Chapter 8

Path Integrals in Statistical Mechanics

The Feynman path integral formulation reveals a deep and fruitful interrelation between quantum mechanics and statistical mechanics. The discretized Euclidean path integrals can be viewed as partition functions for particular lattice spinmodels. Vice versa, the partition function in statistical mechanics is given by a particular path integral with imaginary time. This unified view of quantum and statistical mechanics allows us to apply many powerful methods known in statistical mechanics to calculate correlation functions in Euclidean quantum mechanics.

8.1 Thermodynamic Partition Function

In this section we derive a path integral representation for the canonical partition function belonging to a time-independent Hamiltonian $\hat{H}$. With our previous result in (6.23) we arrived at the following Euclidean path integral representation for the kernel of the 'evolution operator'

$$K(\tau, q, q') = \langle q|\, e^{-\tau \hat{H}/\hbar}|q'\rangle = \int\limits_{w(0)=q'}^{w(\tau)=q} \mathcal{D}w \; e^{-S_E[w]/\hbar}. \tag{8.1}$$

Here one integrates over all paths starting at q' and ending at q. For imaginary times the integrand is real and positive and contains the Euclidean action S_E. Clearly, the object

$$\int dq K(\tau, q, q) = \mathrm{tr}\, e^{-\tau\hat{H}/\hbar} \tag{8.2}$$

is just the quantum *partition function* for temperature $k_B T = \hbar/\tau$. We conclude that the partition function $Z(\beta)$ and *free energy* $F(\beta)$ at inverse temperature[1] $\beta = 1/T$ are given by

$$Z(\beta) = e^{-\beta F(\beta)} = \mathrm{tr}\, e^{-\beta\hat{H}} = \int dq\, K(\hbar\beta, q, q). \tag{8.3}$$

[1]We set $k_B = 1$.

Note that setting $q = q'$ in the last term means that we integrate over periodic paths starting and ending at q in (8.1). Integrating over q is then equivalent to integrating over *all periodic paths* with period $\hbar\beta$. Thus we end up with

$$Z(\beta) = \oint_{w(0)=w(\hbar\beta)} \mathcal{D}w \, e^{-S_E[w]/\hbar} . \tag{8.4}$$

For example, for the Euclidean harmonic oscillator with evolution kernel (6.10)) we have

$$K(\hbar\beta, q, q) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\hbar\omega\beta)}} \exp\left\{-\frac{2m\omega q^2}{\hbar}\frac{\sinh^2(\hbar\omega\beta/2)}{\sin(\hbar\omega\beta)}\right\}, \tag{8.5}$$

so that the partition function takes the form

$$Z(\beta) = \frac{1}{2\sinh(\hbar\omega\beta/2)} = \frac{e^{-\hbar\omega\beta/2}}{1 - e^{-\hbar\omega\beta}} = e^{-\hbar\omega\beta/2}\sum_{n=0}^{\infty} e^{-n\hbar\omega\beta}. \tag{8.6}$$

For a Hamiltonian with discrete energies E_n the partition function has the spectral resolution

$$Z(\beta) = \mathrm{tr}\, e^{-\beta\hat{H}} = \sum_n \langle n|\, e^{-\beta\hat{H}}|n\rangle = \sum_n e^{-\beta E_n}, \tag{8.7}$$

where as orthonormal states $|n\rangle$ we used the eigenfunction of $\hat{H}$. A comparison with equation (8.6) immediately yields the energies of the harmonic oscillator with circular frequency ω,

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \qquad n \in \mathbb{N}. \tag{8.8}$$

For low temperature $\beta \to \infty$ the spectral sum (8.7) is dominated by the contribution of lowest energy such that the free energy will tend to the ground state energy,

$$F(\beta) = -\frac{1}{\beta}\log Z(\beta) \overset{\beta\to\infty}{\longrightarrow} E_0. \tag{8.9}$$

To perform the high-temperature limit is more tricky. We shall investigate this limit later in this lecture. In applications one is also interested in the energies and wave functions of the excited states. Now we shall discuss a method to extract these quantities from the path integral.

8.2 Thermal Correlation Functions

The low lying energies of the Hamiltonian operator $\hat{H}$ can be extracted from the *thermal correlation functions*. These are the expectation values of products of position operators

$$\hat{q}_E(\tau) = e^{\tau\hat{H}/\hbar}\hat{q}\, e^{-\tau\hat{H}/\hbar}, \qquad \hat{q}_E(0) = \hat{q}(0), \tag{8.10}$$

at different imaginary times in the equilibrium state at inverse temperature β,

$$\langle \hat{q}_E(\tau_1)\cdots\hat{q}_E(\tau_n)\rangle_\beta \equiv \frac{1}{Z(\beta)}\,\mathrm{tr}\, e^{-\beta\hat{H}}\hat{q}_E(\tau_1)\cdots\hat{q}_E(\tau_n). \tag{8.11}$$

The normalizing factor in the denominator is the partition function (8.4). At temperature zero these correlation functions are just the *Schwinger functions* we introduced in section 6.1.

