A dancing shape, an image gay,
To haunt, to startle, and waylay
W. Wordsworth (1770–1840), Phantom of Delight

2

Path Integrals — Elementary Properties and Simple Solutions

The operator formalism of quantum mechanics and quantum statistics may not always lead to the most transparent understanding of quantum phenomena. There exists another, equivalent formalism in which operators are avoided by the use of infinite products of integrals, called *path integrals*. In contrast to the Schrödinger equation, which is a differential equation determining the properties of a state at a time from their knowledge at an infinitesimally earlier time, path integrals yield the quantum-mechanical amplitudes in a global approach involving the properties of a system at *all times*.

2.1 Path Integral Representation of Time Evolution Amplitudes

The path integral approach to quantum mechanics was developed by Feynman[1] in 1942. In its original form, it applies to a point particle moving in a Cartesian coordinate system and yields the transition amplitudes of the time evolution operator between the localized states of the particle (recall Section 1.7)

$$(x_b t_b|x_a t_a) = \langle x_b|\hat{U}(t_b, t_a)|x_a\rangle, \quad t_b > t_a. \tag{2.1}$$

For simplicity, we shall at first assume the space to be one-dimensional. The extension to D Cartesian dimensions will be given later. The introduction of curvilinear coordinates will require a little more work. A further generalization to spaces with a nontrivial geometry, in which curvature and torsion are present, will be described in Chapters 10–11.

2.1.1 Sliced Time Evolution Amplitude

We shall be interested mainly in the causal or retarded time evolution amplitudes [see Eq. (1.303)]. These contain all relevant quantum-mechanical information and

[1]For the historical development, see Notes and References at the end of this chapter.

possess, in addition, pleasant analytic properties in the complex energy plane [see the remarks after Eq. (1.310)]. This is why we shall always assume, from now on, the causal sequence of time arguments $t_b > t_a$.

Feynman realized that due to the fundamental composition law of the time evolution operator (see Section 1.7), the amplitude (2.1) could be sliced into a large number, say $N+1$, of time evolution operators, each acting across an infinitesimal time slice of thickness $\epsilon \equiv t_n - t_{n-1}= (t_b - t_a)/(N+1)> 0$:

$$(x_b t_b|x_a t_a) \;=\; \langle x_b|\hat{U}(t_b,t_N)\hat{U}(t_N,t_{N-1})\cdots\hat{U}(t_n,t_{n-1})\cdots\hat{U}(t_2,t_1)\hat{U}(t_1,t_a)|x_a\rangle. \tag{2.2}$$

When inserting a complete set of states between each pair of $\hat{U}$'s,

$$\int_{-\infty}^{\infty} dx_n |x_n\rangle\langle x_n| = 1, \quad n = 1,\dots,N, \tag{2.3}$$

the amplitude becomes a product of N-integrals

$$(x_b t_b|x_a t_a) = \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} dx_n\right]\prod_{n=1}^{N+1}(x_n t_n|x_{n-1}t_{n-1}), \tag{2.4}$$

where we have set $x_b \equiv x_{N+1}$, $x_a \equiv x_0$, $t_b \equiv t_{N+1}$, $t_a \equiv t_0$. The symbol $\Pi[\cdots]$ denotes the product of the quantities within the brackets. The integrand is the product of the amplitudes for the infinitesimal time intervals

$$(x_n t_n|x_{n-1}t_{n-1}) = \langle x_n|e^{-i\epsilon\hat{H}(t_n)/\hbar}|x_{n-1}\rangle, \tag{2.5}$$

with the Hamiltonian operator

$$\hat{H}(t) \equiv H(\hat{p},\hat{x},t). \tag{2.6}$$

The further development becomes simplest under the assumption that the Hamiltonian has the standard form, being the sum of a kinetic and a potential energy:

$$H(p,x,t) = T(p,t) + V(x,t). \tag{2.7}$$

For a sufficiently small slice thickness, the time evolution operator

$$e^{-i\epsilon\hat{H}/\hbar} = e^{-i\epsilon(\hat{T}+\hat{V})/\hbar} \tag{2.8}$$

is factorizable as a consequence of the *Baker-Campbell-Hausdorff formula* (to be proved in Appendix 2A)

$$e^{-i\epsilon(\hat{T}+\hat{V})/\hbar} = e^{-i\epsilon\hat{V}/\hbar}e^{-i\epsilon\hat{T}/\hbar}e^{-i\epsilon^2\hat{X}/\hbar^2}, \tag{2.9}$$

where the operator $\hat{X}$ has the expansion

$$\hat{X} \equiv \frac{i}{2}[\hat{V},\hat{T}] - \frac{\epsilon}{\hbar}\left(\frac{1}{6}[\hat{V},[\hat{V},\hat{T}]] - \frac{1}{3}[[\hat{V},\hat{T}],\hat{T}]\right) + \mathcal{O}(\epsilon^2)\ . \tag{2.10}$$

The omitted terms of order $\epsilon^4, \epsilon^5, \ldots$ contain higher commutators of $\hat{V}$ and $\hat{T}$. If we neglect, for the moment, the $\hat{X}$-term which is suppressed by a factor ϵ^2, we calculate for the local matrix elements of $e^{-i\epsilon\hat{H}/\hbar}$ the following simple expression:

$$\langle x_n|e^{-i\epsilon H(\hat{p},\hat{x},t_n)/\hbar}|x_{n-1}\rangle \approx \int_{-\infty}^{\infty} dx \langle x_n|e^{-i\epsilon V(\hat{x},t_n)/\hbar}|x\rangle\langle x|e^{-i\epsilon T(\hat{p},t_n)/\hbar}|x_{n-1}\rangle$$
$$= \int_{-\infty}^{\infty} dx \langle x_n|e^{-i\epsilon V(\hat{x},t_n)/\hbar}|x\rangle \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} e^{ip_n(x-x_{n-1})/\hbar} e^{-i\epsilon T(p_n,t_n)/\hbar}. \tag{2.11}$$

Evaluating the local matrix elements,

$$\langle x_n|e^{-i\epsilon V(\hat{x},t_n)/\hbar}|x\rangle = \delta(x_n - x) e^{-i\epsilon V(x_n,t_n)/\hbar}, \tag{2.12}$$

this becomes

$$\langle x_n|e^{-i\epsilon H(\hat{p},\hat{x},t_n)/\hbar}|x_{n-1}\rangle \approx$$
$$\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \exp\left\{ip_n(x_n - x_{n-1})/\hbar - i\epsilon[T(p_n,t_n) + V(x_n,t_n)]/\hbar\right\}. \tag{2.13}$$

Inserting this back into (2.4), we obtain *Feynman's path integral formula*, consisting of the multiple integral

$$(x_b t_b|x_a t_a) \approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} dx_n\right] \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar}\right] \exp\left(\frac{i}{\hbar}\mathcal{A}^N\right), \tag{2.14}$$

where $\mathcal{A}^N$ is the sum

$$\mathcal{A}^N = \sum_{n=1}^{N+1}[p_n(x_n - x_{n-1}) - \epsilon H(p_n, x_n, t_n)]. \tag{2.15}$$

2.1.2 Zero-Hamiltonian Path Integral

Note that the path integral (2.14) with zero Hamiltonian produces the Hilbert space structure of the theory via a chain of scalar products:

$$(x_b t_b|x_a t_a) \approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} dx_n\right] \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar}\right] e^{i\sum_{n=1}^{N+1} p_n(x_n - x_{n-1})/\hbar}, \tag{2.16}$$

which is equal to

$$\begin{aligned}(x_b t_b|x_a t_a) &\approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} dx_n\right] \prod_{n=1}^{N+1}\langle x_n|x_{n-1}\rangle = \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} dx_n\right] \prod_{n=1}^{N+1}\delta(x_n - x_{n-1})\\ &= \delta(x_b - x_a).\end{aligned} \tag{2.17}$$

whose continuum limit is

$$(x_b t_b|x_a t_a) = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{i\int dt p(t)\dot{x}(t)/\hbar} = \langle x_b|x_a\rangle = \delta(x_b - x_a). \tag{2.18}$$

In the operator expression (2.2), the right-hand side follows from the fact that for zero Hamiltonian the time evolution operators $\hat{U}(t_n, t_{n-1})$ are all equal to unity.

At this point we make the important observation that a momentum variable p_n *inside* the product of momentuma integrations in the expression (2.16) can be generated by a derivative $\hat{p}_n \equiv -i\hbar\partial_{x_n}$ *outside* of it. In Subsection 2.1.4 we shall go to the *continuum limit* of time slicing in which the slice thickness ϵ goes to zero. In this limit, the discrete variables x_n and p_n become functions $x(t)$ and $p(t)$ of the continuous time t, and the momenta p_n become differential operators $p(t) = -i\hbar\partial_{x(t)}$, satisfying the commutation relations with $x(t)$:

$$[\hat{p}(t), x(t)] = -i\hbar. \tag{2.19}$$

These are the canonical *equal-time commutation relations* of Heisenberg.

This observation forms the basis for deriving, from the path integral (2.14), the Schrödinger equation for the time evolution amplitude.

2.1.3 Schrödinger Equation for Time Evolution Amplitude

Let us split from the product of integrals in (2.14) the final time slice as a factor, so that we obtain the recursion relation

$$(x_b t_b|x_a t_a) \approx \int_{-\infty}^{\infty} dx_N (x_b t_b|x_N t_N)\,(x_N t_N|x_a t_a), \tag{2.20}$$

where

$$(x_b t_b|x_N t_N) \approx \int_{-\infty}^{\infty} \frac{dp_b}{2\pi\hbar} e^{(i/\hbar)[p_b(x_b-x_N)-\epsilon H(p_b,x_b,t_b)]}. \tag{2.21}$$

The momentum p_b *inside* the integral can be generated by a differential operator $\hat{p}_b \equiv -i\hbar\partial_{x_b}$ *outside* of it. The same is true for any function of p_b, so that the Hamiltonian can be moved before the momentum integral yielding

$$(x_b t_b|x_N t_N) \approx e^{-i\epsilon H(-i\hbar\partial_{x_b},x_b,t_b)/\hbar} \int_{-\infty}^{\infty} \frac{dp_b}{2\pi\hbar} e^{ip_b(x_b-x_N)/\hbar} = e^{-i\epsilon H(-i\hbar\partial_{x_b},x_b,t_b)/\hbar}\delta(x_b - x_N). \tag{2.22}$$

Inserting this back into (2.20) we obtain

$$(x_b t_b|x_a t_a) \approx e^{-i\epsilon H(-i\hbar\partial_{x_b},x_b,t_b)/\hbar}(x_b\, t_b - \epsilon|x_a t_a), \tag{2.23}$$

or

$$\frac{1}{\epsilon}\left[(x_b\, t_b+\epsilon|x_a t_a) - (x_b t_b|x_a t_a)\right] \approx \frac{1}{\epsilon}\left[e^{-i\epsilon H(-i\partial_{x_b},x_b,t_b+\epsilon)/\hbar} - 1\right](x_b\, t_b|x_a t_a). \tag{2.24}$$

In the limit $\epsilon \to 0$, this goes over into the differential equation for the time evolution amplitude

$$i\hbar\partial_{t_b}(x_b t_b|x_a t_a) = H(-i\hbar\partial_{x_b}, x_b, t_b)(x_b\, t_b|x_a t_a), \tag{2.25}$$

which is precisely the Schrödinger equation (1.301) of operator quantum mechanics.

