such that, in the parameterization (B.6),

$$\rho(u) = 1 - 4u^m\,. \tag{B.23}$$

Here, $m=1$ corresponds to the double-well potential, $m=2$ to the cosine potential, for $m=3,4$ the potentials are meromorphic elliptic functions. Higher values no longer correspond to meromorphic functions (except for $m=6$ where U^2 is still meromorphic). The case $m\geq 3$ odd corresponds to potentials which diverge on the real axis, m even to periodic and finite potentials on the real axis.

One verifies that the term of order g^l in the expansion is of the form $P_l(u)/u^{2l-1}$, where P_l is polynomial. The expansion of B thus involves only the integral

$$L(\nu) = -\frac{1}{2\,\mathrm{i}\,\pi}\oint_C \mathrm{d}q\, U^{1-2\nu}. \tag{B.24}$$

We change variables $q \mapsto u = U(q)$ in (B.24) and find

$$L_m(\nu) = -\frac{1}{2\,\mathrm{i}\,\pi}\oint_C \mathrm{d}u\, (1-4u^m)^{-1/2}\, u^{1-2\nu}\,. \tag{B.25}$$

Expanding the root in powers of u, we obtain

$$L_m(\nu) = -2^{4(\nu-1)/m}\frac{\Gamma\left(\frac{1}{2}+2\frac{(\nu-1)}{m}\right)}{\Gamma\left(\frac{1}{2}\right)\,\Gamma\left(1+2\frac{(\nu-1)}{m}\right)} \quad \text{for} \quad 2(\nu-1)=0 \pmod m\,. \tag{B.26}$$

For example,

$$
\begin{aligned}
-\frac{1}{2i\pi}\oint_C \mathrm{d}q\, S_0 &= -\sum_{n\geq 0} (2gE)^n \,\frac{\Gamma\left(n-\frac{1}{2}\right)}{\Gamma(n+1)\,\Gamma\left(-\frac{1}{2}\right)} L(n), \\
&= -\sum\nolimits'_{k\geq 0} \frac{(gE)^{1+km/2}\, 2^{1+k(2+m/2)}\,\Gamma\left(\frac{km}{2}+\frac{1}{2}\right)\,\Gamma\left(k+\frac{1}{2}\right)}{\Gamma\left(\frac{km}{2}+2\right)\,\Gamma\left(-\frac{1}{2}\right)\,\Gamma(k+1)\,\Gamma\left(\frac{1}{2}\right)}\,,
\end{aligned}
\tag{B.27}
$$

where $\sum'$ means the sum over k, including only those terms for which $k\,m$ is even.

Appendix C

Multi–Instantons

C.1 Determinant

In this chapter, we give some indication about a few additional technical ingredients that are involved in the calculation of multi-instanton contributions. We can write the operator M defined by equation (4.36) as

$$M = -\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + 1 + \sum_{i=1}^{n} v(t - t_i), \tag{C.1}$$

in which $v(t)$ is a potential localized around $t = 0$:

$$v(t) = \mathcal{O}\left(\mathrm{e}^{-|t|}\right), \quad |t| \to \infty \tag{C.2}$$

and t_i are the positions of the instantons.

We want to calculate

$$\det M\, M_0^{-1} = \det\left\{1 + \left[-\left(\mathrm{d}/\mathrm{d}t\right)^2 + 1\right]^{-1} \sum_{i=1}^{n} v(t - t_i)\right\}. \tag{C.3}$$

Using the identity $\ln\det = \mathrm{Tr}\,\ln$, we expand the r.h.s. in powers of $v(t)$:

$$\ln\det M M_0^{-1} = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \int \prod_{j=1}^{k} \mathrm{d}u_j \Big[\Delta(u_1 - u_2) \sum_{i_1=1}^{n} v(u_2 - t_{i_1})\Delta(u_2 - u_3)\cdots\Delta(u_k - u_1) \sum_{i_k=1}^{n} v(u_1 - t_{i_k})\Big] \tag{C.4}$$

with the definition

$$\Delta(t) = \left\langle 0\middle|\left[-(\mathrm{d}/\mathrm{d}t)^2 + 1\right]^{-1}\middle|t\right\rangle \sim \frac{1}{2}\,\mathrm{e}^{-|t|} \quad \text{for} \quad 1 \ll t \ll \beta\,. \tag{C.5}$$

