Chapter 6

Euclidean Path Integral

The oscillatory nature of the integrand $e^{iS/\hbar}$ in the path integral gives rise to distributions. If the oscillations were suppressed, then it might be possible to define a sensible measure on the set of paths. With this hope much of the rigorous work on path integrals deals with *imaginary time* $t \rightarrow -i\tau$ for which the Lagrangian density undergoes the so-called *Wick rotation*. One analytically continues to imaginary times, calculates the corresponding Greensfunctions and continuous back to real time by the inverse Wick rotation $\tau \rightarrow it$. For imaginary time the measure on the set of paths can rigorously be defined and leads to the *Wiener measure*.

6.1 Quantum Mechanics for Imaginary Times

For a selfadjoint Hamiltonian the unitary time evolution operator has the spectral representation

$$U(t) = e^{-iHt} = \int e^{-iEt} dP_E, \qquad (\hbar = 1)$$
 (6.1)

where the integral has its support on the spectrum of H. Here P_E is the orthogonal projector onto the subspace spanned by the eigenfunction with energy less or equal to E. We assume that the Hamiltonian is bounded from below and add a constant to it, such that it has non-negative spectrum. Then the above integral extends from 0 to ∞ . Now we assume that t becomes complex $t \to t - i\tau$,

$$e^{-(\tau+it)H} = \int_0^\infty e^{-E(\tau+it)H} dP_E.$$
 (6.2)

With our assumption this is a holomorphic semigroup in the half plane

$$\{t - i\tau \in \mathbb{C}, \ \tau \ge 0\}. \tag{6.3}$$

If we would know the operator (6.2) for imaginary times $(t = 0, \tau \ge 0)$ then we could analytically continue it to real times $(t, \tau = 0)$, the time domain of interest in quantum mechanics. If we analytically continue t to $-i\tau$ then the Minkowskian metric $\eta = \text{diag}(1, -1, -1, -1)$ turns into a metric with Euclidean signature. This explains why this continuation is called the transition from the Lorentzian- to the Euclidean sector of the theory.

The evolution operators U(t) are defined for all real times and form a *one-parametric uni*tary group. It satisfies a Schrödinger equation

$$i\frac{d}{dt}U(t) = HU(t), \tag{6.4}$$

and its kernel $K(t,q',q) = \langle q | U(t) | q' \rangle$ is complex and of oscillatory character. For imaginary times the 'evolution operators'

$$U(\tau) = e^{-\tau H} \tag{6.5}$$

are positive (and hence hermitean instead of unitary) with non-negative eigenvalues. The $U(\tau)$ exist for positive τ and form a so-called a *semigroup*. For almost all initial state vectors a propagation backwards in imaginary time is impossible. $U(\tau)$ satisfies a *diffusion* type equation,

$$\frac{d}{d\tau}U(\tau) = -HU(\tau),\tag{6.6}$$

and its kernel

$$K(\tau, q, q') = \langle q | e^{-\tau H} | q' \rangle \quad \text{with} \quad K(0, q, q')) = \delta(q, q'), \tag{6.7}$$

is real for real Hamiltonians¹. This kernel is strictly positive as follows from the

Theorem: Suppose V is continuous and bounded from below, and let $H = H_0 + V$ be essentially selfadjoint. Then the evolution kernel is positive,

$$K(\tau, q, q') = \langle q | e^{-\tau H} | q' \rangle > 0.$$
(6.8)

If a (real) kernel would be negative for q' in an open set \mathcal{O} then we could construct a function $\psi(q) \ge 0$ with support in \mathcal{O} for which $(\psi, U(\tau)\psi) \le 0$. This should not be possible for the positive operator $U(\tau)$. For a rigorous proof of (6.8) I refer to the textbook of Glimm and Jaffe [9], page 50. The positive kernel for a free particle in d dimensions reads

$$K_0(\tau, q, q') = \left(\frac{m}{2\pi\tau}\right)^{d/2} e^{-m(q'-q)^2/2\tau},$$
(6.9)

and the kernel for an oscillator with constant frequency ω is given by *Mehlers formula*

$$K_{\omega}(\tau, q, q') = \left(\frac{m\omega}{2\pi\sinh\omega\tau}\right)^{d/2} \exp\left\{-\frac{m\omega}{2}\left[(q^2 + q'^2)\coth\omega\tau - \frac{2qq'}{\sinh\omega\tau}\right]\right\}.$$
 (6.10)

¹If we couple charged particles to a magnetic field, then the Hamiltonian ceases to be real.

The strict positivity of these kernels is manifest. This positivity allows for a deep connection of Euclidean quantum mechanics (and field theory) to probability theory, see below. The object

$$P(\tau, q) = C \cdot K(\tau, q, 0) \tag{6.11}$$

maybe interpreted as *probability density* for a particle starting at 0 to show up at q after a time interval τ . The probability to end up anywhere should be one,

$$C \cdot \int dq \langle q, \tau | 0, 0 \rangle = C \cdot \int dq K(\tau, q, 0) = 1,$$
(6.12)

and this fixes the constant C. In particular, for the free particle

$$P_0(\tau, q) = \left(\frac{m}{2\pi\tau}\right)^{d/2} e^{-mq^2/2\tau}.$$
(6.13)

This is the probability density for the *Brownian motion* with diffusion coefficient D = 1/2m. It fulfils the same diffusion equation (6.6) as $U(\tau)$, in the present context called *master equation*.