The *gap* between the energies of the ground state and first excited state can be extracted from the thermal 2-point function

$$\begin{aligned}\langle \hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_\beta &= \frac{1}{Z(\beta)}\mathrm{tr}\; e^{-\beta\hat{H}}\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\\ &= \frac{1}{Z(\beta)}\mathrm{tr}\; e^{-(\hbar\beta-\tau_1)\hat{H}/\hbar}\hat{q}\,e^{-(\tau_1-\tau_2)\hat{H}/\hbar}\hat{q}\,e^{-\tau_2\hat{H}/\hbar}\end{aligned} \tag{8.12}$$

as follows: we calculate the trace with the orthonormal energy eigenstates $|n\rangle$ and insert the identity $\sum|m\rangle\langle m|$ after the first position operator. Denoting the energy of $|n\rangle$ by E_n we obtain the following double sum for the thermal 2-point function:

$$\langle\ldots\rangle_\beta = \frac{1}{Z(\beta)}\sum_{n,m} e^{-(\hbar\beta-\tau_1+\tau_2)E_n/\hbar}e^{-(\tau_1-\tau_2)E_m/\hbar}\,\langle n|\,\hat{q}|m\rangle\,\langle m|\,\hat{q}|n\rangle\,. \tag{8.13}$$

Now we consider the low-temperature limit of this expression. For $\beta\to\infty$ the terms containing the energies $E_{n>0}$ of the excited states are exponentially damped and we conclude

$$\lim_{\beta\to\infty}\langle \hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_\beta = \sum_{m\geq 0} e^{-(\tau_1-\tau_2)(E_m-E_0)/\hbar}\,|\,\langle\Omega|\,\hat{q}|m\rangle\,|^2. \tag{8.14}$$

Note that the term $\exp(-\beta E_0)$ chancels against the low temperatur limit of the partition function in the denominator. At low temperature the thermal expectation values tend to the ground state expectation values,

$$\lim_{\beta\to\infty}\langle \hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_\beta = \langle\Omega|\,\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)|\Omega\rangle \tag{8.15}$$

This just expresses the fact that thermal fluctuations freeze out at low temperature. Thermal expectation values become vacuum expectation values at absolute zero. In particular the 1-point function has this property,

$$\lim_{\beta\to\infty}\langle \hat{q}_E(\tau)\rangle_\beta = \langle\Omega|\,\hat{q}|\Omega\rangle\,. \tag{8.16}$$

At this point it is convenient to introduce the *connected thermal* 2*-point function*,

$$\langle \hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_{c,\beta} = \langle \hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_\beta - \langle \hat{q}_E(\tau_1)\rangle\langle \hat{q}_E(\tau_2)\rangle_\beta\,. \tag{8.17}$$

It characterizes the correlations of the differences $\Delta\hat{q}_E = \hat{q}_E - \langle\hat{q}_E\rangle$ at different times,

$$\langle\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_{c,\beta} = \langle\Delta\hat{q}_E(\tau_1)\,\Delta\hat{q}_E(\tau_2)\rangle_\beta\,. \tag{8.18}$$

The connected correlator is exponentially damped for large $|\tau_1-\tau_2|$ since the term with $m=0$ in (8.14) is missing in the spectral resolution for the connected 2-point function,

$$\lim_{\beta\to\infty}\langle\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_{c,\beta} = \sum_{m>0} e^{-(\tau_1-\tau_2)(E_m-E_0)/\hbar}|\,\langle\Omega|\,\hat{q}|m\rangle\,|^2. \tag{8.19}$$

For large (imaginary) time-differences $\tau_1-\tau_2$ it reduces to

$$\lim_{\tau_1-\tau_2\to\infty}\lim_{\beta\to\infty}\langle\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_{c,\beta} = e^{-(E_1-E_0)(\tau_1-\tau_2)/\hbar}|\,\langle\Omega|\,\hat{q}|1\rangle\,|^2, \tag{8.20}$$

and thus one can extract the energy-gap E_1-E_0 and modulus of the matrix element $\langle\Omega|\,\hat{q}|1\rangle$ from the large-time behavior of the connected 2-point function.

To find the path-integral representation for the thermal correlators we proceed similarly as in section 2.4. To calculate the two-point function (8.12) we insert the identity $\mathbb{1}=\int du|u\rangle|u\rangle$ after the two position operators $\hat{q}$ in

$$Z(\beta)\cdot\langle\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_\beta = \int dq\,\langle q|\,e^{-\beta H}\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)|q\rangle\,, \tag{8.21}$$

and in terms of the kernel $K(\tau,u,v)$ for the imaginary time evolution we obtain for the integrand in (8.21) the expression

$$\langle q|\ldots|q\rangle = \int dvdu\,\langle q|\,K(\hbar\beta-\tau_1)|v\rangle v\,\langle v|\,K(\tau_1-\tau_2)|u\rangle\,u\,\langle u|\,K(\tau_2)|q\rangle\,.$$

Now we use the path-integral representation for each evolution kernel separately, similarly as we did for the Greensfunctions in section 2.4. Then the path-integral representation of the is evident: First we sum over all path from q to u in time τ_2 and then multiply with the position u of the particle at time τ_2. Next we sum over all path from u to v in time $\tau_1-\tau_2$ and multiply with the position v of the particle at time τ_1. Finally we sum over all path from v to q in time $\hbar\beta-\tau_1$. The integration over the intermediate positions u and v just means that we must sum over all paths, not only over those which have positions u and v at times τ_2 and τ_1, and include a factor $q(\tau_1)q(\tau_2)$ in the integrand. Since the total traveling time of the particle is $\hbar\beta$, we obtain the representation

$$\langle q|\,e^{-\beta\hat{H}}\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)|q\rangle = \int\limits_{w(0)=q}^{w(\hbar\beta)=q}\mathcal{D}w\,e^{-S_E[w]/\hbar}w(\tau_1)w(\tau_2),\quad \tau_1>\tau_2, \tag{8.22}$$

for the kernel of the thermal 2-point function. Clearly, to get the trace in (8.12) we must integrate over q and then divide by $Z(\beta)$ (whose path-integral representation we derived earlier).