It is clear from the behaviour of $v(t)$ and of $\Delta(t)$, that when the instantons are largely separated, only the terms in which one retains from each potential the same instanton contribution survive. Therefore,

$$\begin{aligned}&\ln\det M M_0^{-1} = \\ &\quad n \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \int \prod_{j=1}^{k} \mathrm{d}u_j \Delta(u_1 - u_2)\, v(u_2)\cdots\Delta(u_k - u_1)\, v(u_1)\,, \\ &\quad \text{for} \quad |t_i - t_j| \gg 1\,.\end{aligned} \tag{C.6}$$

We recognize n times the logarithm of the one-instanton determinant.

C.2 Instanton Interaction

We assume, as in chapter 5, that the potential has two degenerate minima at the points $x = 0$ and $x = x_0$ with

$$V(x) = \tfrac{1}{2}\, x^2 + \mathcal{O}\left(x^3\right) , \tag{C.7a}$$

$$V(x) = \tfrac{1}{2}\, \omega^2\, \left(x - x_0\right)^2 + \mathcal{O}\left((x - x_0)^3\right) . \tag{C.7b}$$

Let us write the one-instanton solution $q_c(t)$ which goes from 0 to $q_0 = x_0/\sqrt{g}$ as

$$q_c(t) = f(t)/\sqrt{g}\,. \tag{C.8}$$

We choose the function $f(t)$ in such a way that it satisfies

$$x_0 - f(t) \sim \sqrt{C_\omega}\, \mathrm{e}^{-\omega t}/\omega \quad \text{for } t \to +\infty \tag{C.9a}$$

$$f(t) \sim \sqrt{C_\omega}\, \mathrm{e}^{t} \quad \text{for } t \to -\infty\,. \tag{C.9b}$$

By solving the equation of motion, it is easy to calculate the constant C_ω:

$$C_\omega = x_0^2\, \omega^{2/(1+\omega)} \exp\left\{ \frac{2\omega}{1+\omega} \left[\int_0^{x_0} \mathrm{d}x \left(\frac{1}{\sqrt{2V(x)}} - \frac{1}{x} - \frac{1}{\omega(x_0 - x)} \right) \right] \right\}. \tag{C.10}$$

We recognize the constant (2.73).

We now construct instanton–anti-instanton pair configurations $q(t)$ which correspond to trajectories starting from, and returning to, $q = q_0$ or $q = 0$. Since we want also to consider the case of two successive instantons, we assume, but only in this last case, that $V(x)$ is an even function and has therefore a third minimum at $x = -x_0$.

According to the discussion of chapter 4, we can take as a two-instanton configuration

$$q_1(t) = \frac{1}{\sqrt{g}} \left(f_+(t) + \varepsilon f_-(t) \right), \qquad \varepsilon = \pm 1 \tag{C.11}$$

with

$$f_+(t) = f(t - \theta/2), \qquad f_-(t) = f(-t - \theta/2)\,. \tag{C.12}$$

Here, θ is a measure of the instanton separation. The case $\varepsilon = 1$ corresponds to an instanton–anti-instanton pair starting from $q = q_0$ at time $-\infty$, approaching $q = 0$ at intermediate times and returning to q_0. The case $\varepsilon = -1$ corresponds to a sequence of two instantons going from $-q_0$ to q_0. Finally, for the classical trajectory which goes, instead, from the origin to q_0 and back, we can take

$$q_2(t) = \left[f(t + \theta/2) + f(\theta/2 - t) - x_0 \right] / \sqrt{g}\,. \tag{C.13}$$