Wightman functions

Of great interest in a relativistic quantum field theory are the *Wightman functions*. These are expectation values of product of field operators in the vacuum state. In quantum mechanics these are the expectation values

$$W^{(n)}(t_1, \dots, t_n) = \langle \Omega | \, \hat{q}(t_1) \cdots \hat{q}(t_n) | \Omega \rangle \,, \qquad \hat{q}(t) = e^{itH} \hat{q} \, e^{-itH}, \tag{6.14}$$

where $|\Omega\rangle$ denotes the ground state. We subtracted the groundstate energy from H such that $|\Omega\rangle$ has zero energy and H becomes a non-negative operator. The $W^{(n)}$ are not symmetric in their arguments, since the position operators at different times do not commute. We may analytically continue the $W^{(n)}$ to $z_i \rightarrow t_i - i\tau_i$,

$$W^{(n)}(z_1,\ldots,z_n) = \langle \Omega | \, \hat{q} e^{-i(z_1-z_2)H} \hat{q} e^{-i(z_2-z_3)H} \hat{q} \cdots \hat{q} \, e^{-i(z_{n-1}-z_n)H} \hat{q} | \Omega \rangle \,, \tag{6.15}$$

provided the imaginary parts of the complex time-differences obey the inequalities

$$\Im(z_k - z_{k+1}) \le 0.$$

In equation (6.15) we used that H annihilates the groundstate, $\exp(i\zeta H)|\Omega\rangle = 0$. From the definition of the z_i it follows that the $W^{(n)}$ are analytic in

$$\tau_1 > \tau_2 \ldots > \tau_n. \tag{6.16}$$

The Wightman functions for real times may be reconstructed as boundary values of the analytic Wightman functions with complex arguments,

$$W^{(n)}(t_1,\ldots,t_n) = \lim_{\substack{\Im z_i \to 0\\ \Im(z_{k+1}-z_k) > 0}} W^{(n)}(z_1,\ldots,z_n).$$
(6.17)

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For purely imaginary times the Wightman functions are called Schwinger functions,

$$S^{(n)}(\tau_1, \dots, \tau_2) = W^{(n)}(-i\tau_1, \dots, -i\tau_n)$$

= $\langle \Omega | \hat{q} e^{-(\tau_1 - \tau_2)H} \hat{q} e^{-(\tau_2 - \tau_3)H} \hat{q} \cdots \hat{q} e^{-(\tau_{n-1} - \tau_n)H} \hat{q} | \Omega \rangle.$ (6.18)

Let us calculate the 2-point Wightman- and Schwinger functions of the harmonic oscillator. The zero-point energy subtracted Hamiltonian reads

$$H = \omega a^{\dagger} a$$
,

where a and a^{\dagger} are the lowering and raising operators

$$q = \frac{1}{\sqrt{2m\omega}}(a^{\dagger} + a)$$
 and $p = i\sqrt{\frac{m\omega}{2}}(a^{\dagger} + a)$ with $[a, a^{\dagger}] = 1$.

By construction the ground state $|\Omega\rangle$ has zero energy and the first excited state $|1\rangle = a^{\dagger}|\Omega\rangle$ has energy $E_1 = \omega$. The two-point Wightman function only depends on $t_1 - t_2$ and reads

$$W^{(2)}(t_1 - t_2) = \langle \Omega | \hat{q}(t_1) \hat{q}(t_2) | \Omega \rangle = \frac{1}{2m\omega} \langle \Omega | (a + a^{\dagger}) e^{-i(t_1 - t_2)H} (a + a^{\dagger}) | \Omega \rangle$$
$$= \frac{1}{2m\omega} \langle a^{\dagger} \Omega | e^{-it\omega a^{\dagger}a} | a^{\dagger} \Omega \rangle = \frac{e^{-i\omega(t_1 - t_2)}}{2m\omega},$$
(6.19)

and the corresponding Schwinger function is

$$S^{(2)}(\tau_1 - \tau_2) = \frac{e^{-\omega(\tau_1 - \tau_2)}}{2m\omega}.$$
(6.20)

In quantum field theory the Schwinger functions are invariant under the Euclidean Lorentzgroup SO(4) which implies that they are symmetric in their arguments. This is not true in quantum mechanics.

6.2 The Euclidean Path Integral

In this section we turn to the path integral formulation of quantum mechanics with imaginary time. For that we recall, that the Trotter product formula (2.25) is obtained from the result (2.24) (which is used for the path integral representation for real times) by replacing *it* by τ . This is possible if the operators in this formula are bounded below. With the same arguments as we used for real times we can now prove the analog of (2.29) for an imaginary time. The only effect being that *i* ϵ is replaced by ϵ . Thus one finds

$$K(\tau, q, q') = \lim_{n \to \infty} \int dw_1 \cdots dw_{n-1} \left(\frac{m}{2\pi\hbar\epsilon}\right)^{n/2} \\ \cdot \exp\left\{-\frac{\epsilon}{\hbar} \sum_{j=0}^{j=n-1} \left[\frac{m}{2} \left(\frac{w_{j+1} - w_j}{\epsilon}\right)^2 + V(w_j)\right]\right\},$$
(6.21)

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where as before $w_0 = q'$ is the initial position and $w_n = q$ the final position.

The right hand side is identical to the *partition function* for a one-dimensional lattice system with sites labeled by the index j and with fixed boundary conditions. The action in the exponent couples nearest-neighbor variables w_j and w_{j+1} . The multiple integral is just a sum over all possible lattice configurations. In this language \hbar is to be interpreted as temperature of the system and the classical limit $\hbar \to 0$ corresponds to the low temperature limit of the lattice system.