2.1.4 Convergence of of the Time-Sliced Evolution Amplitude

Some remarks are necessary concerning the convergence of the time-sliced expression (2.14) to the quantum-mechanical amplitude in the continuum limit, where the thickness of the time slices $\epsilon = (t_b - t_a)/(N+1) \to 0$ goes to zero and the number N of slices tends to ∞. This convergence can be proved for the standard kinetic energy $T = p^2/2M$ only if the potential $V(x,t)$ is sufficiently *smooth*. For time-independent potentials this is a consequence of the *Trotter product formula* which reads

$$e^{-i(t_b-t_a)\hat{H}/\hbar} = \lim_{N\to\infty} \left(e^{-i\epsilon\hat{V}/\hbar} e^{-i\epsilon\hat{T}/\hbar}\right)^{N+1}. \tag{2.26}$$

If T and V are c-numbers, this is trivially true. If they are operators, we use Eq. (2.9) to rewrite the left-hand side of (2.26) as

$$e^{-i(t_b-t_a)\hat{H}/\hbar} \equiv \left(e^{-i\epsilon(\hat{T}+\hat{V})/\hbar}\right)^{N+1} \equiv \left(e^{-i\epsilon\hat{V}/\hbar} e^{-i\epsilon\hat{T}/\hbar} e^{-i\epsilon^2\hat{X}/\hbar^2}\right)^{N+1}.$$

The Trotter formula implies that the commutator term $\hat{X}$ proportional to ϵ^2 does not contribute in the limit $N \to \infty$. The mathematical conditions ensuring this require functional analysis too technical to be presented here (for details, see the literature quoted at the end of the chapter). For us it is sufficient to know that the Trotter formula holds for operators which are bounded from below and that for most physically interesting potentials, it cannot be used to derive Feynman's time-sliced path integral representation (2.14), even in systems where the formula is known to be valid. In particular, the short-time amplitude may be different from (2.13). Take, for example, an attractive Coulomb potential $V(x) \propto -1/|x|$ for which the Trotter formula has been proved to be valid. Feynman's time-sliced formula, however, diverges even for two time slices. This will be discussed in detail in Chapter 12. Similar problems will be found for other physically relevant potentials such as $V(x) \propto l(l+D-2)\hbar^2/|x|^2$ (centrifugal barrier) and $V(\theta) \propto m^2\hbar^2/\sin^2\theta$ (angular barrier near the poles of a sphere). In all these cases, the commutators in the expansion (2.10) of $\hat{X}$ become more and more singular. In fact, as we shall see, the expansion does not even converge, even for an infinitesimally small ϵ. All atomic systems contain such potentials and the Feynman formula (2.14) cannot be used to calculate an approximation for the transition amplitude. A new path integral formula has to be found. This will be done in Chapter 12. Fortunately, it is possible to eventually reduce the more general formula via some transformations back to a Feynman type formula with a bounded potential in an auxiliary space. Thus the above derivation of Feynman's formula for such potentials will be sufficient for the further development in this book. After this it serves as an *independent* starting point for all further quantum-mechanical calculations.

In the sequel, the symbol $\approx$ in all time-sliced formulas such as (2.14) will imply that an equality emerges in the *continuum limit* $N \to \infty$, $\epsilon \to 0$ unless the potential has singularities of the above type. In the action, the continuum limit is without subtleties. The sum $\mathcal{A}^N$ in (2.15) tends towards the integral

$$\mathcal{A}[p,x] = \int_{t_a}^{t_b} dt\, [p(t)\dot{x}(t) - H(p(t), x(t), t)] \tag{2.27}$$

under quite general circumstances. This expression is recognized as the classical canonical action for the path $x(t), p(t)$ in phase space. Since the position variables x_{N+1} and x_0 are fixed at their initial and final values x_b and x_a, the paths satisfy the boundary condition $x(t_b) = x_b,\ x(t_a) = x_a$.

In the same limit, the product of infinitely many integrals in (2.14) will be called a *path integral*. The limiting measure of integration is written as

$$\lim_{N\to\infty} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} dx_n\right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar}\right] \equiv \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar}. \tag{2.28}$$

By definition, there is always one more p_n-integral than x_n-integrals in this product. While x_0 and x_{N+1} are held fixed and the x_n-integrals are done for $n = 1, \dots, N$, each pair (x_n, x_{n-1}) is accompanied by one p_n-integral for $n = 1, \dots, N+1$. The situation is recorded by the prime on the functional integral $\mathcal{D}'x$. With this definition, the amplitude can be written in the short form

$$(x_b t_b | x_a t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{i\mathcal{A}[p,x]/\hbar}. \tag{2.29}$$

The path integral has a simple intuitive interpretation: Integrating over all paths corresponds to summing over all histories along which a physical system can possibly evolve. The exponential $e^{i\mathcal{A}[p,x]/\hbar}$ is the quantum analog of the Boltzmann factor $e^{-E/k_B T}$ in statistical mechanics. Instead of an exponential probability, a pure phase factor is assigned to each possible history: The total amplitude for going from x_a, t_a to x_b, t_b is obtained by adding up the phase factors for all these histories,

$$(x_b t_b | x_a t_a) = \sum_{\substack{\text{all histories} \\ (x_a,t_a)\rightsquigarrow(x_b,t_b)}} e^{i\mathcal{A}[p,x]/\hbar}, \tag{2.30}$$

where the sum comprises all paths in phase space with fixed endpoints x_b, x_a in x-space.

2.1.5 Time Evolution Amplitude in Momentum Space

The above observed asymmetry in the functional integrals over x and p is a consequence of keeping the endpoints fixed in *position space*. There exists the possibility of proceeding in a conjugate way keeping the initial and final *momenta* p_b and p_a fixed. The associated time evolution amplitude can be derived by going through the same steps as before but working in the momentum space representation of the Hilbert space, starting from the matrix elements of the time evolution operator

$$(p_b t_b | p_a t_a) \equiv \langle p_b | \hat{U}(t_b, t_a) | p_a \rangle. \tag{2.31}$$

The time slicing proceeds as in (2.2)–(2.4), with all x's replaced by p's, except in the completeness relation (2.3) which we shall take as

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} |p\rangle\langle p| = 1, \tag{2.32}$$

corresponding to the choice of the normalization of states [compare (1.186)]

$$\langle p_b | p_a \rangle = 2\pi\hbar\delta(p_b - p_a). \tag{2.33}$$

In the resulting product of integrals, the integration measure has an opposite asymmetry: there is now one more x_n-integral than p_n-integrals. The sliced path integral reads

$$\begin{aligned} (p_b t_b | p_a t_a) \approx & \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right] \prod_{n=0}^{N} \left[\int_{-\infty}^{\infty} dx_n \right] \\ & \times \exp\left\{ \frac{i}{\hbar} \sum_{n=0}^{N} [-x_n(p_{n+1} - p_n) - \epsilon H(p_n, x_n, t_n)] \right\}. \end{aligned} \tag{2.34}$$

The relation between this and the x-space amplitude (2.14) is simple: By taking in (2.14) the first and last integrals over p_1 and p_{N+1} out of the product, renaming them as p_a and p_b, and rearranging the sum $\sum_{n=1}^{N+1} p_n(x_n - x_{n-1})$ as follows

$$\begin{aligned} \sum_{n=1}^{N+1} p_n(x_n - x_{n-1}) &= p_{N+1}(x_{N+1} - x_N) + p_N(x_N - x_{N-1}) + \dots \\ & \qquad \dots + p_2(x_2 - x_1) + p_1(x_1 - x_0) \\ &= p_{N+1}x_{N+1} - p_1 x_0 \\ & \quad -(p_{N+1} - p_N)x_N - (p_N - p_{N-1})x_{N-1} - \dots - (p_2 - p_1)x_1 \\ &= p_{N+1}x_{N+1} - p_1 x_0 - \sum_{n=1}^{N} (p_{n+1} - p_n) x_n, \end{aligned} \tag{2.35}$$

the remaining product of integrals looks as in Eq. (2.34), except that the lowest index n is one unit larger than in the sum in Eq. (2.34). In the limit $N \to \infty$ this does not matter, and we obtain the Fourier transform

$$(x_b t_b | x_a t_a) = \int \frac{dp_b}{2\pi\hbar} e^{ip_b x_b/\hbar} \int \frac{dp_a}{2\pi\hbar} e^{-ip_a x_a/\hbar} (p_b t_b | p_a t_a). \tag{2.36}$$

The inverse relation is

$$(p_b t_b | p_a t_a) = \int dx_b \, e^{-ip_b x_b/\hbar} \int dx_a \, e^{ip_a x_a/\hbar} (x_b t_b | x_a t_a). \tag{2.37}$$

In the continuum limit, the amplitude (2.34) can be written as a path integral

$$(p_b t_b | p_a t_a) = \int_{p(t_a)=p_a}^{p(t_b)=p_b} \frac{\mathcal{D}'p}{2\pi\hbar} \int \mathcal{D}x e^{i\bar{\mathcal{A}}[p,x]/\hbar}, \tag{2.38}$$

where

$$\bar{\mathcal{A}}[p,x]=\int_{t_a}^{t_b}dt\,[-\dot{p}(t)x(t)-H(p(t),x(t),t)]=\mathcal{A}[p,x]-p_bx_b+p_ax_a. \tag{2.39}$$

If the Hamiltonian is independent of x and t, the sliced path integral (2.34) becomes trivial. Then the $N+1$ integrals over x_n $(n=0,\dots,N)$ can be done yielding a product of δ-functions $\delta(p_b-p_N)\cdots\delta(p_1-p_0)$. As a conseqence, the integrals over the N momenta p_n $(n=1,\dots,N)$ are all squeezed to the initial momentum $p_N=p_{N-1}=\ldots=p_1=p_a$. A single a final δ-function $2\pi\hbar\delta(p_b-p_a)$ remains, accompanied by the product of $N+1$ factors $\prod_{n=0}^{N}e^{-i\epsilon H(p_a)/\hbar}$, which is equal to $e^{-i(t_b-t_a)H(p)/\hbar}$. Hence we obtain:

$$(p_bt_b|p_at_a)\;=\;2\pi\hbar\delta(p_b-p_a)e^{-i(t_b-t_a)H(p)/\hbar}. \tag{2.40}$$

Inserting this into Eq. (2.36), we find a simple Fourier integral for the time evolution amlitude in x-space:

$$(x_bt_b|x_at_a)=\int\frac{dp}{2\pi\hbar}e^{ip(x_b-x_a)/\hbar-i(t_b-t_a)H(p)/\hbar}. \tag{2.41}$$

Note that in (2.40) contains an equal sign rather than the $\approx$-sign since the right-hand sign is the same for any number of time slices.