Integrating over q means that we integrate over *all periodic paths* with period $\hbar\beta$. When we applied the Trotter product formula we have assumed that τ_1 is bigger than τ_2. The path integral representations for the higher 'time ordered' thermal correlation functions is now evident,

$$\langle \mathbf{T}\, \hat{q}_E(\tau_1)\cdots\hat{q}_E(\tau_n)\rangle_\beta = \frac{1}{Z(\beta)} \oint\limits_{w(0)=w(\hbar\beta)} \mathcal{D}w\, e^{-S_E[w]/\hbar} w(\tau_1)\cdots w(\tau_n). \tag{8.23}$$

These correlators are generated by

$$K(\hbar\beta, q, q'; j) = \int\limits_{w(0)=q'}^{w(\hbar\beta)=q} \mathcal{D}w\; e^{-S_{Ej}[w]/\hbar}, \quad S_{Ej}[w] = S_E[w] - (j, w). \tag{8.24}$$

or the corresponding generating functional, which is just the partition function in the presence of an external source $j(\tau)$,

$$Z[\beta, j] = \int dq K(\hbar\beta, q, q; j) = \oint\limits_{w(0)=w(\hbar\beta)} \mathcal{D}w\, e^{-S_{Ej}[w]/\hbar} \tag{8.25}$$

by differentiating with respect to the source. The source term (j, w) in (8.24) is the scalar product on $L_2[0, \hbar\beta]$. Note that $Z(\beta, 0) = Z(\beta)$ is the previously introduced partition function without source. For example, the thermal two-point function is

$$\langle \mathbf{T}\, \hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_\beta = \frac{1}{Z(\beta,0)} \frac{\hbar^2\delta^2}{\delta j(t_1)\delta j(t_2)}\, Z[\beta, j]|_{j=0}, \tag{8.26}$$

where $\mathbf{T}$ denotes the time ordering.

The *connected* correlation functions are generated by the *finite-temperature Schwinger functional*. It is proportional to the logarithm of the partition function and hence proportional to the free energy with external source,

$$\log Z(\beta, j) = W[\beta, j]/\hbar = -\beta F[\beta, j]. \tag{8.27}$$

In many cases the source is just the applied magnetic field. The *connected correlation functions* are gotten by functionally differentiating $W[\beta, j]$ several times with respect to the source,

$$\langle \mathbf{T}\, \hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\cdots\hat{q}_E(\tau_n)\rangle_{c,\beta} = \frac{\hbar^{n-1}\delta^n}{\delta j(\tau_1)\cdots\delta j(\tau_n)}\, W[\beta, j]|_{j=0}. \tag{8.28}$$

Thermal Schwinger functional for the Oscillator

Let us compute the finite temperature Schwinger functional for the oscillator. We shall calculate the path integral with Euclidian action and additional source term, that is for

$$S_{Ej}[w] = \frac{m}{2}\int\limits_0^{\hbar\beta} d\tau \left\{\dot{w}^2(\tau) + \omega^2(\tau)w^2(\tau)\right\} - \int\limits_0^{\hbar\beta} d\tau j(\tau)w(\tau). \tag{8.29}$$

For later use we allow for a time-dependent frequency. We proceed similarly as in section 3.2 where we calculated the propagator for the driven oscillator. Not to repeat ourselves we just recall the key ideas and point out the main differences as compared to the previous calculation. First one splits w into the classical path $w_{\rm cl}$ from q' to q and the fluctuation $\xi(\tau)$ which vanishes at the endpoints. The classical path is determined by the inhomogeneous equation of motion

$$S''w_{\rm cl}(\tau)=j(\tau),\quad S''=-m\frac{d^2}{d\tau^2}+m\omega^2(\tau),\tag{8.30}$$

and the boundary conditions $w_{\rm cl}(0)=q'$ and $w_{\rm cl}(\hbar\beta)=q$. Expanding the action S_{Ej} about the dominant classical path yields

$$K(\hbar\beta,q,q';j)=e^{-S_{Ej}[w_{\rm cl}]/\hbar}\,K(\hbar\beta,0,0)=e^{-S_{Ej}[w_{\rm cl}]/\hbar}\sqrt{\frac{m}{2\pi\hbar D(\hbar\beta)}},\tag{8.31}$$

where $K(\hbar\beta,0,0)$ is the propagator for the propagation without source from 0 to 0. The D-function solves $S''D=0$ with initial conditions $D(0)=0$ and $\dot D(0)=1$. This formula is just the Euclidean version of the result (3.32). Again we decompose the classical trajectory in two parts,

$$w_{\rm cl}(\tau)=w_h(\tau)+\int_0^{\hbar\beta}G_D(\tau,\sigma)j(\sigma)d\sigma,\tag{8.32}$$

where w_h is the classical path from $q'\to q$ *without* external source and $G_D(\tau,\sigma)$ is the symmetric Dirichlet Greenfunction of the fluctuation operator S''. The second term on the right hand side vanishes at initial and final times and solves the equation of motion with source. Using this information the action of $w_{\rm cl}$ can be rewritten as

$$S_{Ej}[w_{\rm cl}]=S_E[w_h]-(j,w_{\rm h})-\frac{1}{2}\,(j,G_Dj)\,.\tag{8.33}$$

Now we insert this decomposition into (8.31). The term $S_E[w_h]$ converts the source-free propagator for the propagation from $0\to0$ in (8.31) into the source-free propagator for propagation from q' to q such that

$$K(\hbar\beta,q,q';j)=K(\hbar\beta,q,q')\cdot\exp\left\{(j,G_Dj)/2\hbar+(j,w_h)/\hbar\right\}.\tag{8.34}$$