In the limit $n \to \infty$ the right hand side is a path integral, but now with *Euclidean action*

$$S_E[w] = \int_0^\tau d\sigma \left(\frac{m}{2}\dot{w}^2 + V(w(\sigma))\right)$$
(6.22)

and real and positive density

$$K(\tau, q, q') = \int_{w(0)=q'}^{w(\tau)=q} \mathcal{D}w \ e^{-S_E[w]/\hbar}.$$
(6.23)

The kernels for the free particle and the harmonic oscillator are given in (6.9) and (6.10).

6.3 Semiclassical Approximation

Here we discuss the semiclassical approximation for the evolution kernel. The small- \hbar expansion of the Feynman path integral for real time is a stationary phase approximation whereas it is a saddle point approximation for imaginary time. We may recover the real-time kernel K(t) from the imaginary-time kernel $K(\tau)$ by an analytic continuation in time. Since the saddle point approximation is easier to handle then the stationary phase approximation we shall consider the Euclidean path integral in what follows.

6.3.1 Saddle point approximation for ordinary integrals

As a warm up we study the saddle-point approximation for *ordinary integrals*. Let us consider the one-dimensional integral

$$K = \int_{-\infty}^{\infty} dw \, e^{-\alpha S(w)}.$$
(6.24)

Here α replaces $1/\hbar$ in the path integral. We wish to find a good approximation to this integral in the limit $\alpha \to 0$. Let us assume that the function S in the exponent possesses a minimum at $w_{\rm cl}$. Then the main contribution to the integral comes from points near $w_{\rm cl}$. Expanding $S(w_{\rm cl} + \xi)$ about this minimum leads to

$$K = e^{-\alpha S(w_{\rm cl})} \int d\xi \, e^{-\frac{1}{2}\alpha S''(w_{\rm cl})\xi^2 - \alpha P(w_{\rm cl},\xi)},\tag{6.25}$$

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where $P = o(\xi^2)$ contains all higher order terms in the Taylor-expansion of S about its minimum. Let us estimate the *relative error* we make when we approximate K by

$$K_n = e^{-\alpha S(w_{\rm cl})} \int d\xi \, e^{-\frac{1}{2}\alpha S''(w_{\rm cl})\xi^2} \sum_{k=0}^n (-)^k \frac{\alpha^k}{k!} \, P(w_{\rm cl},\xi)^k.$$
(6.26)

We estimate the error relative to the quadratic approximation K_0 ,

$$\Delta_n K = \frac{K - K_n}{K_0} \equiv \int d\mu_\alpha(\xi) \left\{ e^{-\alpha P(\xi)} - \sum_{k=0}^n (-)^k \frac{\alpha^k}{k!} P(w_{\rm cl}, \xi)^k \right\},\tag{6.27}$$

where we have introduced the *probability measure* defined by the quadratic term in the Taylorexpansion of the function S in the exponent,

$$d\mu_{\alpha}(\xi) = \frac{1}{K_0} e^{-\alpha S''(w_{\rm cl})\xi^2/2} d\xi = \sqrt{\frac{\alpha S''}{2\pi}} e^{-\alpha S''\xi^2/2} d\xi.$$
(6.28)

On the right hand side we abbreviated $S'' = S''(w_{cl})$. The measure satisfies the scaling relation

$$d\mu_{\alpha}(\xi) = d\mu_1(\sqrt{\alpha}\xi). \tag{6.29}$$

We recall from the theory of Taylor series expansion, that for a C^{n+1} -function $f(\alpha)$ one has

$$f(\alpha) - \sum_{k=0}^{n} f^{(k)}(0) \frac{\alpha^{k}}{k!} = \frac{f^{(n+1)}(\eta)}{(n+1)!} \alpha^{n+1}$$
(6.30)

for some value η in the interval $[0, \alpha]$. Applied to the expression between the curly brackets in (6.27) we conclude that

$$\{\dots\} = \frac{(-\alpha)^{n+1}}{(n+1)!} P^{n+1} e^{-\eta P}, \quad \text{with} \quad 0 \le \eta \le \alpha.$$
 (6.31)

Without loss of generality we may assume that P is non-negative such that $\exp(-\eta P)$ is less or equal to one. Thus we can bound the relative error from above (6.27) as follows

$$|\Delta_{n-1}K| \le \frac{\alpha^n}{n!} \int d\mu_\alpha(\xi) P^n(w_{\rm cl},\xi).$$
(6.32)

To extract the α -dependence of this bound we use the scaling relation (6.29) which implies

$$|\Delta_{n-1}K| \le \frac{\alpha^n}{n!} \int d\mu_1(u) P^n\left(w_{\rm cl}, u/\sqrt{\alpha}\right).$$
(6.33)

Recall that $P(w_{cl}, \xi)$ contains the higher order terms in the Taylor expansion of S and is of order $O(\xi^3)$. From this we conclude that the relative error in (6.33) tends to zero for large values of the parameter α . For example, for a quartic function $P(\xi) = \lambda \xi^4$ the upper bound reads

$$|\Delta_{n-1}K| \le \frac{1}{n!} \left(\frac{\lambda}{\alpha}\right)^n \int d\mu_1(u) \, u^{4n} \tag{6.34}$$

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which, with the help of the integral formula

$$\int d\mu_1(u)u^{4n} = \sqrt{\frac{S''}{2\pi}} \int e^{-S''u^2/2} u^{4n} = \frac{(4n-1)!!}{(S'')^{2n}}$$

can be written in the form

$$|\Delta_{n-1}K| \le \left(\frac{\lambda}{\alpha}\right)^n \frac{(4n-1)!!}{n!} \frac{1}{(S'')^{2n}}.$$
(6.35)

We see that the saddle-point approximation becomes more accurate when the minimum is deep or the curvature at the minimum is large. Note that for a fixed α the error becomes arbitrarily big for $n \to \infty$. With increasing n the parameter α must increase (or λ decrease) for the saddle point approximation to be applicable.