2.1.6 Quantum-Mechanical Partition Function

A path integral symmetric in p and x arises when considering the quantum-mechanical partition function defined by the trace (recall Section 1.17)

$$Z_{\rm QM}(t_b,t_a)=\mathrm{Tr}\left(e^{-i(t_b-t_a)\hat{H}/\hbar}\right). \tag{2.42}$$

In the local basis, the trace becomes an integral over the amplitude $(x_bt_b|x_at_a)$ with $x_b=x_a$:

$$Z_{\rm QM}(t_b,t_a)=\int_{-\infty}^{\infty}dx_a(x_at_b|x_at_a). \tag{2.43}$$

The additional trace integral over $x_{N+1}\equiv x_0$ makes the path integral for $Z_{\rm QM}$ symmetric in p_n and x_n:

$$\int_{-\infty}^{\infty}dx_{N+1}\prod_{n=1}^{N}\left[\int_{-\infty}^{\infty}dx_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dp_n}{2\pi\hbar}\right]=\prod_{n=1}^{N+1}\left[\iint_{-\infty}^{\infty}\frac{dx_ndp_n}{2\pi\hbar}\right]. \tag{2.44}$$

In the continuum limit, the right-hand side is written as

$$\lim_{N\to\infty}\prod_{n=1}^{N+1}\left[\iint_{-\infty}^{\infty}\frac{dx_ndp_n}{2\pi\hbar}\right]\equiv\oint\mathcal{D}x\int\frac{\mathcal{D}p}{2\pi\hbar}\;, \tag{2.45}$$

and the measures are related by

$$\int_{-\infty}^{\infty} dx_a \int_{x(t_a)=x_a}^{x(t_b)=x_a} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} \equiv \oint \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} \ . \tag{2.46}$$

The symbol $\oint$ indicates the periodic boundary condition $x(t_a) = x(t_b)$. In the momentum representation we would have similarly

$$\int_{-\infty}^{\infty} \frac{dp_a}{2\pi\hbar} \int_{p(t_a)=p_a}^{p(t_b)=p_a} \frac{\mathcal{D}'p}{2\pi\hbar} \int \mathcal{D}x \equiv \oint \frac{\mathcal{D}p}{2\pi\hbar} \int \mathcal{D}x \ , \tag{2.47}$$

with the periodic boundary condition $p(t_a) = p(t_b)$, and the same right-hand side. Hence, the quantum-mechanical partition function is given by the path integral

$$Z_{\rm QM}(t_b, t_a) = \oint \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{i\mathcal{A}[p,x]/\hbar} = \oint \frac{\mathcal{D}p}{2\pi\hbar} \int \mathcal{D}x e^{i\bar{\mathcal{A}}[p,x]/\hbar}. \tag{2.48}$$

In the right-hand exponential, the action $\bar{\mathcal{A}}[p,x]$ can be replaced by $\mathcal{A}[p,x]$, since the extra terms in (2.39) are removed by the periodic boundary conditions. In the time-sliced expression, the equality is easily derived from the rearrangement of the sum (2.35), which shows that

$$\sum_{n=1}^{N+1} p_n(x_n - x_{n-1})\Bigg|_{x_{N+1}=x_0} = -\sum_{n=0}^{N}(p_{n+1} - p_n)x_n\Bigg|_{p_{N+1}=p_0} . \tag{2.49}$$

In the path integral expression (2.48) for the partition function, the rules of quantum mechanics appear as a natural generalization of the rules of classical statistical mechanics, as formulated by Planck. According to these rules, each volume element in phase space $dxdp/h$ is occupied with the exponential probability e^{-E/k_BT}. In the path integral formulation of quantum mechanics, each volume element in the *path phase space* $\prod_n dx(t_n)dp(t_n)/h$ is associated with a pure phase factor $e^{i\mathcal{A}[p,x]/\hbar}$. We see here a manifestation of the correspondence principle which specifies the transition from classical to quantum mechanics. In path integrals, it looks somewhat more natural than in the historic formulation, where it requires the replacement of all classical phase space variables p, x by operators, a rule which was initially hard to comprehend.

2.1.7 Feynman's Configuration Space Path Integral

Actually, in his original paper, Feynman did not give the path integral formula in the above phase space formulation. Since the kinetic energy in (2.7) has usually the form $T(p,t) = p^2/2M$, he focused his attention upon the Hamiltonian

$$H = \frac{p^2}{2M} + V(x,t), \tag{2.50}$$

for which the time-sliced action (2.15) becomes

$$\mathcal{A}^N = \sum_{n=1}^{N+1} \left[p_n(x_n - x_{n-1}) - \epsilon \frac{p_n^2}{2M} - \epsilon V(x_n, t_n) \right]. \tag{2.51}$$

It can be quadratically completed to

$$\mathcal{A}^N = \sum_{n=1}^{N+1} \left[-\frac{\epsilon}{2M} \left(p_n - \frac{x_n - x_{n-1}}{\epsilon} M \right)^2 + \frac{M}{2} \epsilon \left(\frac{x_n - x_{n-1}}{\epsilon} \right)^2 - \epsilon V(x_n, t_n) \right]. \tag{2.52}$$

The momentum integrals in (2.14) may then be performed using the Fresnel integral formula (1.337), yielding

$$\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \exp\left[-\frac{i}{\hbar} \frac{\epsilon}{2M} \left(p_n - M \frac{x_n - x_{n-1}}{\epsilon} \right)^2 \right] = \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}}, \tag{2.53}$$

and we arrive at the alternative representation

$$(x_b t_b | x_a t_a) \approx \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{2\pi\hbar i\epsilon/M}} \right] \exp\left(\frac{i}{\hbar} \mathcal{A}^N \right), \tag{2.54}$$

where $\mathcal{A}^N$ is now the sum

$$\mathcal{A}^N = \epsilon \sum_{n=1}^{N+1} \left[\frac{M}{2} \left(\frac{x_n - x_{n-1}}{\epsilon} \right)^2 - V(x_n, t_n) \right], \tag{2.55}$$

with $x_{N+1} = x_b$ and $x_0 = x_a$. Here the integrals run over all paths in *configuration space* rather than phase space. They account for the fact that a quantum-mechanical particle starting from a given initial point x_a will explore all possible ways of reaching a given final point x_b. The amplitude of each path is $\exp(i\mathcal{A}^N/\hbar)$. See Fig. 2.1 for a geometric illustration of the path integration. In the continuum limit, the sum (2.55) converges towards the action in the Lagrangian form:

$$\mathcal{A}[x] = \int_{t_a}^{t_b} dt L(x, \dot{x}) = \int_{t_a}^{t_b} dt \left[\frac{M}{2} \dot{x}^2 - V(x, t) \right]. \tag{2.56}$$

Note that this action is a local functional of $x(t)$ in the temporal sense as defined in Eq. (1.26).[2]

For the time-sliced Feynman path integral, one verifies the Schrödinger equation as follows: As in (2.20), one splits off the last slice as follows:

$$\begin{aligned} (x_b t_b | x_a t_a) &\approx \int_{-\infty}^{\infty} dx_N \, (x_b t_b | x_N t_N) \, (x_N t_N | x_a t_a) \\ &= \int_{-\infty}^{\infty} d\Delta x \, (x_b t_b | x_b - \Delta x \, t_b - \epsilon) \, (x_b - \Delta x \, t_b - \epsilon | x_a t_a), \end{aligned} \tag{2.57}$$

[2]A functional $F[x]$ is called local if it can be written as an integral $\int dt f(x(t), \dot{x}(t))$; it is called *ultra-local* if it has the form $\int dt f(x(t))$.

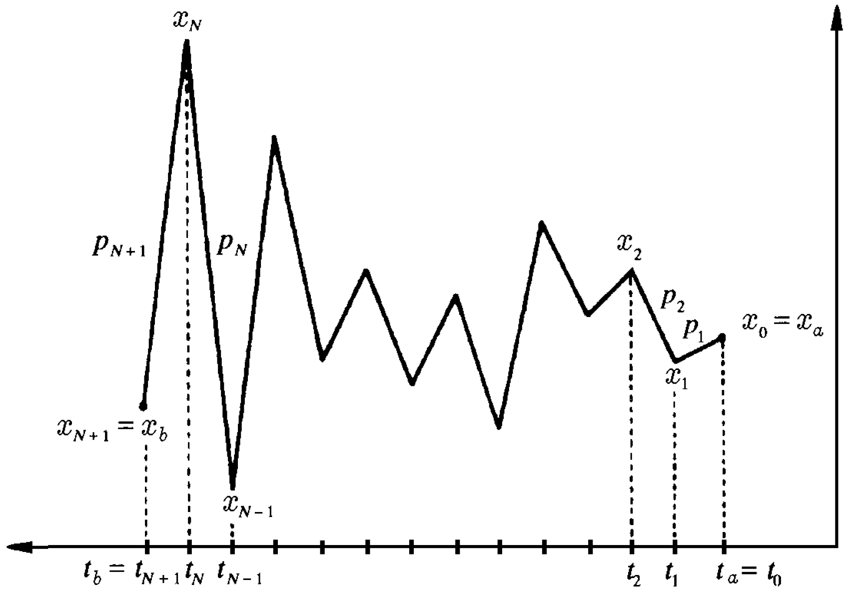

Figure 2.1 Zigzag paths, along which a point particle explores all possible ways of reaching the point x_b at a time t_b, starting from x_a at t_a. The time axis is drawn from right to left to have the same direction as the operator order in Eq. (2.2).

where

$$(x_b t_b | x_b - \Delta x\, t_b - \epsilon) \approx \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}} \exp\left\{ \epsilon \frac{i}{\hbar} \left[\frac{M}{2} \left(\frac{\Delta x}{\epsilon} \right)^2 - V(x_b, t_b) \right] \right\}. \quad (2.58)$$

We now expand the amplitude in the integral of (2.57) in a Taylor series

$$(x_b - \Delta x\, t_b - \epsilon | x_a t_a) = \left[1 - \Delta x\, \partial_{x_b} + \frac{1}{2} (\Delta x)^2 \partial_{x_b}^2 + \ldots \right] (x_b, t_b - \epsilon | x_a t_a). \quad (2.59)$$

Inserting this into (2.57), the odd powers of Δx do not contribute. For the even powers, we perform the integrals using the Fresnel version of formula (1.339), and obtain zero for odd powers of Δx, and

$$\int_{-\infty}^{\infty} \frac{d\Delta x}{\sqrt{2\pi\hbar i\epsilon/M}} (\Delta x)^{2n} \exp\left\{ \epsilon \frac{i}{\hbar} \frac{M}{2} \left(\frac{\Delta x}{\epsilon} \right)^2 \right\} = \left(i \frac{\hbar\epsilon}{M} \right)^n \quad (2.60)$$

for even powers, so that the integral in (2.57) becomes

$$(x_b t_b | x_a t_a) = \left[1 + \epsilon \frac{i\hbar}{2M} \partial_{x_b}^2 + \mathcal{O}(\epsilon^2) \right] \left[1 - \epsilon \frac{i}{\hbar} V(x_b, t_b) + \mathcal{O}(\epsilon^2) \right] (x_b, t_b - \epsilon | x_a t_a). \quad (2.61)$$

In the limit $\epsilon \to 0$, this yields again the Schrödinger equation. (2.23).

In the continuum limit, we write the amplitude (2.54) as a path integral

$$(x_b t_b | x_a t_a) \equiv \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x\, e^{i\mathcal{A}[x]/\hbar}. \quad (2.62)$$

This is Feynman's original formula for the quantum-mechanical amplitude (2.1). It consists of a sum over all paths in configuration space with a phase factor containing the form of the action $\mathcal{A}[x]$.

We have used the same measure symbol $\mathcal{D}x$ for the paths in configuration space as for the completely different paths in phase space in the expressions (2.29), (2.38), (2.46), (2.47). There should be no danger of confusion. Note that the extra dp_n-integration in the phase space formula (2.14) results now in one extra $1/\sqrt{2\pi\hbar i\epsilon/M}$ factor in (2.54) which is not accompanied by a dx_n-integration.

The Feynman amplitude can be used to calculate the quantum-mechanical partition function (2.43) as a configuration space path integral

$$Z_{\rm QM} = \oint \mathcal{D}x\, e^{i\mathcal{A}[x]/\hbar}. \tag{2.63}$$

As in (2.45), (2.46), the symbol $\oint \mathcal{D}x$ indicates that the paths have equal endpoints $x(t_a) = x(t_b)$, the path integral being the continuum limit of the product of integrals

$$\oint \mathcal{D}x \approx \prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{2\pi i\hbar\epsilon/M}}. \tag{2.64}$$

There is no extra $1/\sqrt{2\pi i\hbar\epsilon/M}$ factor as in (2.54) and (2.62), due to the integration over the initial (= final) position $x_b = x_a$ representing the quantum-mechanical trace. The use of the same symbol $\oint \mathcal{D}x$ as in (2.48) should not cause any confusion since (2.48) is always accompanied by an integral $\int \mathcal{D}p$.