In order to obtain the partition function we must set $q'=q$ and integrate over q. To do the integration we need the explicit q-dependence of the action $S_{Ej}[w_{\rm cl}]$ in (8.33). To that aim we introduce a particular solution $\phi(\tau)$ of the homogeneous equation of motion,

$$S''\phi=0\quad\text{and}\quad\phi(0)=\phi(\hbar\beta)=1.\tag{8.35}$$

The classical solution w_h from $q\to q$ in the decomposition (8.32) is just $w_h(\tau)=q\phi(\tau)$. Using the equation of motion and boundary conditions for ϕ the position dependent contributions to S_{Ej} in (8.33) can be isolated,

$$S_{Ej}[w_{\rm cl}]=\frac{1}{2}m_\beta\,q^2-q(j,\phi)-\frac{1}{2}(j,G_Dj),\tag{8.36}$$

where we introduced the source and position-independent function

$$m_\beta = m\dot{\phi}(\hbar\beta) - m\dot{\phi}(0). \tag{8.37}$$

We see that the resulting propagator $K(\hbar\beta, q, q; j)$ is a Gaussian function of q. Integrating over q we obtain the partition function in the presence of an source

$$Z[\beta, j] = Z(\beta)\, e^{W[\beta,j]/\hbar} \tag{8.38}$$

where $Z(\beta)$ is the partition function of the oscillator,

$$Z(\beta) = \sqrt{\frac{2\pi}{m_\beta}}\, K(\hbar\beta, 0, 0) \tag{8.39}$$

and W the its finite temperature Schwinger functional,

$$W[\beta, j] = \frac{1}{2}(j, G_P j), \quad \text{where} \quad G_P(\tau, \sigma) = \frac{\phi(\tau)\phi(\sigma)}{m_\beta} + G_D(\tau, \sigma). \tag{8.40}$$

Actually G_P is just the Greenfunction of S'' for periodic boundary conditions. The term proportional to $\phi(\tau)\phi(\sigma)$ in (8.40) converse the Dirichlet Greenfunction into the periodic Greenfunction. This fact is proven in the appendix to the present chapter.

To compute th connected 2-point function at finite temperature we differentiate $W[\beta, j]$ twice with respect to the source and then set the source to zero. We obtain

$$\langle\, \mathbf{T}\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_{c,\beta} = G_P(\tau_1, \tau_2). \tag{8.41}$$

Note that the partition function $Z(\beta)$ does not enter the result for the connected correlation function. For the oscillator with constant frequency the periodic Greenfunction reads

$$G_P(\tau, \sigma) = \frac{1}{2m\omega} \frac{\cosh(\omega|\tau - \sigma| - \hbar\omega\beta/2)}{\sinh(\hbar\omega\beta/2)} \tag{8.42}$$

and one obtains the following thermal two-point function

$$\langle\, \mathbf{T}\hat{q}_E(\tau_1)\hat{q}_E(\tau_2)\rangle_\beta = \hbar G_P(\tau_1, \tau_2) \stackrel{\beta\to\infty}{\longrightarrow} \frac{\hbar}{2m\omega}\, e^{-\omega|\tau_1 - \tau_2|}. \tag{8.43}$$

Comparing with (8.20) we can extract both the mass gap and modulus of the matrix element of $\hat{q}$ between ground state and first excited state,

$$E_1 - E_0 = \hbar\omega \quad \text{and} \quad |\,\langle\Omega|\,\hat{q}|1\rangle\,|^2 = \frac{\hbar}{2m\omega}, \tag{8.44}$$

a familiar result from the quantum mechanics course.

8.3 Wigner-Kirkwood Expansion

The Wigner-Kirkwood expansion [27] can be used for studying the equilibrium statistical mechanics of a nearly classical system of particles. It is a semiclassical expansion in powers of Planck's constant $\hbar$,

$$Z(\beta) = Z_{\rm cl}(\beta) + O(\hbar^2), \quad Z_{\rm cl}(\beta) = \sqrt{\frac{m}{2\pi\beta\hbar^2}} \int dq\, e^{-\beta V(q)}, \tag{8.45}$$

or equivalently of the thermal de Broglie wavelength $\lambda = \hbar(\beta/m)^{1/2}$. The $\hbar$-expansion for the partition function $Z(\beta) = \operatorname{tr}\exp(-\beta\hat{H})$ is different from that for the evolution kernel in quantum mechanics. The small expansion parameter $\hbar$ enters $Z(\beta)$ only via $\hbar^2$ in the kinetic energy whereas in the kernel $\langle q|\exp(it\hat{H}/\hbar)|q'\rangle$ it also enters as overall factor in the exponent. Here we shall derive the Wigner-Kirkwood expansion from the path integral representation for the partition function

$$Z(\beta) = \oint\limits_{w(0)=w(\hbar\beta)} \mathcal{D}w\; e^{-S_E[w]/\hbar}. \tag{8.46}$$