We now calculate the classical action corresponding to $q_1(t)$. We separate the action into two parts, corresponding at leading order to the two instanton contributions:

$$\mathcal{S}(q_1) = \mathcal{S}_+(q_1) + \mathcal{S}_-(q_1) \tag{C.14}$$

with

$$\mathcal{S}_+(q_1) = \int_0^{+\infty} \left[\frac{1}{2}\, \dot{q}_1^2 + \frac{1}{g}\, V\left(\sqrt{g}\, q_1(t)\right) \right] \mathrm{d}t,$$

$$\mathcal{S}_-(q_1) = \int_{-\infty}^{0} \left[\frac{1}{2}\, \dot{q}_1^2 + \frac{1}{g}\, V\left(\sqrt{g}\, q_1(t)\right) \right] \mathrm{d}t\,. \tag{C.15}$$

The value $t = 0$ of the separation point is somewhat arbitrary and can be replaced by any value which remains finite when θ becomes infinite. We then use the properties that for θ large $f_+(t)$ is small for $t < 0$, and $f_-(t)$ is small for $t > 0$, to expand both terms. For example, for $\mathcal{S}_+$ we find

$$\begin{aligned} \mathcal{S}_+(q_1) = \frac{1}{g} \int_0^{+\infty} \mathrm{d}t \, \Big\{ & \left[\frac{1}{2} \left[\dot{f}_+^2(t) \right] + V\left(f_+(t)\right) \right] \\ & + \varepsilon \left[\dot{f}_-(t)\, \dot{f}_+(t) + V'\big(f_+(t)\big)\, f_-(t) \right] \\ & + \frac{1}{2} \left[\dot{f}_-^2(t) + V''\big(f_+(t)\big)\, f_-^2(t) \right] \Big\} . \end{aligned} \tag{C.16}$$

Since $f_-(t)$ decreases exponentially, only values of t small compared to $\theta/2$ contribute to the last term of equation (C.16) which is proportional to V''. For such values of t, we have

$$\tfrac{1}{2}\,V''\big(f_+(t)\big)\,f_-^2 \sim V\big(f_-(t)\big)\,. \tag{C.17}$$

For the terms linear in $f_-(t)$, we integrate by parts the kinetic term and use the equation of motion

$$\ddot{f}(t) = V'[f(t)]\,. \tag{C.18}$$

Only the integrated term survives and yields

$$\int_0^{+\infty} \mathrm{d}t\,\left[\dot{f}_-(t)\,\dot{f}_+(t) + V'\big(f_+(t)\big)\,f_-(t)\right] = -\dot{f}(-\theta/2)\,f(-\theta/2)\,. \tag{C.19}$$

The contribution $\mathcal{S}_-$ can be evaluated by exactly the same method. We note that the sum of the two contributions reconstructs twice the classical action a. We then find

$$\mathcal{S}(q_1) = \frac{1}{g}\,\left[2\,a - 2\,\varepsilon\,f(-\theta/2)\dot{f}(-\theta/2) + \cdots\right] \tag{C.20}$$

with

$$a = \int_0^{x_0} \sqrt{2V(x)}\mathrm{d}x\,. \tag{C.21}$$

Replacing, for θ large, f by its asymptotic form (C.9), we finally obtain the classical action

$$\mathcal{S}(q_1) = g^{-1}\left[2a - 2C\varepsilon\,\mathrm{e}^{-\theta} + \mathcal{O}\left(\mathrm{e}^{-2\theta}\right)\right] \tag{C.22}$$

and thus the instanton interaction.

Following the same steps, we can calculate the classical action corresponding to $q_2(t)$. The result is

$$\mathcal{S}(q_2) = \frac{1}{g}\,\left\{2a - 2\left[f(\theta/2) - x_0\right]\dot{f}(\theta/2) + \cdots\right\}\,, \tag{C.23}$$

which for θ large is equivalent to

$$\mathcal{S}(q_2) = \frac{1}{g}\,\left[2a - 2(C/\omega)\mathrm{e}^{-\omega\theta}\right]\,. \tag{C.24}$$

Finally, if we consider the case of a finite time interval β with periodic boundary conditions, we can combine both results to find the action of a periodic trajectory passing close to $q = 0$ and $q = q_0$:

$$\mathcal{S}(q) = g^{-1}\left[2a - 2C\left(\mathrm{e}^{-\beta+\theta} + \mathrm{e}^{-\omega\theta}/\omega\right)\right]\,, \tag{C.25}$$

in agreement with equations (5.5) and (5.8).