For the sake of generality we might point out that it is not necessary to slice the time axis in an equidistant way. In the continuum limit $N \to \infty$, the canonical path integral (2.14) is *indifferent* to the choice of the infinitesimal spacings

$$\epsilon_n = t_n - t_{n-1}. \tag{2.65}$$

The configuration space formula contains the different spacings ϵ_n in the following way: When performing the p_n integrations, we obtain a formula of the type (2.54), with each ϵ replaced by ϵ_n, i.e.,

$$(x_b t_b|x_a t_a) \approx \frac{1}{\sqrt{2\pi\hbar i\epsilon_b/M}} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{2\pi i\hbar\epsilon_n/M}} \right] \times \exp\left\{ \frac{i}{\hbar} \sum_{n=1}^{N+1} \left[\frac{M}{2} \frac{(x_n - x_{n-1})^2}{\epsilon_n} - \epsilon_n V(x_n, t_n) \right] \right\}. \tag{2.66}$$

To end this section, an important remark is necessary: It would certainly be possible to *define* the path integral for the time evolution amplitude (2.29), without going through Feynman's time-slicing procedure, as the solution of the Schrödinger differential equation [see Eq. (1.308))]:

$$[\hat{H}(-i\hbar\partial_x, x) - i\hbar\partial_t](x\, t|x_a t_a) = -i\hbar\delta(t - t_a)\delta(x - x_a). \tag{2.67}$$

If one possesses an orthonormal and complete set of wave functions $\psi_n(x)$ solving the time-independent Schrödinger equation $\hat{H}\psi_n(x)=E_n\psi_n(x)$, this solution is given by the spectral representation (1.323)

$$(x_b t_b | x_a t_a) = \Theta(t_b - t_a) \sum_n \psi_n(x_b)\psi_n^*(x_a) e^{-iE_n(t_b-t_a)/\hbar}, \tag{2.68}$$

where $\Theta(t)$ is the Heaviside function (1.304). This definition would, however, run contrary to the very purpose of Feynman's path integral approach, which is to understand a quantum system from the global all-time fluctuation point of view. The goal is to find all properties from the globally defined time evolution amplitude, in particular the Schrödinger wave functions.[3] The global approach is usually more complicated than Schrödinger's and, as we shall see in Chapters 8 and 12–14, contains novel subtleties caused by the finite time slicing. Nevertheless, it has at least four important advantages. First, it is conceptually very attractive by formulating a quantum theory without operators which describe quantum fluctuations by close analogy with thermal fluctuations (as will be seen later in this chapter). Second, it links quantum mechanics smoothly with classical mechanics (as will be shown in Chapter 4). Third, it offers new variational procedures for the approximate study of complicated quantum-mechanical and -statistical systems (see Chapter 5). Fourth, it gives a natural geometric access to the dynamics of particles in spaces with curvature and torsion (see Chapters 10–11). This has recently led to results where the operator approach has failed due to operator-ordering problems, giving rise to a unique and correct description of the quantum dynamics of a particle in spaces with curvature and torsion. From this it is possible to derive a unique extension of Schrödinger's theory to such general spaces whose predictions can be tested in future experiments.[4]

2.2 Exact Solution for the Free Particle

In order to develop some experience with Feynman's path integral formula we consider in detail the simplest case of a free particle, which in the canonical form reads

$$(x_b t_b | x_a t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt \left(p\dot{x} - \frac{p^2}{2M}\right)\right], \tag{2.69}$$

and in the pure configuration form:

$$(x_b t_b | x_a t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt \frac{M}{2}\dot{x}^2\right]. \tag{2.70}$$

Since the integration limits are obvious by looking at the left-hand sides of the equations, they will be omitted from now on, unless clarity requires their specification.

[3] Many publications claiming to have solved the path integral of a system have violated this rule by implicitly using the Schrödinger equation, although camouflaged by complicated-looking path integral notation.

[4] H. Kleinert, Mod. Phys. Lett. A *4*, 2329 (1989) (`http://www.physik.fu-berlin.de/~kleinert/199`); Phys. Lett. B *236*, 315 (1990) (*ibid.*`http/202`).

2.2.1 Trivial Solution

Since the Hamiltonian of a free particle $H = p^2/2M$ does not depend on x, the path integral in momentum space yields the simple result (2.40). In configuration space it reduces to simple Fourier integral Eq. (2.41). Inserting the above Hamiltonian, the integral reads

$$(x_b t_b|x_a t_a) = \int \frac{dp}{2\pi\hbar} e^{ip(x_b-x_a)/\hbar - i(t_b-t_a)p^2/2M\hbar}, \tag{2.71}$$

and can be done with the help of the Fresnel formula (2.53). The result is

$$(x_b t_b|x_a t_a) = \frac{1}{\sqrt{2\pi i\hbar(t_b-t_a)/M}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x_b-x_a)^2}{t_b-t_a}\right]. \tag{2.72}$$

This result is easily generalized to D dimensions, where the free-particle amplitude (2.40) reads

$$(\mathbf{p}_b t_b|\mathbf{p}_a t_a) = (2\pi\hbar)^D \delta^{(D)}(\mathbf{p}_b - \mathbf{p}_a) e^{-i(t_b-t_a)\mathbf{p}^2/2M\hbar}, \tag{2.73}$$

and the Fourier transform yields

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \frac{1}{\sqrt{2\pi i\hbar(t_b-t_a)/M}^D} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\mathbf{x}_b-\mathbf{x}_a)^2}{t_b-t_a}\right], \tag{2.74}$$

in agreement with the quantum-mechanical result in D dimensions (1.341).

2.2.2 Solution in Configuration Space

The problem can also be solved with little effort starting from Eq. (2.70). The time-sliced expression to be integrated is given by Eqs. (2.54), (2.55) with $V(x)$ set equal to zero. The resulting product of Gaussian integrals can easily be done successively using formula (1.337), from which we derive the simple rule

$$\begin{aligned}\int dx' \frac{1}{\sqrt{2\pi i\hbar A\epsilon/M}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x''-x')^2}{A\epsilon}\right] \frac{1}{\sqrt{2\pi i\hbar B\epsilon/M}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x'-x)^2}{B\epsilon}\right] \\ = \frac{1}{\sqrt{2\pi i\hbar(A+B)\epsilon/M}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x''-x)^2}{(A+B)\epsilon}\right],\end{aligned} \tag{2.75}$$

which leads directly to the free-particle amplitude

$$(x_b t_b|x_a t_a) = \frac{1}{\sqrt{2\pi i\hbar(N+1)\epsilon/M}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x_b-x_a)^2}{(N+1)\epsilon}\right]. \tag{2.76}$$

After inserting $(N+1)\epsilon = t_b - t_a$, this agrees with the previous result (2.72). Note that the free-particle amplitude happens to be independent of the number $N+1$ of time slices.

The calculation shows that the path integrals (2.69) and (2.70) possess a simple solvable generalization to a time-dependent mass $M(t) = Mg(t)$:

$$(x_b t_b | x_a t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt \left(p\dot{x} - \frac{p^2}{2Mg(t)}\right)\right], \tag{2.77}$$

and in the pure configuration form:

$$(x_b t_b | x_a t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x\sqrt{g} \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt \frac{M}{2} g(t)\dot{x}^2(t)\right]. \tag{2.78}$$

Here the measure of integration $\int \mathcal{D}x\sqrt{g}$ symbolizes the continuum limit of the product [compare (2.54)]:

$$\int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x\sqrt{g} \equiv \frac{1}{\sqrt{2\pi\hbar i\epsilon/Mg(t_b)}} \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{2\pi\hbar i\epsilon/Mg(t_n)}}\right]. \tag{2.79}$$

The factor $g(t_n)$ enters in each of the integrations (2.75), where the previous time slicing parameters ϵ becomes now $\epsilon_n = \epsilon/g(t_n)$, and we find instead of (2.72) the amplitude

$$(x_b t_b | x_a t_a) \;=\; \frac{1}{\sqrt{2\pi i\hbar M^{-1}\int_{t_a}^{t_b} g^{-1}(t)}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x_b - x_a)^2}{\int_{t_a}^{t_b} g^{-1}(t)}\right]. \tag{2.80}$$

This has the Fourier representation

$$(x_b t_b | x_a t_a) \;=\; \int \frac{dp}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\left[ip(x_b - x_a) - \frac{p^2}{2M}\int_{t_a}^{t_b} g^{-1}(t)\right]\right\}. \tag{2.81}$$

2.2.3 Fluctuations around the Classical Path

There exists yet another method of calculating this amplitude which is somewhat involved than the simple case at hand deserves, but which turns out to be useful for the treatment of a certain class of more complicated path integrals, after a suitable generalization. This method is based on summing aver all path deviations from the classical path, i.e., all paths are split into the classical path

$$x_{\rm cl}(t) = x_a + \frac{x_b - x_a}{t_b - t_a}(t - t_a), \tag{2.82}$$

along which the free particle would run following the equation of motion

$$\ddot{x}_{\rm cl}(t) = 0, \tag{2.83}$$

plus deviations $\delta x(t)$:

$$x(t) = x_{\rm cl}(t) + \delta x(t). \tag{2.84}$$

Since the initial and final points are fixed at x_a, x_b, respectively, the deviations vanish at the endpoints:

$$\delta x(t_a) = \delta x(t_b) = 0. \tag{2.85}$$

The deviations $\delta x(t)$ are referred to as the *quantum fluctuations* of the particle orbit. In mathematics, the boundary conditions (2.85) are referred to as *Dirichlet boundary conditions*. When inserting the decomposition (2.84) into the action we observe that due to the equation of motion (2.83) for the classical path, the action separates into the sum of a classical and a purely quadratic fluctuation term

$$\begin{aligned}
&\frac{M}{2}\int_{t_a}^{t_b} dt\left\{\dot{x}_{\rm cl}^2(t) + 2\dot{x}_{\rm cl}(t)\delta\dot{x}(t) + [\delta\dot{x}(t)]^2\right\}\\
&\quad = \frac{M}{2}\int_{t_a}^{t_b} dt\dot{x}_{\rm cl}^2 + M\dot{x}\delta x\Big|_{t_a}^{t_b} - M\int_{t_a}^{t_b} dt\ddot{x}_{\rm cl}\delta x + \frac{M}{2}\int_{t_a}^{t_b} dt(\delta\dot{x})^2\\
&\quad = \frac{M}{2}\left[\int_{t_a}^{t_b} dt\dot{x}_{\rm cl}^2 + \int_{t_a}^{t_b} dt(\delta\dot{x})^2\right].
\end{aligned}$$

The absence of a mixed term is a general consequence of the extremality property of the classical path,

$$\delta\mathcal{A}\Big|_{x(t)=x_{\rm cl}(t)} = 0. \tag{2.86}$$

It implies that a quadratic *fluctuation expansion* around the classical action

$$\mathcal{A}_{\rm cl} \equiv \mathcal{A}[x_{\rm cl}] \tag{2.87}$$

can have no linear term in $\delta x(t)$, i.e., it must start as

$$\mathcal{A} = \mathcal{A}_{\rm cl} + \frac{1}{2}\int_{t_a}^{t_b} dt\int_{t_a}^{t_b} dt'\frac{\delta^2\mathcal{A}}{\delta x(t)\delta x(t')}\delta x(t)\delta x(t')\Big|_{x(t)=x_{\rm cl}(t)} + \dots\,. \tag{2.88}$$

With the action being a sum of two terms, the amplitude factorizes into the product of a classical amplitude $e^{i\mathcal{A}_{\rm cl}/\hbar}$ and a fluctuation factor $F_0(t_b - t_a)$,

$$(x_bt_b|x_at_a) = \int\mathcal{D}x\, e^{i\mathcal{A}[x]/\hbar} = e^{i\mathcal{A}_{\rm cl}/\hbar}F_0(t_b, t_a). \tag{2.89}$$

For the free particle with the classical action

$$\mathcal{A}_{\rm cl} = \int_{t_a}^{t_b} dt\frac{M}{2}\dot{x}_{\rm cl}^2, \tag{2.90}$$

the function factor $F_0(t_b - t_a)$ is given by the path integral

$$F_0(t_b - t_a) = \int\mathcal{D}\delta x(t)\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\frac{M}{2}(\delta\dot{x})^2\right]. \tag{2.91}$$

Due to the vanishing of $\delta x(t)$ at the endpoints, this does not depend on x_b, x_a but only on the initial and final times t_b, t_a. The time translational invariance reduces this dependence further to the time difference $t_b - t_a$. The subscript zero of $F_0(t_b - t_a)$ indicates the free-particle nature of the fluctuation factor. After inserting (2.82) into (2.90), we find immediately

$$\mathcal{A}_{\rm cl} = \frac{M}{2}\frac{(x_b - x_a)^2}{t_b - t_a}. \tag{2.92}$$

The fluctuation factor, on the other hand, requires the evaluation of the multiple integral

$$F_0^N(t_b - t_a) = \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \frac{d\delta x_n}{\sqrt{2\pi\hbar i\epsilon/M}}\right] \exp\left(\frac{i}{\hbar}\mathcal{A}_{\rm fl}^N\right), \tag{2.93}$$

where $\mathcal{A}_{\rm fl}^N$ is the time-sliced fluctuation action

$$\mathcal{A}_{\rm fl}^N = \frac{M}{2}\epsilon \sum_{n=1}^{N+1} \left(\frac{\delta x_n - \delta x_{n-1}}{\epsilon}\right)^2. \tag{2.94}$$

At the end, we have to take the continuum limit

$$N \to \infty, \quad \epsilon = (t_b - t_a)/(N+1) \to 0.$$

2.2.4 Fluctuation Factor

The remainder of this section will be devoted to calculating the fluctuation factor (2.93). Before doing this, we shall develop a general technique for dealing with such time-sliced expressions. Due to the frequent appearance of the fluctuating δx-variables, we shorten the notation by omitting all δ's and working only with x-variables.