The normalization of the (formal) path integral is fixed by the classical limit $Z_{\rm cl}(\beta)$ in (8.45). We rescale imaginary time such that the periodicity of the paths is β instead of $\hbar\beta$,

$$\tau \longrightarrow \hbar\tau. \tag{8.47}$$

After this rescaling of time the path integral reads

$$Z(\beta) = \int\limits_{w(0)=w(\beta)} \mathcal{D}w\; \exp\left\{-\int_0^\beta \Big[\frac{m}{2}\dot{w}^2/\hbar^2 + V(w)\Big] d\tau\right\}. \tag{8.48}$$

Observe that for a moving particle the kinetic energy dominates the potential energy for small $\hbar$ whereas for a particle at rest the potential term is dominant. This suggest to split a path into its constant part (for which the kinetic energy vanishes) and fluctuations about it. Thus we change variables from $w(\tau) \to q + \hbar\xi(\tau)$ such that $\xi(0) = \xi(\beta) = 0$. We obtain

$$Z(\beta) = \int dq \int\limits_{\xi(0)=\xi(\beta)=0} \mathcal{D}\xi \exp\left\{-\frac{m}{2}\int_0^\beta \dot{\xi}^2 d\tau\right\}\; \exp\left\{-\int_0^\beta V(q+\hbar\xi)\, d\tau\right\}. \tag{8.49}$$

Now we expand the last exponential factor containing the potential in powers of $\hbar$,

$$\begin{aligned}\exp\{\dots\} \;=\;& e^{-\beta V}\Big\{1 - \hbar V' I(\xi) + \frac{\hbar^2}{2}\Big(V'^2 I^2(\xi) - V'' I(\xi^2)\Big)\\ &- \frac{\hbar^3}{3!}\Big(V'^3 I^3(\xi) - 3V'V'' I(\xi) I(\xi^2) + V''' I(\xi^3)\Big) + \dots\Big\},\end{aligned} \tag{8.50}$$

where the argument of V and its derivatives is the constant path q and we abbreviated the time integrals of powers of the fluctuation field by

$$\int \xi^n(\tau)d\tau \equiv I(\xi^n). \tag{8.51}$$

The remaining path integral in (8.49) leads to correlators of the time integrated fluctuations, for example

$$\langle I(\xi^2)I(\xi)\rangle = \int\limits_{\xi(0)=\xi(\beta)=0} \mathcal{D}\xi\, \exp\left\{-\frac{m}{2}\int \dot{\xi}^2\right\} \int \xi^2(\tau)d\tau \int \xi(\sigma)d\sigma. \tag{8.52}$$

The explicit form of the lowest order terms in the resulting series is

$$Z(\beta) = \int dq\, e^{\beta V}\left\{\langle 1\rangle - \hbar V'\langle I(\xi)\rangle + \frac{\hbar^2}{2}\left(V'^2\langle I^2(\xi)\rangle - V''\langle I(\xi^2)\rangle\right) + \dots\right\} \tag{8.53}$$

The expectation values (8.52) before time-integration are generated by the generating functional of the free particle with Dirichlet boundary conditions and $\hbar = 1$,

$$K(\beta, 0, 0; j) = \sqrt{\frac{m}{2\pi\beta}}\, \exp\left\{\frac{1}{m\beta}\int_0^\beta d\tau \int_0^\tau d\sigma\, (\beta-\tau)\sigma j(\tau)j(\sigma)\right\}. \tag{8.54}$$

To determine the expansion up to order $\hbar^2$ we need

$$\langle 1\rangle = \sqrt{\frac{m}{2\pi\beta}}, \quad \langle \xi(\tau)\rangle = 0 \quad \text{and} \quad \langle \xi(\tau)\xi(\sigma)\rangle = \frac{\langle 1\rangle}{m\beta}(\beta-\sigma)\tau \quad (\tau < \sigma). \tag{8.55}$$

Finally we must integrate over τ (and σ) which, after a partial integration in q, leads to

$$Z(\beta) = \sqrt{\frac{m}{2\pi\beta\hbar^2}} \int dq\, e^{-\beta V(q)}\left(1 - \hbar^2\frac{\beta^3}{24m}V'^2 + O(\hbar^4)\right), \tag{8.56}$$

where we have already anticipated that the odd powers of $\hbar$ vanish in this expansion, since the odd moments of the free measure vanish.[2]

The first term in this power series in $\hbar$ is the classical partition function. The coefficients of $O(\hbar^n)$ contain exactly n derivatives of the potential, e.g. the $\hbar^4$ coefficient contains terms like

$$V'''', \quad V'^4, \quad V'''V' \quad \text{and} \quad V''^2. \tag{8.57}$$

We see that the $\hbar$-expansion is actually a gradient expansion. A strongly coupled system behaves classically and we may expect that its behavior is described by a Wigner-Kirkwood gradient expansion. The first few terms in the semiclassical expansion have been derived by WIGNER AND KIRKWOOD [27].

[2]One needs to restore an additional factor of $1/\hbar$ to find the correct classical limit. This is due to the different rescaling of the constant path and the fluctuations $\xi(\tau)$.

8.4 High Temperature Expansion

Besides the perturbative expansion in the powers of the interaction term or the semi-classical expansion in powers of $\hbar$ there exits another approximation of considerable interest, namely the high temperature expansion in powers of the inverse temperature β. Actually we shall need this expansion later when we discuss certain gauge field theories and in particular their anomalies.