Inserting the Taylor series

$$e^{-\alpha P} = \sum_{m=0}^{\infty} (-)^m \frac{\alpha^m}{m!} P^m$$

for a quartic $P(\xi)$ into the complete integral we obtain the perturbation series

$$\frac{K}{K_0} = \int d\mu_{\alpha}(w) \, e^{-\alpha P(w)} = 1 + \sum_{m=1}^{\infty} \frac{(-)^m}{(S'')^{2m}} \frac{(4m-1)!!}{m!} \left(\frac{\lambda}{\alpha}\right)^m \equiv \sum A_m.$$

It is easy to see that the quotients of two successive terms in this series grow with m,

$$\frac{A_{m+1}}{A_m} \xrightarrow{m \to \infty} -\frac{\lambda}{\alpha} \cdot \frac{16m}{(S'')^2}$$
(6.36)

which proves that the series has zero-radius of convergence. But from (6.35) it follows that it is still an *asymptotic series*: for given ϵ and n there exists an $\alpha(n)$ such that for all $\alpha > \alpha(n)$

$$\left|\frac{K}{K_0} - \sum_{m=0}^n A_m\right| < \epsilon.$$

Note that for a non-convergent asymptotic series $\alpha(n)$ depends on n, contrary to the situation for a convergent series. Asymptotic series is the best we can hope for in a perturbative expansion of the propagator². For the quartic function $S = w^2/2 + \lambda w^4$ with $w_{cl} = 0$ the exact integral (6.24) for $\alpha = 1$ is given by a modified Bessel function,

$$K = 2\sqrt{\kappa} e^{\kappa} K_{1/4}(\kappa), \quad \kappa = 1/32\lambda.$$
(6.37)

The saddle point approximations of order 3 is given by the polynomial

$$K_3 = \sqrt{2\pi} \left(1 - 3\lambda + 105\lambda^2/2 - 3465\lambda^3/2 \right)$$
(6.38)

The exact result together with the approximations K_1, K_2, K_3 are depicted in figure 6.1.

²there is a general argument due to Dyson which shows that perturbative expansion cannot be analytic at the point where the coupling constant vanishes.

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Figure 6.1: The integral K for a quartic function and its lowest saddle point approximations.

6.3.2 Saddle point approximation in Euclidean Quantum Mechanics

To find the semiclassical approximation to the kernel $K(\tau, q, q')$ we start with the path integral representation (6.23), where the potential may include a source term. Note that for imaginary time we can apply the saddle point approximation. For ordinary quantum mechanics with real time we would perform a stationary phase approximation instead.

As for the ordinary integrals we expand the classical action about an extremum, that is about a classical solution of the equation of motion

$$S'_E[w_{\rm cl}] = 0 \iff m\ddot{w}_{\rm cl} = V'(w_{\rm cl}),\tag{6.39}$$

subject to the boundary conditions

$$w(0) = q'$$
 and $w(\tau) = q.$ (6.40)

An arbitrary path $w(\sigma)$ is the sum of the classical path and a fluctuation $\xi(\sigma)$ and the Euclidean action has the expansion

$$S_E[w_{\rm cl} + \xi] = S_E[w_{\rm cl}] + \frac{1}{2}(\xi, S_E''(w_{\rm cl})\xi) + P[w_{\rm cl}, \xi],$$
(6.41)

where P contains all terms of cubic or higher orders

$$P[w_{\rm cl},\xi] = \frac{1}{3!} \int_0^\tau V'''(w_{\rm cl}(\sigma))\xi^3(\sigma) + \cdots, \qquad (6.42)$$

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and the fluctuation operator has the explicit form

$$S_E''(w_{\rm cl}) = -m\frac{d^2}{d\sigma^2} + V''(w_{\rm cl}(\sigma)).$$
(6.43)

Inserting these results into (6.23) yields

$$K(\tau, q, q') = \sqrt{\frac{m}{2\pi\hbar D(\tau)}} e^{-S_E[w_{\rm cl}]/\hbar} \int d\mu_{\hbar}(\xi) e^{-P[w_{\rm cl},\xi]/\hbar}, \tag{6.44}$$

where one integrates over all fluctuating paths starting at the origin and returning to this point after a time τ and the *D*-function in the first factor belongs to the fluctuation operator S''. As for the ordinary integrals we have introduced the Gaussian probability measure

$$d\mu_{\hbar}(\xi) = \frac{1}{K_0} e^{-(\xi, S_E''\xi)/2\hbar} \mathcal{D}\xi \quad \text{with} \quad K_0 = \int \mathcal{D}\xi \ e^{-(\xi, S_E''\xi)/2\hbar}. \tag{6.45}$$

The relative errors are bounded by

$$|\Delta_{n-1}K| = \left| \int d\mu_{\hbar} \left\{ e^{-P/\hbar} - \sum_{k=0}^{n-1} \frac{1}{k!} (-P/\hbar)^k \right\} \right| \le \frac{1}{n! \hbar^n} \int d\mu_{\hbar} P^n.$$
(6.46)

Note that the measure $d\mu_{\hbar}$ possesses the scaling property (6.29) with α replaced by $1/\hbar$. Using this property for the quartic function $P = \lambda \int \xi^4(\sigma) d\sigma$ one obtains

$$|\Delta_{n-1}K| \le \frac{\lambda^n \hbar^n}{n!} \int d\mu_1(\xi) \left(\int d\sigma \,\xi^4(\sigma) \right)^n.$$
(6.47)

Since the path integral is calculated with the Gaussian measure with $d\mu_1$ it is independent of \hbar . This shows that the relative error $\Delta_{n-1}K$ is of the order $O(\hbar^n)$ for a quartic P.