A useful device for manipulating sums on a sliced time axis such as (2.94) is the difference operator ∇ and its conjugate $\overline{\nabla}$, defined by

$$\nabla x(t) \equiv \frac{1}{\epsilon}[x(t+\epsilon) - x(t)], \qquad \overline{\nabla} x(t) \equiv \frac{1}{\epsilon}[x(t) - x(t-\epsilon)]. \tag{2.95}$$

They are two different discrete versions of the time derivative ∂_t, to which both reduce in the continuum limit $\epsilon \to 0$:

$$\nabla, \overline{\nabla} \xrightarrow{\epsilon \to 0} \partial_t, \tag{2.96}$$

if they act upon differentiable functions. Since the discretized time axis with $N+1$ steps constitutes a one-dimensional lattice, the difference operators $\nabla, \overline{\nabla}$ are also called *lattice derivatives*.

For the coordinates $x_n = x(t_n)$ at the discrete times t_n we write

$$\begin{aligned} \nabla x_n &= \frac{1}{\epsilon}(x_{n+1} - x_n), \qquad N \geq n \geq 0, \\ \overline{\nabla} x_n &= \frac{1}{\epsilon}(x_n - x_{n-1}), \qquad N+1 \geq n \geq 1. \end{aligned} \tag{2.97}$$

The time-sliced action (2.94) can then be expressed in terms of ∇x_n or $\overline{\nabla} x_n$ as (writing x_n instead of δx_n)

$$\mathcal{A}_{\rm fl}^N = \frac{M}{2}\epsilon\sum_{n=0}^{N}(\nabla x_n)^2 = \frac{M}{2}\epsilon\sum_{n=1}^{N+1}(\overline{\nabla} x_n)^2. \qquad (2.98)$$

In this notation, the limit $\epsilon \to 0$ is most obvious: The sum $\epsilon\sum_n$ goes into the integral $\int_{t_a}^{t_b} dt$, whereas both $(\nabla x_n)^2$ and $(\overline{\nabla} x_n)^2$ tend to $\dot{x}^2$, so that

$$\mathcal{A}_{\rm fl}^N \to \int_{t_a}^{t_b} dt \frac{M}{2}\dot{x}^2. \qquad (2.99)$$

Thus, the time-sliced action becomes the Lagrangian action.

Lattice derivatives have properties quite similar to ordinary derivatives. One only has to be careful in distinguishing ∇ and $\overline{\nabla}$. For example, they allow for the useful operation *summation by parts* which is analogous to integration by parts. Recall the rule for the integration by parts

$$\int_{t_a}^{t_b} dt g(t)\dot{f}(t) = g(t)f(t)\Big|_{t_a}^{t_b} - \int_{t_a}^{t_b} dt\dot{g}(t)f(t). \qquad (2.100)$$

On the lattice, this relation yields for functions $f(t) \to x_n$ and $g(t) \to p_n$:

$$\epsilon\sum_{n=1}^{N+1} p_n\overline{\nabla} x_n = p_n x_n\big|_0^{N+1} - \epsilon\sum_{n=0}^{N}(\nabla p_n)x_n. \qquad (2.101)$$

This follows directly by rewriting (2.35).

For functions vanishing at the endpoints, i.e., for $x_{N+1} = x_0 = 0$, we can omit the surface terms and shift the range of the sum on the right-hand side to obtain the simple formula [see also Eq. (2.49)]

$$\sum_{n=1}^{N+1} p_n\overline{\nabla} x_n = -\sum_{n=0}^{N}(\nabla p_n)x_n = -\sum_{n=1}^{N+1}(\nabla p_n)x_n. \qquad (2.102)$$

The same thing holds if both $p(t)$ and $x(t)$ are periodic in the interval $t_b - t_a$, so that $p_0 = p_{N+1},\ x_0 = x_{N+1}$. In this case, it is possible to shift the sum on the right-hand side by one unit arriving at the more symmetric-looking formula

$$\sum_{n=1}^{N+1} p_n\overline{\nabla} x_n = -\sum_{n=1}^{N+1}(\nabla p_n)x_n. \qquad (2.103)$$

In the time-sliced action (2.94) the quantum fluctuations x_n ($\hat{=}\delta x_n$) vanish at the ends, so that (2.102) can be used to rewrite

$$\sum_{n=1}^{N+1}(\overline{\nabla} x_n)^2 = -\sum_{n=1}^{N} x_n\nabla\overline{\nabla} x_n. \qquad (2.104)$$

In the ∇x_n -form of the action (2.98), the same expression is obtained by applying formula (2.102) from the right- to the left-hand side and using the vanishing of x_0 and x_{N+1}:

$$\sum_{n=0}^{N}(\nabla x_n)^2 = -\sum_{n=1}^{N+1} x_n \overline{\nabla}\nabla x_n = -\sum_{n=1}^{N} x_n \overline{\nabla}\nabla x_n. \tag{2.105}$$

The right-hand sides in (2.104) and (2.105) can be written in matrix form as

$$\begin{aligned}
-\sum_{n=1}^{N} x_n \nabla\overline{\nabla} x_n &\equiv -\sum_{n,n'=1}^{N} x_n (\nabla\overline{\nabla})_{nn'} x_{n'}, \\
-\sum_{n=1}^{N} x_n \overline{\nabla}\nabla x_n &\equiv -\sum_{n,n'=1}^{N} x_n (\overline{\nabla}\nabla)_{nn'} x_{n'},
\end{aligned} \tag{2.106}$$

with the same $N \times N$ -matrix

$$\nabla\overline{\nabla} \equiv \overline{\nabla}\nabla \equiv \frac{1}{\epsilon^2}\begin{pmatrix} -2 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & -2 \end{pmatrix}. \tag{2.107}$$

This is obviously the lattice version of the double time derivative ∂_t^2, to which it reduces in the continuum limit $\epsilon \to 0$. It will therefore be called the *lattice Laplacian*.

A further common property of lattice and ordinary derivatives is that they can both be diagonalized by going to Fourier components. When decomposing

$$x(t) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} x(\omega), \tag{2.108}$$

and applying the lattice derivative ∇, we find

$$\begin{aligned}
\nabla x(t_n) &= \int_{-\infty}^{\infty} d\omega \, \frac{1}{\epsilon}\left(e^{-i\omega(t_n+\epsilon)} - e^{-i\omega t_n}\right) x(\omega) \\
&= \int_{-\infty}^{\infty} d\omega e^{-i\omega t_n} \frac{1}{\epsilon}(e^{-i\omega\epsilon} - 1) \; x(\omega).
\end{aligned} \tag{2.109}$$

Hence, on the Fourier components, ∇ has the eigenvalues

$$\frac{1}{\epsilon}(e^{-i\omega\epsilon} - 1). \tag{2.110}$$

In the continuum limit $\epsilon \to 0$, this becomes the eigenvalue of the ordinary time derivative ∂_t, i.e., $-i$ times the frequency of the Fourier component ω. As a reminder of this we shall denote the eigenvalue of $i\nabla$ by Ω and have

$$(i\nabla x)(\omega) = \Omega \; x(\omega) \equiv \frac{i}{\epsilon}(e^{-i\omega\epsilon} - 1) \; x(\omega). \tag{2.111}$$

For the conjugate lattice derivative we find similarly

$$(i\overline{\nabla}x)(\omega) = \overline{\Omega}\ x(\omega) \equiv -\frac{i}{\epsilon}(e^{i\omega\epsilon} - 1)\ x(\omega), \tag{2.112}$$

where $\overline{\Omega}$ is the complex-conjugate number of Ω, i.e., $\overline{\Omega} \equiv \Omega^*$. As a consequence, the eigenvalues of the negative lattice Laplacian $-\nabla\overline{\nabla}\equiv-\overline{\nabla}\nabla$ are real and nonnegative:

$$\frac{i}{\epsilon}(e^{-i\omega\epsilon} - 1)\frac{i}{\epsilon}(1 - e^{i\omega\epsilon}) = \frac{1}{\epsilon^2}[2 - 2\cos(\omega\epsilon)] \geq 0. \tag{2.113}$$

Of course, Ω and $\bar{\Omega}$ have the same continuum limit ω.

When decomposing the quantum fluctuations $x(t)$ [$\hat{=}\delta x(t)$] into their Fourier components, not all eigenfunctions occur. Since $x(t)$ vanishes at the initial time $t = t_a$, the decomposition can be restricted to the sine functions and we may expand

$$x(t) = \int_0^\infty d\omega \sin\omega(t - t_a)\ x(\omega). \tag{2.114}$$

The vanishing at the final time $t = t_b$ is enforced by a restriction of the frequencies ω to the discrete values

$$\nu_m = \frac{\pi m}{t_b - t_a} = \frac{\pi m}{(N+1)\epsilon}. \tag{2.115}$$

Thus we are dealing with the Fourier series

$$x(t) = \sum_{m=1}^{\infty} \sqrt{\frac{2}{(t_b - t_a)}} \sin\nu_m(t - t_a)\, x(\nu_m) \tag{2.116}$$

with real Fourier components $x(\nu_m)$. A further restriction arises from the fact that for finite ϵ, the series has to represent $x(t)$ only at the discrete points $x(t_n)$, $n = 0, \dots, N+1$. It is therefore sufficient to carry the sum only up to $m = N$ and to expand $x(t_n)$ as

$$x(t_n) = \sum_{m=1}^{N} \sqrt{\frac{2}{N+1}} \sin\nu_m(t_n - t_a)\, x(\nu_m), \tag{2.117}$$

where a factor $\sqrt{\epsilon}$ has been removed from the Fourier components, for convenience. The expansion functions are orthogonal,

$$\frac{2}{N+1}\sum_{n=1}^{N} \sin\nu_m(t_n - t_a)\ \sin\nu_{m'}(t_n - t_a) = \delta_{mm'}, \tag{2.118}$$

and complete:

$$\frac{2}{N+1}\sum_{m=1}^{N} \sin\nu_m(t_n - t_a)\ \sin\nu_m(t_{n'} - t_a) = \delta_{nn'} \tag{2.119}$$

(where $0 < m, m' < N+1$). The orthogonality relation follows by rewriting the left-hand side of (2.118) in the form

$$\frac{2}{N+1}\frac{1}{2}\,\mathrm{Re}\sum_{n=0}^{N+1}\left\{\exp\left[\frac{i\pi(m-m')}{N+1}n\right]-\exp\left[\frac{i\pi(m+m')}{N+1}n\right]\right\}, \tag{2.120}$$

with the sum extended without harm by a trivial term at each end. Being of the geometric type, this can be calculated right away. For $m = m'$ the sum adds up to 1, while for $m \neq m'$ it becomes

$$\frac{2}{N+1}\frac{1}{2}\mathrm{Re}\left[\frac{1-e^{i\pi(m-m')}e^{i\pi(m-m')/(N+1)}}{1-e^{i\pi(m-m')/(N+1)}}-(m'\to -m')\right]. \tag{2.121}$$

The first expression in the curly brackets is equal to 1 for even $m - m' \neq 0$; while being imaginary for odd $m - m'$ [since $(1+e^{i\alpha})/(1-e^{i\alpha})$ is equal to $(1+e^{i\alpha})(1-e^{-i\alpha})/|1-e^{i\alpha}|^2$ with the imaginary numerator $e^{i\alpha}-e^{-i\alpha}$]. For the second term the same thing holds true for even and odd $m + m' \neq 0$, respectively. Since $m - m'$ and $m + m'$ are either both even or both odd, the right-hand side of (2.118) vanishes for $m \neq m'$ [remembering that $m,\ m' \in [0, N+1]$ in the expansion (2.117), and thus in (2.121)]. The proof of the completeness relation (2.119) can be carried out similarly.