The temperature dependence of finite temperature expectation values comes from the β-periodicity (more accurately $\hbar/k_BT$-periodicity) of the trajectories in the path integral. As in the previous section we split a path into its constant part q and the fluctuations $\xi(\tau)$ about q. This way the partition function becomes the q-integral over the fluctuation part,

$$Z(\beta) = \int dq\, Z(\beta, q). \tag{8.58}$$

The *heat kernel* $K(\beta, q)$ is the path integral over the fluctuations in (8.49) (to simplify the notation we set $\hbar = 1$). Now we rescale time such the fluctuation have periodicity 1 and at the same time rescale the amplitude of the fluctuations such the kinetic term becomes β-independent:

$$\tau \longrightarrow \beta\tau \quad \text{and} \quad \xi \longrightarrow \sqrt{\beta}\,\xi. \tag{8.59}$$

After these rescaling the β-dependence comes only from the temperature-dependent potential:

$$Z(\beta, q) = \frac{1}{\sqrt{\beta}} \int\limits_{\xi(0)=\xi(1)=0} \mathcal{D}\xi \exp\left\{-\frac{m}{2}\int_0^1 \dot{\xi}^2\right\} \exp\left\{-\beta \int V(q+\sqrt{\beta}\,\xi)\, d\tau\right\}. \tag{8.60}$$

Now we expand the last exponential in powers of β. Again we are lead to calculate time integrals of correlators of the fluctuation field. Using $\langle \xi(\tau)\rangle = 0$ we find the following expansion for the heat kernel

$$\begin{aligned} Z(\beta, q) \;=\; & \sqrt{\beta}\Big\langle 1 - \beta V(q) + \frac{\beta^2}{2} V^2(q) - \frac{\beta^2}{2} V''(q)\, I(\xi^2) \\ & -\frac{\beta^3}{3!}V^3 + \frac{\beta^3}{2} V'V' I^2(\xi) + \frac{\beta^3}{2} VV'' I(\xi^2) - \frac{\beta^3}{24} V'''' I(\xi^4) \dots \Big\rangle. \end{aligned} \tag{8.61}$$

Inserting the correlators (8.55) with $\beta = 1$ we can compute the remaining correlators and time-integrals. This way one obtains

$$\begin{aligned} Z(\beta, q) \;=\; & \sqrt{\frac{m}{2\pi\beta}} \Big\{ 1 - \beta V + \frac{\beta^2}{2} V^2 - \frac{\beta^2}{12m} V'' \\ & -\frac{\beta^3}{6} V^3 + \frac{\beta^3}{24m} V'V' + \frac{\beta^3}{12m} VV'' - \frac{\beta^3}{240m^2} V''' + \dots \Big\}, \end{aligned} \tag{8.62}$$

where the potential and its derivatives are evaluated on the constant path q. The partition function is the space integral of this kernel. If the potential is localized near the origin or alternatively if space is compact we obtain the series expansion

$$Z(\beta)-Z_0(\beta)=\sqrt{\frac{m}{2\pi\beta}}\int dq\left\{-\beta V+\frac{\beta^2}{2}V^2-\frac{\beta^3}{6}V^3-\frac{\beta^3}{12m}V'^2+\dots\right\} \tag{8.63}$$

For very high temperature the particles move almost freely and as expected $Z(\beta)$ tends to the partition function $Z_0(\beta)$ of a gas of free particles with mass m. Note that besides the overall factor $\beta^{-1/2}$ the density and the partition function have an expansion in integer powers of β, although the argument of V in (8.60) contains $\sqrt{\beta}$. The corresponding expansion for a particle propagating in d-dimensions reads

$$Z(\beta)-Z_0(\beta)=\left(\frac{m}{2\pi\beta}\right)^{d/2}\int d^dq\left\{-\beta V+\frac{\beta^2}{2}V^2-\frac{\beta^3}{6}V^3-\frac{\beta^3}{12m}(\nabla V)^2+\dots\right\}. \tag{8.64}$$

In [28] the high temperature expansion was completely computerized using the algebraic language FORM. The calculation was performed up to order β^{11}. For the coefficient of β^n in the expansion of $Z(\beta)$ the number of terms are:

n	7	8	9	10	11
# of terms	37	114	380	1373	5301

The high temperature expansion enters the inverse mass expansion of worldline path integrals occuring in one-loop effective action.

8.5 High-T Expansion for the Dirac-Hamiltonian

The heat kernel expansion of the previous section is of great importance in relativistic quantum field theories. The Lagrangian for the electron- or quark-field contains the Dirac operator $\not{D}$ and the fermionic path integral leads to the determinant of this operator. This determinant in turn can be related to the partition function of $-\not{D}^2$. Here we shall compute the high temperature expansion of the heat kernel

$$Z(\beta,q)=\langle q|\,e^{\beta\not{D}^2}|q\rangle\,, \tag{8.65}$$

where the Euclidean Dirac-operator

$$\not{D}=\gamma^\mu D_\mu. \tag{8.66}$$

contains the *covariant derivative* which couples the fermionic field to the gauge potential A_μ,

$$D_\mu=\partial_\mu-iA_\mu. \tag{8.67}$$

In Quantum Electrodynamics (QED) the electric and magnetic fields entering the field strength tensor $F_{\mu\nu}$ are given by $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. In non-Abelian gauge theories the potential A_μ and field strength $F_{\mu\nu}$ are matrix values functions. They take their values in the Lie-algebra of the underlying gauge group. Besides the gauge potential the Dirac operator contains the Euclidean matrices γ^μ obeying the anti-commutation relations