C.3 Multi–Instantons from Constraints

Although multi-instanton configurations do not correspond to solutions of the equation of motion, it is nevertheless possible to modify the classical action by introducing constraints and integrating over all possible constraints. The main problem with such a method is to find a system of constraints which are both theoretically reasonable, and convenient for practical calculations.

One can, for instance, fix the positions of the instantons by introducing in the path integral (in the example of the double-well)

$$1 = \int \prod_{i=1}^{n} \left[\int \mathrm{d}t\,\dot{q}^2_{\varepsilon_i}(t-t_i)\right]\,\delta\left[\int \mathrm{d}t\,\dot{q}_{\varepsilon_i}(t-t_i)\,\big(q(t) - q_{\varepsilon_i}(t-t_i)\big)\right]\mathrm{d}t_i\,, \tag{C.26}$$

where t_i are the instanton positions and ε_i a succession of $\pm$ indicating instantons and anti-instantons. One then uses an integral representation of the δ-functions, so that the path integral becomes

$$\left(\frac{||\dot{q}_+||^2}{2i\pi}\right)^n \int \prod_{i=1}^{n} \mathrm{d}t_i\,\mathrm{d}\lambda_i\,\int[\mathrm{d}q(t)]\,\prod_{i=1}^{n}\exp\left[-\mathcal{S}(q,\lambda_i)\right] \quad \text{with}$$

$$\mathcal{S}(q,\lambda_i) = \mathcal{S}(q) + \sum_{i=1}^{n}\lambda_i\,\int \mathrm{d}t\,\dot{q}_{\varepsilon_i}(t-t_i)\,\big(q(t) - q_{\varepsilon_i}(t-t_i)\big)\,. \tag{C.27}$$

Appendix D

Dispersion Relations and (non-)Borel Summability

D.1 Dispersion Relations

(*The simplest example.*) The nonalternating ($g > 0$) factorially divergent series

$$f(g) \sim \sum_{n=0}^{\infty} n!\, g^n \tag{D.1}$$

is generated by expanding in powers of g the following integral,

$$f(g) = \int_0^{\infty \pm \mathrm{i}\,\epsilon} \mathrm{d}t\, \frac{1}{1-gt}\, \exp(-t)\,. \tag{D.2}$$

The imaginary part due to the (half-)pole at $t = 1/g$ is

$$\mathrm{Im}\, f(g) = \pm \frac{\pi}{g}\, \exp(-1/g)\,. \tag{D.3}$$

Because $f(g)$ has a cut along the positive real axis, one may write a dispersion relation in an obvious way as

$$0 = -2\pi\mathrm{i} \operatorname*{Res}_{z=z_0} \frac{f(z)}{z-z_0} + \int_0^{\infty} \mathrm{d}x\, \left[\frac{1}{x-z_0} \left(f(x+\mathrm{i}\,\epsilon) - f(x-\mathrm{i}\,\epsilon) \right) \right]. \tag{D.4}$$

(*Dispersion relation.*) The equality

$$f(z_0) = \frac{1}{\pi} \int_0^{\infty} \mathrm{d}x\, \frac{1}{x-z_0}\, \mathrm{Im}\, f(x) \tag{D.5}$$

follows immediately. Let us now start from this dispersion relation as the fundamental property of a function which has a cut along the positive real axis and fulfills sufficient conditions in order to ensure the convergence of the integral. Let us assume furthermore, that $f(z_0)$ can be expanded as a formal power series,

$$f(z_0) \sim \sum_{n=0}^{\infty} a_n\, z_0^n\,. \tag{D.6}$$

Expanding the right-hand side of (D.5) into a power series in z_0,

$$\frac{1}{x-z_0} = \frac{1}{x} \sum_{n=0}^{\infty} \left(\frac{z_0}{x} \right)^n\,, \tag{D.7}$$

we immediately have

$$a_n = \frac{1}{\pi} \int_0^\infty \mathrm{d}x \, \frac{1}{x^{n+1}} \, \mathrm{Im}\, f(x) \,. \tag{D.8}$$

In many cases, possible convergence problems near $x = 0$ are eliminated due to a nonanalytic factor of the form $\exp(-1/x)$ that enters into $\mathrm{Im}\, f(x)$.