Inserting now the expansion (2.117) into the time-sliced fluctuation action (2.94), the orthogonality relation (2.118) yields

$$\mathcal{A}_{\mathrm{fl}}^N = \frac{M}{2}\epsilon\sum_{n=0}^{N}(\overline{\nabla}x_n)^2 = \frac{M}{2}\epsilon\sum_{m=1}^{N+1}x(\nu_m)\Omega_m\overline{\Omega}_m x(\nu_m). \tag{2.122}$$

Thus the action decomposes into a sum of independent quadratic terms involving the discrete set of eigenvalues

$$\Omega_m\overline{\Omega}_m = \frac{1}{\epsilon^2}[2-2\cos(\nu_m\epsilon)] = \frac{1}{\epsilon^2}\left[2-2\cos\left(\frac{\pi m}{N+1}\right)\right], \tag{2.123}$$

and the fluctuation factor (2.93) becomes

$$\begin{aligned} F_0^N(t_b-t_a) = {} & \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}}\prod_{n=1}^{N}\left[\int_{-\infty}^{\infty}\frac{dx_n}{\sqrt{2\pi\hbar i\epsilon/M}}\right] \\ & \times\prod_{m=1}^{N}\exp\left\{\frac{i}{\hbar}\frac{M}{2}\epsilon\Omega_m\overline{\Omega}_m\,[x(\nu_m)]^2\right\}. \end{aligned} \tag{2.124}$$

Before performing the integrals, we must transform the measure of integration from the local variables x_n to the Fourier components $x(\nu_m)$. Due to the orthogonality relation (2.118), the transformation has a unit determinant implying that

$$\prod_{n=1}^{N}dx_n = \prod_{m=1}^{N}dx(\nu_m). \tag{2.125}$$

With this, Eq. (2.124) can be integrated with the help of Fresnel's formula (1.337). The result is

$$F_0^N(t_b - t_a) = \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}} \prod_{m=1}^{N} \frac{1}{\sqrt{\epsilon^2 \Omega_m \overline{\Omega}_m}}. \tag{2.126}$$

To calculate the product we use the formula[5]

$$\prod_{m=1}^{N} \left(1 + x^2 - 2x \cos \frac{m\pi}{N+1}\right) = \frac{x^{2(N+1)} - 1}{x^2 - 1}. \tag{2.127}$$

Taking the limit $x \to 1$ gives

$$\prod_{m=1}^{N} \epsilon^2 \Omega_m \overline{\Omega}_m = \prod_{m=1}^{N} 2\left(1 - \cos \frac{m\pi}{N+1}\right) = N + 1. \tag{2.128}$$

The time-sliced fluctuation factor of a free particle is therefore simply

$$F_0^N(t_b - t_a) = \frac{1}{\sqrt{2\pi i\hbar(N+1)\epsilon/M}}, \tag{2.129}$$

or, expressed in terms of $t_b - t_a$,

$$F_0(t_b - t_a) = \frac{1}{\sqrt{2\pi i\hbar(t_b - t_a)/M}}. \tag{2.130}$$

As in the amplitude (2.72) we have dropped the superscript N since this final result is independent of the number of time slices.

Note that the dimension of the fluctuation factor is 1/length. In fact, one may introduce a length scale associated with the time interval $t_b - t_a$,

$$l(t_b - t_a) \equiv \sqrt{2\pi\hbar(t_b - t_a)/M}, \tag{2.131}$$

and write

$$F_0(t_b - t_a) = \frac{1}{\sqrt{i}\, l(t_b - t_a)}. \tag{2.132}$$

With (2.130) and (2.92), the full time evolution amplitude of a free particle (2.89) is again given by (2.72)

$$(x_b t_b | x_a t_a) = \frac{1}{\sqrt{2\pi i\hbar(t_b - t_a)/M}} \exp\left[\frac{i}{\hbar} \frac{M}{2} \frac{(x_b - x_a)^2}{t_b - t_a}\right]. \tag{2.133}$$

It is instructive to present an alternative calculation of the product of eigenvalues in (2.126) which does not make use of the Fourier decomposition and works entirely in configuration space. We observe that the product

$$\prod_{m=1}^{N} \epsilon^2 \Omega_m \overline{\Omega}_m \tag{2.134}$$

[5] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formula 1.396.2.

is the determinant of the diagonalized $N \times N$ -matrix $-\epsilon^2\nabla\overline{\nabla}$. This follows from the fact that for any matrix, the determinant is the product of its eigenvalues. The product (2.134) is therefore also called the *fluctuation determinant* of the free particle and written

$$\prod_{m=1}^{N} \epsilon^2 \Omega_m \overline{\Omega}_m \equiv \det{}_N(-\epsilon^2\nabla\overline{\nabla}). \tag{2.135}$$

With this notation, the fluctuation factor (2.126) reads

$$F_0^N(t_b - t_b) = \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}} \left[\det{}_N(-\epsilon^2\nabla\overline{\nabla})\right]^{-1/2}. \tag{2.136}$$

Now one realizes that the determinant of $\epsilon^2\overline{\nabla}\nabla$ can be found very simply from the explicit $N \times N$ matrix (2.107) by induction: For $N = 1$ we see directly that

$$\det{}_{N=1}(-\epsilon^2\nabla\overline{\nabla}) = |2| = 2. \tag{2.137}$$

For $N = 2$, the determinant is

$$\det{}_{N=2}(-\epsilon^2\nabla\overline{\nabla}) = \begin{vmatrix} 2 & -1 \\ -1 & 2 \end{vmatrix} = 3. \tag{2.138}$$

A recursion relation is obtained by developing the determinant twice with respect to the first row:

$$\det{}_N(-\epsilon^2\nabla\overline{\nabla}) = 2 \det{}_{N-1}(-\epsilon^2\nabla\overline{\nabla}) - \det{}_{N-2}(-\epsilon^2\nabla\overline{\nabla}). \tag{2.139}$$

With the initial condition (2.137), the solution is

$$\det{}_N(-\epsilon^2\nabla\overline{\nabla}) = N + 1, \tag{2.140}$$

in agreement with the previous result (2.128).

2.2.5 Finite Slicing Properties of Free-Particle Amplitude

The time-sliced free-particle time evolution amplitude (2.76) happens to be independent of the number N of time slices used for their calculation. We have pointed this out earlier for the fluctuation factor (2.129). Let us study the origin of this independence for the classical action in the exponent. The difference equation of motion

$$-\overline{\nabla}\nabla x(t) = 0 \tag{2.141}$$

is solved by the same linear function

$$x(t) = At + B, \tag{2.142}$$

as in the continuum. Imposing the initial conditions gives

$$x_{\rm cl}(t_n) = x_a + (x_b - x_a)\frac{n}{N+1}. \tag{2.143}$$

The time-sliced action of the fluctuations is calculated, via a summation by parts on the lattice [see (2.101)]. Using the difference equation $\overline{\nabla}\nabla x_{\rm cl} = 0$, we find

$$\begin{aligned}
\mathcal{A}_{\rm cl} &= \epsilon \sum_{n=1}^{N+1} \frac{M}{2}(\overline{\nabla} x_{\rm cl})^2 \qquad (2.144)\\
&= \frac{M}{2}\left(x_{\rm cl}\nabla x_{\rm cl}\Big|_{n=0}^{N+1} - \epsilon \sum_{n=0}^{N} x_{\rm cl}\nabla\overline{\nabla} x_{\rm cl}\right)\\
&= \frac{M}{2} x_{\rm cl}\nabla x_{\rm cl}\Big|_{n=0}^{N+1} = \frac{M}{2}\frac{(x_b - x_a)^2}{t_b - t_a}.
\end{aligned}$$

This coincides with the continuum action for any number of time slices.

In the operator formulation of quantum mechanics, the ϵ-independence of the amplitude of the free particle follows from the fact that in the absence of a potential $V(x)$, the two sides of the Trotter formula (2.26) coincide for any N.

2.3 Exact Solution for Harmonic Oscillator

A further problem to be solved along similar lines is the time evolution amplitude of the linear oscillator

$$\begin{aligned}
(x_b t_b | x_a t_a) &= \int \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\mathcal{A}[p,x]\right\}\\
&= \int \mathcal{D}x \exp\left\{\frac{i}{\hbar}\mathcal{A}[x]\right\}, \qquad (2.145)
\end{aligned}$$

with the canonical action

$$\mathcal{A}[p,x] = \int_{t_a}^{t_b} dt \left(p\dot{x} - \frac{1}{2M}p^2 - \frac{M\omega^2}{2}x^2 \right), \tag{2.146}$$

and the Lagrangian action

$$\mathcal{A}[x] = \int_{t_a}^{t_b} dt\, \frac{M}{2}(\dot{x}^2 - \omega^2 x^2). \tag{2.147}$$

2.3.1 Fluctuations around the Classical Path

As before, we proceed with the Lagrangian path integral, starting from the time-sliced form of the action

$$\mathcal{A}^N = \epsilon \frac{M}{2} \sum_{n=1}^{N+1} \left[(\overline{\nabla} x_n)^2 - \omega^2 x_n^2 \right]. \tag{2.148}$$

The path integral is again a product of Gaussian integrals which can be evaluated successively. In contrast to the free-particle case, however, the direct evaluation is now quite complicated; it will be presented in Appendix 2B. It is far easier to employ the fluctuation expansion, splitting the paths into a classical path $x_{\rm cl}(t)$ plus fluctuations $\delta x(t)$. The fluctuation expansion makes use of the fact that the action is quadratic in $x = x_{\rm cl} + \delta x$ and decomposes into the sum of a classical part

$$\mathcal{A}_{\rm cl} = \int_{t_a}^{t_b} dt \frac{M}{2}(\dot{x}_{\rm cl}^2 - \omega^2 x_{\rm cl}^2), \tag{2.149}$$

and a fluctuation part

$$\mathcal{A}_{\rm fl} = \int_{t_a}^{t_b} dt \frac{M}{2}[(\delta\dot{x})^2 - \omega^2(\delta x)^2], \tag{2.150}$$

with the boundary condition

$$\delta x(t_a) = \delta x(t_b) = 0. \tag{2.151}$$

There is no mixed term, due to the extremality of the classical action. The equation of motion is

$$\ddot{x}_{\rm cl} = -\omega^2 x_{\rm cl}. \tag{2.152}$$

Thus, as for a free-particle, the total time evolution amplitude splits into a classical and a fluctuation factor:

$$(x_b t_b|x_a t_a) = \int \mathcal{D}x \, e^{i\mathcal{A}[x]/\hbar} = e^{i\mathcal{A}_{\rm cl}/\hbar} F_\omega(t_b - t_a). \tag{2.153}$$

The subscript of F_ω records the frequency of the oscillator.