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}, \quad \mu, \nu = 1, .., d. \tag{8.68}$$

In d dimensions they are $2^{[d/2]}$-dimensional hermitian matrices. The explicit form of the second order hermitian matrix differential operator $\not{D}^2$ is

$$\not{D}^2 = \frac{1}{2}\{\gamma^\mu, \gamma^\nu\} D_\mu D_\nu + \frac{1}{4}[\gamma^\mu, \gamma^\nu][D_\mu, D_\nu] = D^\mu D_\mu + \Sigma^{\mu\nu} F_{\mu\nu}, \tag{8.69}$$

where we have introduced the components $F_{\mu\nu}$ of the field strength tensor which for non-Abelian gauge theories contain additional commutators,

$$F_{\mu\nu} = i[D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu - i[A_\mu, A_\nu]. \tag{8.70}$$

The squared Dirac operator also contains the $d(d-1)/2$ matrices

$$\Sigma^{\mu\nu} = \frac{1}{4i}[\gamma^\mu, \gamma^\nu] \tag{8.71}$$

generating the spin rotations in Euclidean spacetime.

Similar as in section 5.2 one proves that the Euclidean evolution kernel has the following path integral representation:

$$\langle q | \, e^{\beta \not{D}^2} | q' \rangle = \int \mathcal{D}w \; \mathcal{P} \, e^{-S_E[w,A]}, \tag{8.72}$$

where the Euclidean action is given by the Wick-rotated Legendre transform of $\not{D}^2$,

$$S_E = \int_0^\beta d\tau \int d^{d-1}\boldsymbol{x} \; \mathcal{L}_E(w, A), \quad \mathcal{L}_E = \frac{1}{4}\dot{w}^2 - i\dot{w}A - \Sigma F, \tag{8.73}$$

and we abbreviated $w^\mu w_\mu = w^2$, $w^\mu A_\mu = wA$ and $\Sigma^{\mu\nu} F_{\mu\nu} = \Sigma F$. The potential and field strength are evaluated along the trajectory $w(\tau) \in \mathbb{R}^d$. In (8.72) we needed the time ordering $\mathcal{P}$ since the matrix-values Lagrangian $\mathcal{L}_E$ at different times do not commute for non-homogeneous background gauge fields. In the following we shall consider Abelian gauge fields in which case no path ordering is required.

With the same change of variables as the one leading to (8.60) we obtain the following density for the partition function,

$$Z(\beta, q) = \beta^{-d/2} \int\limits_{\xi(0)=\xi(1)=0} \mathcal{D}\xi \exp\left\{ -\int \left(\frac{\dot{\xi}^2}{4} - i\sqrt{\beta}\,\dot{\xi} A(q + \sqrt{\beta}\xi) - \beta \Sigma F(q + \sqrt{\beta}\xi) \right) \right\}. \tag{8.74}$$

As in the scalar case one expands the exponent in powers of $\beta^{1/2}$ and uses that $\int \dot\xi = 0$ and that integrated moments like $\int\langle\dot\xi f(\xi)\rangle$ vanish due to the invariance of the measure under $\tau \to 1-\tau$. Then one obtains for Abelian fields the expansion

$$\begin{aligned}\beta^{d/2} Z(\beta,q) \;\sim\; & \Big\langle 1+\beta\Sigma\cdot F+\frac{\beta^2}{2}(\Sigma\cdot F)^2+\frac{\beta^2}{2}(\Sigma\cdot F)_{,\alpha\beta}\int d\tau\,\xi^\alpha(\tau)\xi^\beta(\tau)\\ & -\frac{\beta^2}{2}A_{\mu,\alpha}A_{\nu,\beta}\int d\tau d\sigma\,\dot\xi^\mu(\tau)\xi^\alpha(\tau)\dot\xi^\nu(\sigma)\xi^\beta(\sigma)+\dots\Big\rangle,\end{aligned} \tag{8.75}$$

where the external fields are evaluated on the constant path q. From the result (8.55) with $m = 1/2$ and $\beta = 1$ we read off the two point function,

$$\langle \xi^\alpha(\tau)\xi^\beta(\sigma)\rangle = \frac{2}{(4\pi)^{d/2}}\,(1-\sigma)\,\tau\delta^{\alpha\beta}, \qquad \tau<\sigma. \tag{8.76}$$

The 4-point function can be calculated with the help of Wicks theorem. One obtains for the last average in (8.75)

$$\begin{aligned}&(4\pi)^{d/2}\Big\langle\dot\xi^\mu(\tau)\xi^\alpha(\tau)\dot\xi^\nu(\sigma)\xi^\beta(\sigma)\Big\rangle\\ &=(1-2\tau)(1-2\sigma)\delta^{\mu\alpha}\delta^{\nu\beta}\\ &\quad+4\Big\{(\delta(\tau-\sigma)-1)\delta^{\mu\nu}\delta^{\alpha\beta}-4\delta^{\mu\beta}\delta^{\alpha\nu}\Big\}\,\sigma(1-\tau).\end{aligned} \tag{8.77}$$

The least trivial term is the δ-function coming from a careful evaluation of $\langle\dot\xi^\mu\dot\xi^\nu\rangle$. Finally, after integrating over τ (and σ) one ends up with the following heat kernel expansion

$$Z(\beta,q)=\frac{1}{(4\pi\beta)^{d/2}}\Big\{1+\beta\,\Sigma F+\frac{\beta^2}{12}\Big(2\Delta(\Sigma F)+6(\Sigma F)^2-F_{\mu\nu}F^{\mu\nu}\Big)+\dots\Big\}. \tag{8.78}$$