(*A calculational example*.) We now replace $x \to g$. For a function whose imaginary part is

$$\mathrm{Im}\, f(g) = \frac{1}{g} \, \exp\left(-\frac{1}{a\, g}\right) \, (1 + bg + cg^2 + dg^3 + \ldots) \,, \tag{D.9a}$$

the evaluation of the integral on the right-hand side of (D.8) leads to

$$a_n = \frac{a^{n+1}}{\pi} \, n! \, \left(1 + \frac{b}{n} + \frac{c}{n\,(n+1)} + \frac{d}{n\,(n+1)\,(n+2)} + \ldots\right) \,. \tag{D.9b}$$

This example shows that correction terms to the imaginary part of order g to the imaginary part along the positive real axis (the cut) correspond to subleading corrections to the factorial growth of the "perturbative coefficients" a_n of relative order n^{-1}. The correction terms can be summarized in a natural way in terms of an inverse factorial series. This consideration is the basis for the "matching" discussed in chapter 8.2.

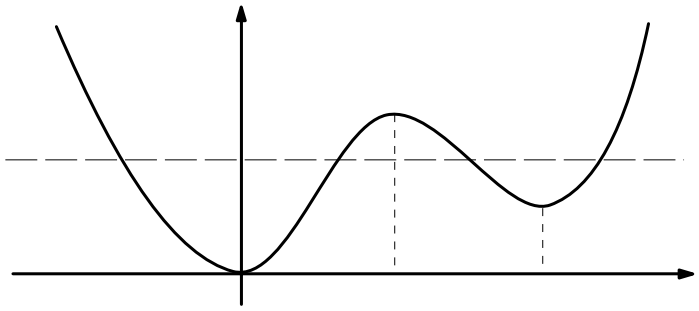

Figure D.1: The four roots of equation (D.14).

D.2 A Simple Example of non–Borel Summability

Let us try to illustrate the problem of non-Borel summability with the example of a simple integral, which shares some of the features of the problem in quantum mechanics which we have studied in chapter 4. We consider the function

$$I(g) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}q \, \exp\left[-\frac{1}{g} V(q\sqrt{g})\right] \,, \tag{D.10}$$

where $V(x)$ is an entire function with an absolute minimum at $x = 0$, $V(0) = 0$. For g small $I(g)$ can be calculated by steepest descent, expanding V around $q = 0$:

$$I(g) = \sum_{k \geq 0} I_k \, g^k. \tag{D.11}$$

It is easy to write a finite dimensional integral of the form (D.10) as a generalized Borel or Laplace transform,

$$I(g) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}q \, \mathrm{d}t \, \delta \, [V(q\sqrt{g}) - t] \, \mathrm{e}^{-t/g}. \tag{D.12}$$

We integrate over q:

$$I(g) = \frac{1}{\sqrt{2\pi g}} \int_0^\infty \mathrm{d}t \, \mathrm{e}^{-t/g} \, \sum_i \frac{1}{|V'\,[x_i(t)]|} \,, \tag{D.13}$$

in which $\{x_i(t)\}$ are the solutions of the equation

$$V\left[x_i(t)\right] = t\,. \tag{D.14}$$

When the function $V(x)$ is monotonic both for x positive and negative, the equation (D.14) has two solutions for all values of t and the equation (D.13) is directly the Borel representation of the function $I(g)$, which has a Borel summable power series expansion.