The classical orbit connecting initial and final points is obviously

$$x_{\rm cl}(t) = \frac{x_b \sin\omega(t - t_a) + x_a \sin\omega(t_b - t)}{\sin\omega(t_b - t_a)}. \tag{2.154}$$

Note that this equation only makes sense if $t_b - t_a$ is not equal to an integer multiple of π/ω which we shall always assume from now on.[6]

After an integration by parts we can rewrite the classical action $\mathcal{A}_{\rm cl}$ as

$$\mathcal{A}_{\rm cl} = \int_{t_a}^{t_b} dt \frac{M}{2}\left[x_{\rm cl}(-\ddot{x}_{\rm cl} - \omega^2 x_{\rm cl})\right] + \frac{M}{2} x_{\rm cl}\dot{x}_{\rm cl}\Big|_{t_a}^{t_b} . \tag{2.155}$$

The first term vanishes due to the equation of motion (2.152), and we obtain the simple expression

$$\mathcal{A}_{\rm cl} = \frac{M}{2}[x_{\rm cl}(t_b)\dot{x}_{\rm cl}(t_b) - x_{\rm cl}(t_a)\dot{x}_{\rm cl}(t_a)]. \tag{2.156}$$

[6]For subtleties in the immediate neighborhood of the singularities which are known as *caustic phenomena*, see Notes and References at the end of the chapter, as well as Section 4.8.

Since

$$\dot{x}_{\rm cl}(t_a) = \frac{\omega}{\sin\omega(t_b-t_a)}[x_b - x_a\cos\omega(t_b-t_a)], \tag{2.157}$$

$$\dot{x}_{\rm cl}(t_b) = \frac{\omega}{\sin\omega(t_b-t_a)}[x_b\cos\omega(t_b-t_a) - x_a], \tag{2.158}$$

we can rewrite the classical action as

$$\mathcal{A}_{\rm cl} = \frac{M\omega}{2\sin\omega(t_b-t_a)}\left[(x_b^2+x_a^2)\cos\omega(t_b-t_a) - 2x_bx_a\right]. \tag{2.159}$$

2.3.2 Fluctuation Factor

We now turn to the fluctuation factor. With the matrix notation for the lattice operator $-\nabla\overline{\nabla} - \omega^2$, we have to solve the multiple integral

$$F_\omega^N(t_b,t_a) = \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}}\prod_{n=1}^N\left[\int_{-\infty}^{\infty}\frac{d\delta x_n}{\sqrt{2\pi\hbar i\epsilon/M}}\right] \times\exp\left\{\frac{i}{\hbar}\frac{M}{2}\epsilon\sum_{n,n'=1}^N \delta x_n[-\nabla\overline{\nabla}-\omega^2]_{nn'}\delta x_{n'}\right\}. \tag{2.160}$$

When going to the Fourier components of the paths, the integral factorizes in the same way as for the free-particle expression (2.124). The only difference lies in the eigenvalues of the fluctuation operator which are now

$$\Omega_m\overline{\Omega}_m - \omega^2 = \frac{1}{\epsilon^2}[2-2\cos(\nu_m\epsilon)] - \omega^2 \tag{2.161}$$

instead of $\Omega_m\overline{\Omega}_m$. For times t_b, t_a where all eigenvalues are positive (which will be specified below) we obtain from the upper part of the Fresnel formula (1.337) directly

$$F_\omega^N(t_b,t_a) = \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}}\prod_{m=1}^N\frac{1}{\sqrt{\epsilon^2\Omega_m\overline{\Omega}_m - \epsilon^2\omega^2}}. \tag{2.162}$$

The product of these eigenvalues is found by introducing an auxiliary frequency $\tilde{\omega}$ satisfying

$$\sin\frac{\epsilon\tilde{\omega}}{2} \equiv \frac{\epsilon\omega}{2}. \tag{2.163}$$

Then we decompose the product as

$$\prod_{m=1}^N[\epsilon^2\Omega_m\overline{\Omega}_m - \epsilon^2\omega^2] = \prod_{m=1}^N\left[\epsilon^2\Omega_m\overline{\Omega}_m\right]\prod_{m=1}^N\left[\frac{\epsilon^2\Omega_m\overline{\Omega}_m - \epsilon^2\omega^2}{\epsilon^2\Omega_m\overline{\Omega}_m}\right] = \prod_{m=1}^N\left[\epsilon^2\Omega_m\overline{\Omega}_m\right]\left[\prod_{m=1}^N\left(1-\frac{\sin^2\frac{\epsilon\tilde{\omega}}{2}}{\sin^2\frac{m\pi}{2(N+1)}}\right)\right]. \tag{2.164}$$

The first factor is equal to $(N+1)$ by (2.128). The second factor, the product of the ratios of the eigenvalues, is found from the standard formula[7]

$$\prod_{m=1}^{N}\left(1-\frac{\sin^2 x}{\sin^2\frac{m\pi}{2(N+1)}}\right)=\frac{1}{\sin 2x}\frac{\sin[2(N+1)x]}{(N+1)}. \tag{2.165}$$

With $x=\tilde{\omega}\epsilon/2$, we arrive at the fluctuation determinant

$$\det{}_N(-\epsilon^2\nabla\overline{\nabla}-\epsilon^2\omega^2)=\prod_{m=1}^{N}[\epsilon^2\Omega_m\overline{\Omega}_m-\epsilon^2\omega^2]=\frac{\sin\tilde{\omega}(t_b-t_a)}{\sin\epsilon\tilde{\omega}}, \tag{2.166}$$

and the fluctuation factor is given by

$$F_\omega^N(t_b,t_a)=\frac{1}{\sqrt{2\pi i\hbar/M}}\sqrt{\frac{\sin\tilde{\omega}\epsilon}{\epsilon\sin\tilde{\omega}(t_b-t_a)}},\qquad t_b-t_a<\pi/\tilde{\omega}, \tag{2.167}$$

where, as we have agreed earlier in Eq. (1.337), $\sqrt{i}$ means $e^{i\pi/4}$, and t_b-t_a is always larger than zero.

2.3.3 The $i\eta$-Prescription and Maslov-Morse Index

The result (2.167) is initially valid only for

$$t_b-t_a<\pi/\tilde{\omega}. \tag{2.168}$$

In this time interval, all eigenvalues in the fluctuation determinant (2.166) are positive, and the upper version of the Fresnel formula (1.337) applies to each of the integrals in (2.160) [this was assumed in deriving (2.162)]. If t_b-t_a grows larger than $\pi/\tilde{\omega}$, the smallest eigenvalue $\Omega_1\overline{\Omega}_1-\omega^2$ becomes negative and the integration over the associated Fourier component has to be done according to the lower case of the Fresnel formula (1.337). The resulting amplitude carries an extra phase factor $e^{-i\pi/2}$ and remains valid until t_b-t_a becomes larger than $2\pi/\tilde{\omega}$, where the second eigenvalue becomes negative introducing a further phase factor $e^{-i\pi/2}$.

All phase factors emerge naturally if we associate with the oscillator frequency ω an infinitesimal negative imaginary part, replacing everywhere ω by $\omega-i\eta$ with an infinitesimal $\eta>0$. This is referred to as the *$i\eta$-prescription*. Physically, it amounts to attaching an infinitesimal damping term to the oscillator, so that the amplitude behaves like $e^{-i\omega t-\eta t}$ and dies down to zero after a very long time (as opposed to an unphysical antidamping term which would make it diverge after a long time). Now, each time that t_b-t_a passes an integer multiple of $\pi/\tilde{\omega}$, the square root of $\sin\tilde{\omega}(t_b-t_a)$ in (2.167) passes a singularity in a specific way which ensures the proper phase.[8] With such an $i\eta$-prescription it will be superfluous to restrict t_b-t_a to the

[7] I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 1.391.1.

[8] In the square root, we may equivalently assume t_b-t_a to carry a small negative imaginary part. For a detailed discussion of the phases of the fluctuation factor in the literature, see Notes and References at the end of the chapter.

range (2.168). Nevertheless it will sometimes be useful to exhibit the phase factor arising in this way in the fluctuation factor (2.167) for $t_b - t_a > \pi/\tilde{\omega}$ by writing

$$F_\omega^N(t_b, t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}} \sqrt{\frac{\sin\tilde{\omega}\epsilon}{\epsilon|\sin\tilde{\omega}(t_b - t_a)|}} e^{-i\nu\pi/2}, \tag{2.169}$$

where ν is the number of zeros encountered in the denominator along the trajectory. This number is called the *Maslov-Morse index* of the trajectory[9].

2.3.4 Continuum Limit

Let us now go to the continuum limit, $\epsilon \to 0$. Then the auxiliary frequency $\tilde{\omega}$ tends to ω and the fluctuation determinant becomes

$$\det{}_N(-\epsilon^2\nabla\overline{\nabla} - \epsilon^2\omega^2) \xrightarrow{\epsilon\to 0} \frac{\sin\omega(t_b - t_a)}{\omega\epsilon}. \tag{2.170}$$

The fluctuation factor $F_\omega^N(t_b - t_a)$ goes over into

$$F_\omega(t_b - t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}} \sqrt{\frac{\omega}{\sin\omega(t_b - t_a)}}, \tag{2.171}$$

with the phase for $t_b - t_a > \pi/\omega$ determined as above.

In the limit $\omega \to 0$, both fluctuation factors agree, of course, with the free-particle result (2.130).

In the continuum limit, the ratios of eigenvalues in (2.164) can also be calculated in the following simple way. We perform the limit $\epsilon \to 0$ directly in each factor. This gives

$$\begin{aligned} \frac{\epsilon^2\Omega_m\overline{\Omega}_m - \epsilon^2\omega^2}{\epsilon^2\Omega_m\overline{\Omega}_m} &= 1 - \frac{\epsilon^2\omega^2}{2 - 2\cos(\nu_m\epsilon)} \\ &\xrightarrow{\epsilon\to 0} 1 - \frac{\omega^2(t_b - t_a)^2}{\pi^2 m^2}. \end{aligned} \tag{2.172}$$

As the number N goes to infinity we wind up with an infinite product of these factors. Using the well-known infinite-product formula for the sine function[10]

$$\sin x = x \prod_{m=1}^{\infty}\left(1 - \frac{x^2}{m^2\pi^2}\right), \tag{2.173}$$

we find, with $x = \omega(t_b - t_a)$,

$$\prod_m \frac{\Omega_m\overline{\Omega}_m}{\Omega_m\overline{\Omega}_m - \omega^2} \xrightarrow{\epsilon\to 0} \prod_{m=1}^{\infty} \frac{\nu_m^2}{\nu_m^2 - \omega^2} = \frac{\omega(t_b - t_a)}{\sin\omega(t_b - t_a)}, \tag{2.174}$$

[9] V.P. Maslov and M.V. Fedoriuk, *Semi-Classical Approximations in Quantum Mechanics*, Reidel, Boston, 1981.

[10] I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 1.431.1.

and obtain once more the fluctuation factor in the continuum (2.171).

Multiplying the fluctuation factor with the classical amplitude, the time evolution amplitude of the linear oscillator in the continuum reads

$$\begin{aligned}(x_bt_b|x_at_a) &= \int \mathcal{D}x(t)\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}dt\frac{M}{2}(\dot{x}^2-\omega^2x^2)\right] \\ &= \frac{1}{\sqrt{2\pi i\hbar/M}}\sqrt{\frac{\omega}{\sin\omega(t_b-t_a)}} \\ &\quad\times\exp\left\{\frac{i}{2\hbar}\frac{M\omega}{\sin\omega(t_b-t_a)}[(x_b^2+x_a^2)\cos\omega(t_b-t_a)-2x_bx_a]\right\}.\end{aligned} \tag{2.175}$$

The result can easily be extended to any number D of dimensions, where the action is

$$\mathcal{A}=\int_{t_a}^{t_b}dt\frac{M}{2}\left(\dot{\mathbf{x}}^2-\omega^2\mathbf{x}^2\right). \tag{2.176}$$

Being quadratic in $\mathbf{x}$, the action is the sum of the actions of each component leading to the factorized amplitude:

$$\begin{aligned}(\mathbf{x}_bt_b|\mathbf{x}_at_a)=\prod_{i=1}^{D}(x_b^it_b|x_a^it_a) &= \frac{1}{\sqrt{2\pi i\hbar/M}^D}\sqrt{\frac{\omega}{\sin\omega(t_b-t_a)}}^D \\ \times\exp\left\{\frac{i}{2\hbar}\frac{M\omega}{\sin\omega(t_b-t_a)}\right.&\left.[(\mathbf{x}_b^2+\mathbf{x}_a^2)\cos\omega(t_b-t_a)-2\mathbf{x}_b\mathbf{x}_a]\right\},\end{aligned} \tag{2.177}$$

where the phase of the second square root for $t_b-t_a>\pi/\omega$ is determined as in the one-dimensional case [see Eq. (1.546)].