Note that all terms in this high-temperature expansion are gauge covariant, as required. Up to an overall factor $\beta^{-d/2}$ only integer powers of β occur, very much like in the scalar case. The reason is that all odd moments of the free measure vanish. To obtain the high temperature expansion of the *partition function* one takes the trace with respect to the Dirac indices and integrates over the Euclidean spacetime. The coefficients in the expansion are finite for spacetimes with finite volumes. For non-Abelian gauge fields the calculation is not much different and the result (8.78) also holds in this case if we only replace the Laplacian by the gauge-covariant Laplacian and in addition take the trace over internal indices.

8.6 Appendix B: From Dirichlet to periodic Greenfunction

In this appendix we prove that

$$G_P(\tau,\sigma)=\frac{1}{m_\beta}\phi(\tau)\phi(\sigma)+G_D(\tau,\sigma) \tag{B.1}$$

is the Greenfunction of the fluctuation operator

$$S'' = -m\frac{d^2}{d\tau^2} + m\omega^2(\tau). \tag{B.2}$$

with respect to periodic boundary conditions. Here $G_D(\tau,\sigma)$ is the Greenfunction for Dirichlet boundary conditions. ϕ is a solution of $S''\phi = 0$ and takes the values 1 at initial and final time 0 and β. The normalizing constant m_β is[3]

$$m_\beta = m\left(\dot\phi(\beta) - \dot\phi(0)\right). \tag{B.3}$$

For the proof we introduce two fundamental solutions $D(\tau)$ and $E(\tau)$ with boundary conditions

$$D(0) = 0, \quad \dot D(0) = 1 \quad \text{and} \quad E(0) = 1, \quad E(\hbar\beta) = 0. \tag{B.4}$$

Their time-independent Wronskian is

$$W(D,E) = D\dot E - E\dot D = -1. \tag{B.5}$$

Two typical fundamental solutions are depicted in figure 8.1. It is easy to prove that the Dirichlet

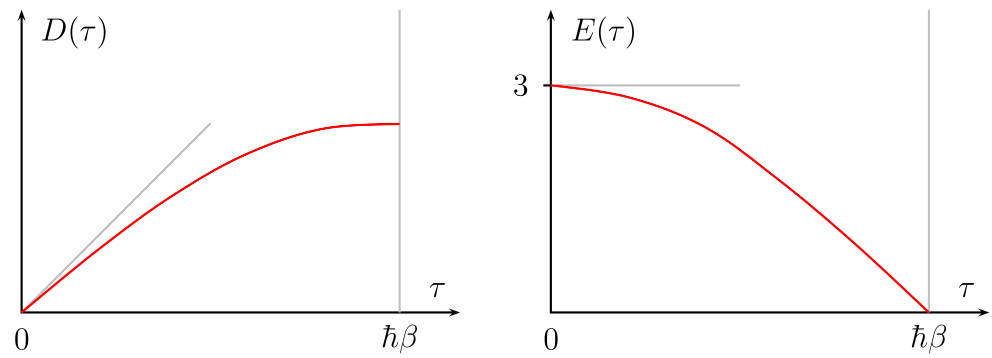

Figure 8.1: *Two fundamental solutions obeying $S''D = S''E = 0$.*

Greenfunction is given by

$$mG_D(\tau,\sigma) = \begin{cases} D(\tau)E(\sigma) & \text{for } \tau<\sigma \\ D(\sigma)E(\tau) & \text{for } \tau>\sigma \end{cases} \tag{B.6}$$

and the particular function ϕ is given by

$$\phi(\tau) = E(\tau) + \frac{D(\tau)}{D(\beta)}. \tag{B.7}$$

[3]In this appendix we set $\hbar = 1$.

We can make the following ansatz for the periodic Greenfunction,

$$G_P(\tau,\sigma) = \frac{\alpha}{m}\phi(\tau)\phi(\sigma) + G_D(\tau,\sigma). \tag{B.8}$$

Clearly this function is symmetric in both arguments and has the value α/m at initial and final (imaginary) time. The constant α is fixed by the periodicity condition

$$\frac{\partial}{\partial\tau}G_P(\tau,\sigma)|_{\tau=0} = \frac{\partial}{\partial\tau}G_P(\tau,\sigma)|_{\tau=\beta}$$

which implies

$$\alpha\left\{\dot\phi(0)-\dot\phi(\beta)\right\}\phi(\sigma) = m\frac{\partial}{\partial\tau}G_D(\tau,\sigma)|_{\tau=\beta} - m\frac{\partial}{\partial\tau}G_D(\tau,\sigma)|_{\tau=0}. \tag{B.9}$$

Inserting the Dirichlet Greenfunction (B.6) the right hand side becomes

$$\dot E(\beta)D(\sigma) - E(\sigma)) = -\frac{D(\sigma)}{D(\beta)} - E(\sigma) = -\phi(\sigma), \tag{B.10}$$

where we used $\dot D(0) = 1$ and that the Wronskian at final time is $\dot E(\beta)D(\beta) = -1$. Comparing with (B.9) we conclude that $\alpha = -1$ and this proves that G_P in (B.1) with m_β given in (B.3) is the Greenfunction of S'' with respect to periodic boundary conditions.