The first correction to the classical contribution $\exp(-S[w_{cl}]\hbar)$ coming from the quadratic fluctuation is called the semiclassical correction or *one-loop correction*. According to (6.44) the one-loop approximation to the evolution kernel consisting of the classical part and the one-loop correction is

$$K_0(\tau, q, q') = \sqrt{\frac{m}{2\pi\hbar D(\tau)}} e^{-S_E[w_{\rm cl}]/\hbar}.$$
(6.48)

The higher order terms can be computed systematically by calculating the corresponding moments of the Gaussian measure defined by the fluctuation operator.

To determine the function D appearing in the above expansions we first solve the classical equation of motion with given *initial position* q' and *initial momentum* p'. Next we differentiate the equation for the classical solution w_{cl} with respect to the initial momentum and obtain

$$m\frac{d^2}{d\sigma^2}\frac{dw_{\rm cl}}{dp'} = V''(w_{\rm cl})\frac{dw_{\rm cl}}{dp'}.$$
(6.49)

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For very short times the particles moves freely such that $w_{\rm cl}(\sigma) \sim q' + p'\sigma/m + O(\sigma^2)$ for small σ . We conclude that

$$m\frac{dw_{\rm cl}}{dp'}(0) = 0 \quad \text{and} \quad m\frac{d}{d\sigma}\frac{dw_{\rm cl}}{dp'}(0) = 1.$$
(6.50)

Since $m dw_{cl}/dp'$ obeys the same differential equation and the same initial condition as the *D*-function the two functions must be identical. It follows that the 1-loop approximation to the kernel can be written as

$$K(\tau, q, q') = \left(2\pi\hbar \frac{dw_{\rm cl}(\tau)}{dp(0)}\right)^{-1/2} e^{-S_E[w_{\rm cl}]/\hbar}.$$
(6.51)

This means that the correction to the classical result is given by the spread in the final position of the classical particle (area where a projective may land) in terms of the spread in the initial momentum (spread in the angle of projection). Thus, for artillery computation at least, it is an important quantity!

The result can further be simplified by noting that the variation of the action when one varies the end points is

$$\delta S = pq - p'q' + \int \left(-m\ddot{w} + V'(w)\right)\delta w.$$
(6.52)

For a classical trajectory the integral vanishes and we conluce that

$$\frac{\partial S_{\rm cl}}{\partial q'} = -p' = -p(0). \tag{6.53}$$

The variation of the initial momentum with respect to the final position is given by the second variation of the action of the classical trajectory (the Hamilton-Jacobi function) with respect to the two end points

$$K(\tau, q, q') = \frac{1}{\sqrt{2\pi\hbar}} \left(-\frac{\partial^2 S_{\rm cl}}{\partial q' \partial q} \right)^{1/2} e^{-S_E[w_{\rm cl}]/\hbar}.$$
(6.54)

This formula shows that it suffices to calculate the classical path for arbitrary endpoints q' and q to calculate the 1-loop approximation. According to (6.47) the 1-loop result deviates from the exact answer at most by the term $K_0 \int d\mu_1(\xi) P[w_{\rm cl}, \sqrt{\hbar} \xi]/\hbar$.

6.4 Functional Determinants

In this section we shall study more carefully determinants of second order differential operators we did encounter in section 3.3, that is of the fluctuation operators of the form

$$M = M_0 + U(s), \quad \text{where} \quad M_0 = \frac{d^2}{ds^2} + U_0 \quad \text{(real time)}$$
$$M = M_0 + U(\sigma), \quad \text{where} \quad M_0 = -\frac{d^2}{d\sigma^2} + U_0 \quad \text{(imag. time)}. \quad (6.55)$$

Here U_0 is either zero or a positive constant. The first determinant appears in ordinary quantum mechanics and the second in Euclidean quantum mechanics. Such determinant show up in many applications of path integrals and it is worth studying these objects in detail.

If λ_n and λ_n^0 are the eigenvalues of M and M_0 , respectively, then both the numerator and denominator in

$$\frac{\det M}{\det M_0} = \frac{\prod \lambda_n}{\prod \lambda_n^0} = \frac{\infty}{\infty}$$

are not well defined. Hence we consider the determinant of the ratio of these two operators and define

$$\det \frac{M}{M_0} := \prod \frac{\lambda_n}{\lambda_n^0},\tag{6.56}$$

which in quantum mechanics at least leads to a finite and well-defined result. For example, for the harmonic oscillator with frequency ω , the eigenvalues of the fluctuation operator on the time interval [0, t] or $[0, \tau]$ are

$$\lambda_n(\omega) = -\left(\frac{n\pi}{t}\right)^2 + \omega^2 \quad \text{or} \quad \lambda_n(\omega) = \left(\frac{n\pi}{\tau}\right)^2 + \omega^2$$
(6.57)

so that the infinite products (6.56), in which we skip the divergent factor with n = 0, are

real time:
$$\prod_{n \neq 0} \frac{\lambda_n(\omega)}{\lambda_n(0)} = \prod \left(1 - \left(\frac{\omega t}{n\pi}\right)^2 \right) = \frac{\sin(\omega t)}{\omega t}$$

imag. time:
$$\prod_{n \neq 0} \frac{\lambda_n(\omega)}{\lambda_n(0)} = \prod \left(1 + \left(\frac{\omega \tau}{n\pi}\right)^2 \right) = \frac{\sinh(\omega \tau)}{\omega \tau}.$$
 (6.58)

We *defined* the determinant of the operator M/M_0 as the product of the ratios of the eigenvalues. These seems to be reasonable for commuting operators M and M_0 which can be diagonalized simultaneously. For non-commuting operators it needs some further justification and this will be given below. In the remainder of this this section the explicit calculations are done for real time. The corresponding results for imaginary time are gotten by an analytic continuation.