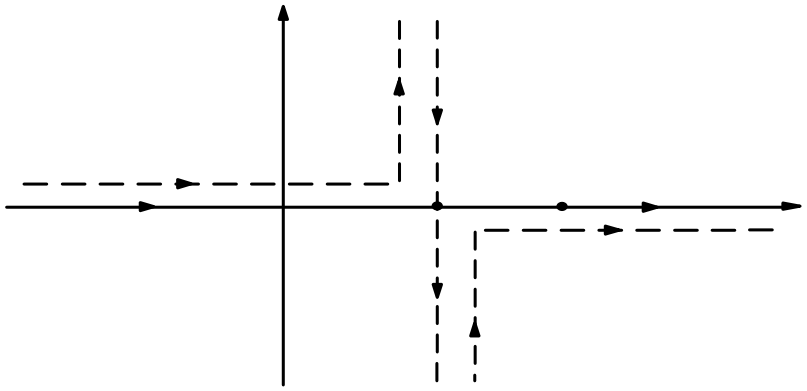

Figure D.2: The different contours in the x-plane.

We now assume, instead, that $V(x)$ has a second local minimum which gives a negligible contribution to $I(g)$ for g small. A simple example is

$$V(x) = \tfrac{1}{2}x^2 - \frac{1}{3a}\,x^3\,(1+a) + \frac{1}{4a}\,x^4, \quad \tfrac{1}{2} < a < 1\,, \tag{D.15}$$

which has a minimum at $x = 1$. Between its two minima the potential $V(x)$ has a maximum, located at $x = a$, whose contribution dominates the large order behaviour of the expansion in powers of g:

$$I_k \underset{k\to\infty}{\propto} \Gamma(k)\,\left[V(a)\right]^{-k}\,, \qquad V(a) > 0 \tag{D.16}$$

(in the example (D.15) $V(a) = a^2\,(1 - a/2)/6$) and the series is not Borel summable.

The *naive* Borel transform of $I(g)$ is obtained by retaining in equation (D.13) only the roots of equation (D.14) which exists for t small. The singularities of the Borel transform then correspond to the zeros of $V''(x)$.

For the potential (D.15) the expression (D.13) has the form

$$\begin{aligned} I(g) \;\; = \;\; & \frac{1}{\sqrt{2\pi g}} \int_0^{+\infty} \mathrm{d}t\, \mathrm{e}^{-t/g} \left[\frac{1}{\left|V'\big(x_1(t)\big)\right|} + \frac{\theta\big(V(a)-t\big)}{\left|V'\big(x_2(t)\big)\right|} \right. \\ & \left. + \frac{\theta\big(V(a)-t\big)\,\theta\big(t-V(1)\big)}{\left|V'\big(x_3(t)\big)\right|} + \frac{\theta\big(t-V(1)\big)}{\left|V'\big(x_4(t)\big)\right|} \right] \end{aligned} \tag{D.17}$$

with the definitions (see figure D.1): $x_1(t) \le 0 \le x_2(t) \le a \le x_3(t) \le 1 \le x_4(t)$.

The idea of the analytic continuation is to integrate each contribution up to $t = +\infty$ following a contour which passes below or above the cut along the positive real axis. This means that we consider $x_2(t)$ to solve the equation:

$$V\left[x_2(t)\right] = t \pm \mathrm{i}\,\varepsilon\,. \tag{D.18}$$

The sign is arbitrary. Let us, for instance, choose the positive sign. We then have to subtract this additional contribution. We proceed in the same way for $x_3(t)$ for $t > V(a)$. Since $x_2(t)$ and $x_3(t)$ meet at $t = V(a)$, the analytic continuation will correspond to take for $x_3(t)$ the other solution

$$V\left[x_3(t)\right] = t \mp \mathrm{i}\,\varepsilon\,. \tag{D.19}$$

We thus have to subtract from the total expression the contributions of two roots of the equation. But it is easy to verify that this is just the contribution of the saddle point located at $x = a$, which corresponds to a maximum of the potential.

Therefore, we have succeeded in writing expression (D.17) as the sum of three saddle point contributions (see figure D.2). There is some arbitrariness in this decomposition which here corresponds to the choice $\varepsilon = \pm 1$.

In the complex x plane, we have replaced the initial contour C on the real positive axis, by a sum of three contours C_1, C_2 and C_3 corresponding to the three saddle points located at $0, a, 1$.

Appendix E

Degenerate Minima: Energy Splitting and Schrödinger Equation

We consider the Hamiltonian

$$H = -\tfrac{1}{2}\mathrm{d}_x^2 + V(x) \tag{E.1}$$

where the potential is analytic on the real axis, even: $V(x) = V(-x)$ and has an absolute minimum located at $x = \pm x_m$ (choosing $x_m > 0$) where it vanishes. Eigenfunctions and eigenvalues can be calculated in a perturbative expansion in each well of the potential. There are twice degenerate to all orders. We call $\psi_N(x)$ the WKB eigenfunction corresponding to the expansion near the well around $x = x_m$:

$$-\tfrac{1}{2}\psi_N''(x) + V(x)\psi_N(x) = E_N\psi_N(x)\,. \tag{E.2}$$

Then the second eigenfunction with the same perturbative energy is $\psi_N(-x)$ and it is a WKB approximation near $-x_m$. We know that the true eigenfunctions are even or odd. To calculate the energy difference $\delta E_N = E_{+,N} - E_{-,N}$ we construct trial wave functions $\phi_{N,\varepsilon}(x)$, which are even or odd depending on the value $\varepsilon = \pm 1$,

$$\phi_{N,\varepsilon}(x) = \begin{cases} \psi_N(x)\,\left(1 + \varepsilon\,\frac{\psi_N(-\alpha)}{\psi_N(\alpha)}\right) & \text{for} \quad \alpha < x\,, \\ \psi_N(x) + \varepsilon\psi_N(-x), & \text{for} \quad -\alpha < x < \alpha\,, \\ \psi_N(-x)\,\left(\varepsilon + \frac{\psi_N(-\alpha)}{\psi_N(\alpha)}\right) & \text{for} \quad x < -\alpha\,, \end{cases} \tag{E.3}$$

where $x_m > \alpha > 0$. At the points $x = \pm\alpha$ the function $\psi_N(x)$ is exponentially small in the semi-classical limit and $\psi_N(-\alpha) \ll \psi_N(\alpha)$.

The trial wave functions are continuous, satisfy locally the Schrödinger equation, but are not differentiable at the points $x \pm \alpha$. We now calculate

$$E_{N,\varepsilon} = \frac{\langle\phi_{N,\varepsilon}\,|\,H\,|\phi_{N,\varepsilon}\rangle}{\langle\phi_{N,\varepsilon}\,|\phi_{N,\varepsilon}\rangle}. \tag{E.4}$$

Integrating by parts, one finds

$$\begin{aligned} &\int_{-\infty}^{+\infty} \mathrm{d}x\,\left[\tfrac{1}{2}\left(\phi'_{N,\varepsilon}(x)\right)^2 + V(x)\,\phi_{N,\varepsilon}^2(x)\right] \\ &\quad = \quad E_N \int_{-\infty}^{+\infty} \mathrm{d}x\,\left\{\phi_{N,\varepsilon}^2(x) + \phi_{N,\varepsilon}(\alpha)\,\left[\phi'_{N,\varepsilon}(\alpha_-) - \phi'_{N,\varepsilon}(\alpha_+)\right]\right\}\,. \end{aligned} \tag{E.5}$$

It follows, that up to smaller exponential corrections,

$$\delta E_N = -\frac{\psi_N(\alpha)\psi'_N(-\alpha) + \psi_N(-\alpha)\psi'_N(\alpha)}{\int \mathrm{d}x\,\psi_N^2(x)}, \tag{E.6}$$

where only the neighbourhood of $x = x_m$ contributes to the integral in the denominator. We note that since $\psi_N(\pm x)$ are two eigenfunctions with the same energy, the quantity

$$\begin{aligned} W(\alpha) &= -\psi_N(\alpha)\,\psi'_N(-\alpha) - \psi_N(-\alpha)\,\psi'_N(\alpha) \\ &= -\psi_N(\alpha)\,\psi_N(-\alpha)\,\left(\frac{\psi'_N(-\alpha)}{\psi_N(-\alpha)} + \frac{\psi'_N(\alpha)}{\psi_N(\alpha)}\right) \end{aligned} \tag{E.7}$$

is a Wronskian and thus independent of α. The calculation then follows closely the lines of chapter (3.3), where the inverse quantity is calculated. Equation (E.6) can easily be generalized to the Schrödinger equation in higher dimensions.