Convergence of infinite products: Tor proceed we consider the one-parametric family of fluctuation operators

$$M_{\alpha} = M_0 + \alpha U(s), \quad \alpha \in [0, 1], \tag{6.59}$$

interpolating between the operator without potential M_0 and the operator of interest $M = M_1$. According to the *Feynman-Hellman formula* the variation of an eigenvalue $\lambda(\alpha)$ is given by

$$\frac{d}{d\alpha}\lambda_n(\alpha) = (\psi_n(\alpha), U\psi_n(\alpha)), \tag{6.60}$$

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where $\psi_n(\alpha)$ is a normalized eigenfunction of the fluctuation operator M_{α} with eigenvalue $\lambda_n(\alpha)$. We immediately obtain the inequality

$$\left|\frac{d}{d\alpha}\lambda_n(\alpha)\right| \le \Omega^2$$
, where $\Omega^2 = \max_{s\in[t',t]}|U(s)|.$ (6.61)

Integrating these inequality with respect to α from 0 to 1 yields the following two inequalities for the eigenvalues λ_n of M and the eigenvalues λ_n^0 of M_0 :

$$\lambda_n^0 - \Omega^2 \le \lambda_n \le \lambda_n^0 + \Omega^2. \tag{6.62}$$

For example, if we choose for M_0 the operator ∂^2 with eigenvalues $\lambda_n^0 = -(n\pi/t)^2$ then these inequalities yield the following upper and lower bounds for the infinite product,

$$\frac{1}{\Omega t}\sin(\Omega t) \le \prod \frac{\lambda_n}{\lambda_n^0} \le \frac{1}{\Omega t}\sinh(\Omega t),\tag{6.63}$$

where one of the inequalities becomes an equality for constant potentials. In particular we see that the infinite products are always convergent. Actually, one can prove a stronger statement, namely that for any *square-integrable potential*

$$\lambda_n - \lambda_n^0 = \frac{1}{t} \int_{t'}^t ds \ U(s) + r_n$$

holds true, where the sum of the r_n^2 exists. This inequality guarantees that the infinite product in (6.56) converges.

From infinite products to determinants and traces: Now we wish to show that

$$\prod \frac{\lambda_n}{\lambda_n^0} = \det \left(1 + U M_0^{-1} \right) \tag{6.64}$$

can be defined in terms of the spectrum of the operator UM_0^{-1} alone and that the definition agrees with the previous one. This statement is not empty, since for non-commuting M and M_0 their eigenfunctions may be rather different.

The operator $A = UM_0^{-1}$ of interest is a socalled *trace class operator*. These are operators with the property that tr |A| is finite, where |A| is the positive square root of $A^{\dagger}A$. Trace-class operators are compact and possess a discrete spectrum $\{\mu_1 \ge \mu_2, \ldots\}$ and a representation

$$A\phi_n = \mu_n \phi_n + \sum_{m=1}^{n-1} \alpha_{nm} \phi_m, \qquad (\phi_n, \phi_m) = \delta_{mn}.$$
 (6.65)

In the adapted basis $\{\phi_n\}$ a compact operator is represented by a triangular matrix with eigenvalues on the diagonal. Now one defines the determinant of 1 + A similarly as for matrices as the product of the eigenvalues

$$\det(1+A) = \prod (1+\mu_n).$$
 (6.66)

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The sum of the eigenvalues of a trace-class operator is absolute convergent [24]

$$\sum |\mu_n| \leq \operatorname{tr} |A|$$

It follows at once that the determinant of a trace-class operator is always finite and can easily be bounded above as follows

$$\det(1+A) = \prod(1+\mu_n) \le \exp\left(\sum |\mu_n|\right) \le e^{\operatorname{tr}|A|}.$$
(6.67)

We see that for a trace-class operator the infinite product (6.66) is always absolute convergent³. From the definition of the determinant and the spectral decomposition (6.65) it is clear that

$$\log \det(1+A) = \operatorname{tr} \log(1+A).$$
 (6.68)

This formula will play an important role when we discuss the quantization of fermions in external fields or the one-loop effective actions for bosons.

Next we determine the variation of det(1 + A) if A is slightly perturbed by a trace class operator ϵB . Without loss of generality we may assume that the perturbed operator is sufficiently small so that we may expand as follows

$$\log \det(1 + A + \epsilon B) = \operatorname{tr} \log(1 + A + \epsilon B)$$
$$= \operatorname{tr} \left[(A + \epsilon B) - \frac{1}{2} (A + \epsilon B)^2 + \cdots \right]$$
$$= \operatorname{tr} \left[\log(1 + A) + \epsilon (1 + A)^{-1} B + O(\epsilon^2) \right].$$

Thus we have shown that

$$\frac{d}{d\epsilon}\log\det(1+A+\epsilon B)|_{\epsilon=0} = \operatorname{tr}(1+A)^{-1}B.$$
(6.69)

Now its easy to prove the *product rule* applies to the determinant of two operators,

$$\det \{ (1+A)(1+B) \} = \det(1+A) \det(1+B), \tag{6.70}$$

which holds true for two trace-class operators A and B. To prove this product rule we multiply A with a deformation parameter α and show that the α -derivatives of the logarithm of both sides in (6.70) are the same.

After these general remarks let us now prove the identity (6.64). Again we introduce a deformation parameter such that $M = M_0 + \alpha U$ and compute the α -derivative of the logarithm of the determinant appearing on the right hand side of (6.64). Using the identity (6.69) with

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³More generally one can prove the following useful theorem: If for any k > 0 the series $\sum \mu_n$, $\sum \mu_n^2$, $\sum \mu_n^{k-1}$ and $\sum |\mu_n|^k$ are convergent, then the infinite product $\prod (1 + \mu_n)$ is convergent as well.

 $A = UM_0^{-1}$ and the cyclicity of the trace (which holds for a trace-class and a bounded operator) one sees at once that

$$\frac{d}{d\alpha}\log\det\left(1+\alpha UM_0^{-1}\right) = \operatorname{tr} UM^{-1}.$$
(6.71)

On the other hand, using again the Feynman-Hellman formula one can compute the variation of the logarithm of the infinite product in (6.64) directly as follows:

$$\frac{d}{d\alpha} \sum \log \frac{\lambda_n(\alpha)}{\lambda_n^0} = \sum \frac{(\psi_n, U\psi_n)}{\lambda_n} = \operatorname{tr} U M^{-1}.$$
(6.72)

Comparing (6.71) with (6.72) we see that both sides of (6.64) possess the same α -derivative. Since they are equal for $\alpha = 0$ they must be equal for $\alpha = 1$ and this proves (6.64) as required.

6.4.1 Calculating determinants

Let us now compute the functional determinants (6.64). We shall use the identity (6.71) and compute the trace on the right hand side explicitly. To that end we introduce two fundamental solutions C(s) and D(s) of

$$MC(s) = MD(s) = 0, \quad M = M_0 + \alpha U,$$
 (6.73)

subject to the initial conditions

$$C(t') = \dot{D}(t') = 1$$
 and $\dot{C}(t') = D(t') = 0,$ (6.74)

so that their time-independent Wronskian is

$$W(C,D) = C\dot{D} - \dot{C}D = 1.$$
 (6.75)

In terms of these fundamental solutions the Dirichlet Greenfunction for M reads for s < s':

$$G_D(s,s') = \frac{C(t)}{D(t)} D(s') D(s) - C(s') D(s).$$
(6.76)

With this explicit expression for the Green function we can now calculate the trace in (6.71),

$$\operatorname{tr} UM^{-1} = \int_{t'}^{t} G_D(s,s)U(s) = \frac{C(t)}{D(t)} \int_{t'}^{t} D^2(s)U(s) - \int_{t'}^{t} C(s)D(s)U(s).$$
(6.77)

Let us finally define the function

$$W(t,t') = D(t) \operatorname{tr} U M^{-1}.$$
(6.78)

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It depends on the initial time t' as well, but here we are interested in its dependence on the final time t and on α . By using (6.73) together with (6.75) one finds that W obeys the differential equation

$$(MW)(s) = -U(s)D(s),$$
 (6.79)

where the fluctuation operator M acts on s. On the other hand, when differentiating (6.74) with respect to α (recall that $M = M_0 + \alpha U$) on obtains

$$M \partial_{\alpha} D(s, t') = -U(s)D(s, t') \tag{6.80}$$

which shows that W(t) and $\partial_{\alpha}D(t)$ are solutions of the same differential equation. Finally it follows from the initial conditions (6.74) and from the representation (6.77,6.78) that both functions and their first derivatives vanish at t = t' and thus we have

$$W(t) = \partial_{\alpha} D(t). \tag{6.81}$$

Integrating the identity (6.72) from $\alpha = 0$ to $\alpha = 1$ and noting that the infinite product is one for $\alpha = 0$ finally yields

$$\log \prod \frac{\lambda_n}{\lambda_n^0} = \log D(t) - \log D_0(t), \tag{6.82}$$

where D is the D-function of $M = M_0 + U$ and D_0 that of M_0 . Hence we end up with the explicit result

$$\det \frac{M}{M_0} = \prod \frac{\lambda_n}{\lambda_n^0} = \frac{D(t)}{D_0(t)},\tag{6.83}$$

for the functional determinants appearing in the path integrals. Nowhere did we assume that M_0 is the free fluctuation operator such that the above formula holds true if U_0 in $M_0 = \partial^2 + U_0(t)$ is time-dependent.

We could have anticipated (6.83) by noting that

$$\det \frac{M_0 + \alpha U}{M_0}$$

is an analytic function of α with simple zeros at values of α for which one of the eigenvalues $\lambda_n(\alpha)$ vanishes. For these α the function $D_{\alpha}(s)$ vanishes at t and is proportional to the corresponding eigenfunction. Hence, the infinite product and the analytic function $D_{\alpha}(t)$ share the same zeros. Clearly, since for $\alpha = 0$ the determinant is one, we must divide D_{α} by the α -independent D_0 , but this normalization does not remove or add zeros/poles. According to a theorem by Weierstrass the quotient $D_{\alpha}(t)/D_0(t)$ must then be an analytic function $\exp(f(\alpha))$

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without zeros times the determinant. Finally from the asymptotic growth of the zeros of D_{α} one can deduce that $f(\alpha) = 0$ and this proves (6.83).