We now apply this result to the Schrödinger equation in the normalization (2.10). At leading order in the semi-classical limit, the eigenfunction $\psi_N(q)$ can be written, for $0 \leq q < q_0$, as

$$\begin{aligned} \psi_N(q) &= q^N \sqrt{q/U(q)}\,\exp\left[-\frac{1}{g}\int_0^q \mathrm{d}q'\,U(q')\right] \\ &\quad \times \exp\left[(N+\tfrac{1}{2})\int_0^q \mathrm{d}q'\,\left(\frac{1}{U(q')} - \frac{1}{q'}\right)\right]. \end{aligned} \tag{E.8}$$

At this order $\psi'_N(q)/\psi_N(q) \sim -U(q)/g$. The value of the Wronskian $W(q)$ thus is

$$\begin{aligned} W(q) &= -\psi_N(q)\,\psi_N(q_0-q)\,\left(\frac{\psi'_N(q_0-q)}{\psi_N(q_0-q)} + \frac{\psi'_N(q)}{\psi_N(q)}\right) \\ &= \frac{2}{g}\,C^{N+1/2}\,\mathrm{e}^{-a/2g}, \end{aligned} \tag{E.9}$$

with [see equations (2.58), (2.60) and (3.35)]

$$a = 2\int_0^{q_0} \mathrm{d}q\,U(q), \tag{E.10a}$$

$$C = q_0^2\,\exp\left[\int_0^{q_0}\left(\frac{1}{U(q)} - \frac{1}{q} - \frac{1}{q_0-q}\right)\right]. \tag{E.10b}$$

For the denominator, we need the perturbative eigenfunction near $q = 0$ with the same normalization. We thus set $q = x\sqrt{g}$ and obtain

$$\psi_N(x\sqrt{g}) \underset{g\to 0}{\sim} g^{N/2} x^N \mathrm{e}^{-x^2/2}. \tag{E.11}$$

This result, however, yields the coefficient of $\mathrm{e}^{-x^2/2}$ in the WKB limit $q = x\sqrt{g}$ fixed, that is x large. Actually, we know that at leading order the wave function is simply the eigenfunction of the harmonic oscillator. The eigenfunction with norm $\sqrt{\pi}$ is

$$\varphi_N(x) = \frac{1}{2^{N/2}\sqrt{N!}}\,(x - \mathrm{d}_x)^N\,\mathrm{e}^{-x^2/2} \underset{x\to\infty}{\sim} \frac{2^{N/2}}{\sqrt{N!}} x^N \mathrm{e}^{-x^2/2}. \tag{E.12}$$

We conclude

$$\psi_N(x\sqrt{g}) \sim \sqrt{N!}\,(g/2)^{N/2}. \tag{E.13}$$

Therefore,

$$\int \mathrm{d}q\,\psi_N^2(q) = \sqrt{\pi g}\,N!\,(g/2)^N. \tag{E.14}$$

Finally, we notice that in the q variable and with the form (E.1) of the Schrödinger operator the spectrum is E/g. The one-instanton contribution to the energy difference follows:

$$\delta E_N(g) \sim \frac{2}{\sqrt{2\pi}}\frac{1}{N!}\left(\frac{2C}{g}\right)^{N+1/2}\,\mathrm{e}^{-a/2g}, \tag{E.15}$$

a result consistent with the expansion of the zeros of expression (5.18).

Note that to go beyond leading order by this method is simple for N fixed, but not for generic N because the WKB expansion yields the perturbative eigenfunction under the form of an expansion only valid for large arguments.

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