What we have shown then is that the kernel (3.62) is given by

$$K(t,q,t',q') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}} \left(\frac{D_0(t,t')}{D(t,t')}\right)^{1/2} e^{iS[w_{\rm cl}]/\hbar},$$
(6.84)

where $D_0(s, t')$ and D(s, t') are the Gelfand-Yaglom *D*-functions belonging *M* and *M*₀. They fulfill the initial conditions

$$D(t',t') = D_0(t',t') = 0$$
 and $\frac{\partial D(s,t')}{\partial s}\Big|_{s=t'} = \frac{\partial D_0(s,t')}{\partial s}\Big|_{s=t'} = 1.$ (6.85)

For the free particle $D_0(s) = (s - t')$ and its only role in (6.84) is to chancel the t - t' in the square root. We thus recover our result for the kernel of the oscillator with time dependent force in (3.21).

6.4.2 Generalizing the result of Gelfand and Yaglom

For a quantum mechanical system with several degrees of freedom is the fluctuation operator M a matrix differential operator,

$$M = -\mathbb{1}\frac{d^2}{ds^2} + P(s)\frac{d}{ds} + Q(s),$$
(6.86)

with matrix-functions P and Q. Following KIRSTEN and MCKANE in [19] we convert the second order fluctuation problem

$$\ddot{\boldsymbol{\xi}} = P\dot{\boldsymbol{\xi}} + Q\boldsymbol{\xi} \tag{6.87}$$

into the equivalent first order problem

$$\frac{d}{ds}\begin{pmatrix}\boldsymbol{\xi}\\ \dot{\boldsymbol{\xi}}\end{pmatrix} = K\begin{pmatrix}\boldsymbol{\xi}\\ \dot{\boldsymbol{\xi}}\end{pmatrix}, \quad K = \begin{pmatrix}0 & 1\\Q & P\end{pmatrix}.$$
(6.88)

There are interesting applications where one needs the determinant of M not only for Dirichlet boundary conditions but for periodic, Neumann- or general Robin boundary conditions. The most general linear boundary conditions can be written as

$$B_L\begin{pmatrix}\boldsymbol{\xi}\\\dot{\boldsymbol{\xi}}\end{pmatrix}(t') + B_R\begin{pmatrix}\boldsymbol{\xi}\\\dot{\boldsymbol{\xi}}\end{pmatrix}(t) = 0$$
(6.89)

with 'boundary operators' B_L and B_R . For Dirichlet boundary conditions at t' and t we have

$$B_L = \begin{pmatrix} \mathbb{1} & 0\\ 0 & 0 \end{pmatrix} \quad \text{and} \quad B_R = \begin{pmatrix} 0 & 0\\ \mathbb{1} & 0 \end{pmatrix}.$$
(6.90)

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To calculate the determinant of the fluctuation operator M one solves the *initial value problem*

$$\frac{d}{ds}\boldsymbol{\psi} = K\boldsymbol{\psi}, \quad \boldsymbol{\psi}(t') = \mathbb{1}.$$
(6.91)

The columns of the matrix $\psi(s)$ form a complete set of linearly independent solutions of the first order differential equation (6.88): any solution of this equation must be a linear combination of the columns of ψ . Let us assume that the determinant of

$$B_L \boldsymbol{\psi}(t') + B_R \boldsymbol{\psi}(t) \stackrel{(6.91)}{=} B_L + B_R \boldsymbol{\psi}(t)$$

vanishes. Then there exists a linear combination of the columns of ψ which satisfies the boundary condition (6.89). This linear combination gives rise a solution of the second order fluctuation problem (6.87) fulfilling the boundary conditions. This means that det(M) vanishes when the determinant of $B_L + B_R \psi(t)$ vanishes. Since the converse statement holds as well, it is not surprising that the ratio of two fluctuation determinants is given by [19]

$$\frac{\det M_1}{\det M_2} = \frac{\det(-\partial^2 + P_1\partial + Q_1)}{\det(-\partial^2 + P_2\partial + Q_2)} = \frac{\det(B_L + B_R\psi_1(t))}{\det(B_L + B_R\psi_2(t))}.$$
(6.92)

For one degree of freedom and Dirichlet boundary condition with boundary operators (6.90) one recovers the original Gelfand-Yaglom formula for the ratio of functional determinants.

Zeta-function determinants

Finally we introduce another representation for determinants which is popular in field theory, namely the *zeta-function* definition of determinants. The zeta-function of a (elliptic) selfadjoint M is defined as

$$\zeta_M(s) = \sum \lambda_n^{-s} = -\frac{1}{\Gamma(s)} \int dt \, t^{s-1} \sum e^{-t\lambda_n} = -\frac{1}{\Gamma(s)} \int dt \, t^{s-1} \mathrm{tr} \, e^{-tM}, \tag{6.93}$$

where $\Gamma(s)$ is the Riemann zeta-function. From the bounds (6.62) one infers that the difference

$$\zeta_M(s) - \zeta_{M_0}(s) = -s \sum \log \frac{\lambda_n}{\lambda_n^0} + O(s^2)$$

is analytic at the origin and that its derivative at his point is related to the determinant of M/M_0 as follows:

$$\log \det \frac{M}{M_0} = -\{\zeta'_M(0) - \zeta'_{M_0}(0)\}.$$
(6.94)

The advantage of this representation is that one only needs to know the derivative of the zeta function at s = 0 to compute the determinants of interest. In addition, the zeta-function defined determinants have some nice properties. In particular they respect a local gauge symmetry. Later we shall see that in certain field theoretical models (e.g. the massless Schwinger model) the value $\zeta'_M(0)$ can be calculated explicitly.

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