2.3.5 Useful Fluctuation Formulas

It is worth realizing that when performing the continuum limit in the ratio of eigenvalues (2.174), we have actually calculated the ratio of the functional determinants of the *differential* operators

$$\frac{\det(-\partial_t^2-\omega^2)}{\det(-\partial_t^2)}. \tag{2.178}$$

Indeed, the eigenvalues of $-\partial_t^2$ in the space of real fluctuations vanishing at the endpoints are simply

$$\nu_m^2=\left(\frac{\pi m}{t_b-t_a}\right)^2, \tag{2.179}$$

so that the ratio (2.178) is equal to the product

$$\frac{\det(-\partial_t^2-\omega^2)}{\det(-\partial_t^2)}=\prod_{m=1}^{\infty}\frac{\nu_m^2-\omega^2}{\nu_m^2}, \tag{2.180}$$

which is the same as (2.174). This observation should, however, not lead us to believe that the entire fluctuation factor

$$F_\omega(t_b-t_a)=\int\mathcal{D}\delta x\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\frac{M}{2}[(\delta\dot{x})^2-\omega^2(\delta x)^2]\right\} \tag{2.181}$$

could be calculated via the continuum determinant

$$F_\omega(t_b,t_a) \xrightarrow{\epsilon\to 0} \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}}\frac{1}{\sqrt{\det(-\partial_t^2-\omega^2)}} \qquad \text{(false)}. \tag{2.182}$$

The product of eigenvalues in $\det(-\partial_t^2-\omega^2)$ would be a strongly divergent expression

$$\det(-\partial_t^2-\omega^2) = \prod_{m=1}^{\infty}(\nu_m^2-\omega^2) \tag{2.183}$$
$$= \prod_{m=1}^{\infty}(\nu_m^2)\prod_{m=1}^{\infty}\left[\frac{\nu_m^2-\omega^2}{\nu_m^2}\right] = \prod_{m=1}^{\infty}\left[\frac{\pi^2 m^2}{(t_b-t_a)^2}\right]\times\frac{\sin\omega(t_b-t_a)}{\omega(t_b-t_a)}.$$

Only *ratios* of determinants $-\nabla\overline{\nabla}-\omega^2$ with different ω's can be replaced by their differential limits. Then the common divergent factor in (2.183) cancels.

Let us look at the origin of this strong divergence. The eigenvalues on the lattice and their continuum approximation start both out for small m as

$$\Omega_m\overline{\Omega}_m \approx \nu_m^2 \approx \frac{\pi^2 m^2}{(t_b-t_a)^2}. \tag{2.184}$$

For large $m \leq N$, the eigenvalues on the lattice saturate at $\Omega_m\overline{\Omega}_m \to 2/\epsilon^2$, while the ν_m^2's keep growing quadratically in m. This causes the divergence.

The correct time-sliced formulas for the fluctuation factor of a harmonic oscillator is summarized by the following sequence of equations:

$$\begin{aligned} F_\omega^N(t_b-t_a) &= \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}}\prod_{n=1}^{N}\left[\int\frac{d\delta x_n}{\sqrt{2\pi\hbar i\epsilon/M}}\right]\exp\left[\frac{i}{\hbar}\frac{M}{2\epsilon}\delta x^T(-\epsilon^2\nabla\overline{\nabla}-\epsilon^2\omega^2)\delta x\right] \\ &= \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}}\frac{1}{\sqrt{\det_N(-\epsilon^2\nabla\overline{\nabla}-\epsilon^2\omega^2)}}, \end{aligned} \tag{2.185}$$

where in the first expression, the exponent is written in matrix notation with x^T denoting the transposed vector x whose components are x_n. Taking out a free-particle determinant $\det_N(-\epsilon^2\overline{\nabla}\nabla)$, formula (2.140), leads to the ratio formula

$$F_\omega^N(t_b-t_a) = \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}}\left[\frac{\det_N(-\epsilon^2\nabla\overline{\nabla}-\epsilon^2\omega^2)}{\det_N(-\epsilon^2\nabla\overline{\nabla})}\right]^{-1/2}, \tag{2.186}$$

which yields

$$F_\omega^N(t_b-t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}}\sqrt{\frac{\sin\tilde{\omega}\epsilon}{\epsilon\sin\tilde{\omega}(t_b-t_a)}}, \tag{2.187}$$

If with $\tilde{\omega}$ of Eq. (2.163). If we are only interested in the continuum limit, we may let ϵ go to zero on the right-hand side of (2.186) and evaluate

$$\begin{aligned} F_\omega(t_b-t_a) &= \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}}\left[\frac{\det(-\partial_t^2-\omega^2)}{\det(-\partial_t^2)}\right]^{-1/2} \\ &= \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}}\prod_{m=1}^{\infty}\left[\frac{\nu_m^2-\omega^2}{\nu_m^2}\right]^{-1/2} \\ &= \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}}\sqrt{\frac{\omega(t_b-t_a)}{\sin\omega(t_b-t_a)}}. \end{aligned} \tag{2.188}$$

Let us calculate also here the time evolution amplitude in momentum space. The Fourier transform of initial and final positions of (2.177) [as in (2.73)] yields

$$
\begin{aligned}
(\mathbf{p}_b t_b|\mathbf{p}_a t_a) = & \int d^D x_b\, e^{-i\mathbf{p}_b\mathbf{x}_b/\hbar} \int d^D x_a\, e^{i\mathbf{p}_a\mathbf{x}_a/\hbar} (\mathbf{x}_b t_b|\mathbf{x}_a t_a) \\
= & \frac{(2\pi\hbar)^D}{\sqrt{2\pi i\hbar}^D} \frac{1}{\sqrt{M\omega \sin\omega(t_b-t_a)}^D} \\
\times & \exp\left\{\frac{i}{\hbar}\frac{1}{2M\omega\sin\omega(t_b-t_a)}\left[(\mathbf{p}_b^2+\mathbf{p}_a^2)\cos\omega(t_b-t_a)-2\mathbf{p}_b\mathbf{p}_a\right]\right\}.
\end{aligned}
\tag{2.189}
$$

The limit $\omega \to 0$ reduces to the free-particle expression (2.73), not quite as directly as in the $\mathbf{x}$-space amplitude (2.177). Expanding the exponent

$$
\begin{aligned}
& \frac{1}{2M\omega\sin\omega(t_b-t_a)}\left[(\mathbf{p}_b^2+\mathbf{p}_a)\cos\omega(t_b-t_a)-2\mathbf{p}_b\mathbf{p}_a^2\right] \\
& = \frac{1}{2M\omega^2(t_b-t_a)}\left\{(\mathbf{p}_b-\mathbf{p}_a)^2-\frac{1}{2}(\mathbf{p}_b^2+\mathbf{p}_a^2)[\omega(t_b-t_a)]^2+\ldots\right\},
\end{aligned}
\tag{2.190}
$$

and going to the limit $\omega \to 0$, the leading term in (2.189)

$$
\frac{(2\pi)^D}{\sqrt{2\pi i\omega^2(t_b-t_a)\hbar M}^D}\exp\left\{\frac{i}{\hbar}\frac{1}{2M\omega^2(t_b-t_a)}(\mathbf{p}_b-\mathbf{p}_a)^2\right\}
\tag{2.191}
$$

tends to $(2\pi\hbar)^D\delta^{(D)}(\mathbf{p}_b-\mathbf{p}_a)$ [recall (1.534)], while the second term in (2.190) yields a factor $e^{-i\mathbf{p}^2(t_b-t_a)/2M\hbar}$, so that we recover indeed (2.73).

2.3.6 Oscillator Amplitude on Finite Time Lattice

Let us calculate the exact time evolution amplitude for a finite number of time slices. In contrast to the free-particle case in Section 2.2.5, the oscillator amplitude is no longer equal to its continuum limit but ϵ-dependent. This will allow us to study some typical convergence properties of path integrals in the continuum limit. Since the fluctuation factor was initially calculated at a finite ϵ in (2.169), we only need to find the classical action for finite ϵ. To maintain time reversal invariance at any finite ϵ, we work with a slightly different sliced potential term in the action than before in (2.148), using

$$
\mathcal{A}^N = \epsilon\frac{M}{2}\sum_{n=1}^{N+1}\left[(\overline{\nabla}x_n)^2-\omega^2(x_n^2+x_{n-1}^2)/2\right],
\tag{2.192}
$$

or, written in another way,

$$
\mathcal{A}^N = \epsilon\frac{M}{2}\sum_{n=0}^{N}\left[(\nabla x_n)^2-\omega^2(x_{n+1}^2+x_n^2)/2\right].
\tag{2.193}
$$

This differs from the original time-sliced action (2.148) by having the potential $\omega^2 x_n^2$ replaced by the more symmetric one $\omega^2(x_n^2+x_{n-1}^2)/2$. The gradient term is the same in both cases and can be rewritten, after a summation by parts, as

$$
\epsilon\sum_{n=1}^{N+1}(\overline{\nabla}x_n)^2 = \epsilon\sum_{n=0}^{N}(\nabla x_n)^2 = \left[x_b\overline{\nabla}x_b - x_a\nabla x_a\right] - \epsilon\sum_{n=1}^{N}x_n\nabla\overline{\nabla}x_n.
\tag{2.194}
$$

This leads to a time-sliced action

$$\mathcal{A}^N = \frac{M}{2}\left(x_b\overline{\nabla}x_b - x_a\nabla x_a\right) - \epsilon\frac{M}{4}\omega^2(x_b^2+x_a^2) - \epsilon\frac{M}{2}\sum_{n=1}^{N} x_n(\nabla\overline{\nabla}+\omega^2)x_n. \tag{2.195}$$

Since the variation of $\mathcal{A}^N$ is performed at fixed endpoints x_a and x_b, the fluctuation factor is the same as in (2.160). The equation of motion on the sliced time axis is

$$(\nabla\overline{\nabla}+\omega^2)x_{\rm cl}(t) = 0. \tag{2.196}$$

Here it is understood that the time variable takes only the discrete lattice values t_n. The solution of this difference equation with the initial and final values x_a and x_b, respectively, is given by

$$x_{\rm cl}(t) = \frac{1}{\sin\tilde{\omega}(t_b-t_a)}\left[x_b\sin\tilde{\omega}(t-t_a) + x_a\sin\tilde{\omega}(t_b-t)\right], \tag{2.197}$$

where $\tilde{\omega}$ is the auxiliary frequency introduced in (2.163). To calculate the classical action on the lattice, we insert (2.197) into (2.195). After some trigonometry, and replacing $\epsilon^2\omega^2$ by $4\sin^2(\tilde{\omega}\epsilon/2)$, the action resembles closely the continuum expression (2.159):

$$\mathcal{A}^N_{\rm cl} = \frac{M}{2\epsilon}\frac{\sin\tilde{\omega}\epsilon}{\sin\tilde{\omega}(t_b-t_a)}\left[(x_b^2+x_a^2)\cos\tilde{\omega}(t_b-t_a) - 2x_bx_a\right]. \tag{2.198}$$

The total time evolution amplitude on the sliced time axis is

$$(x_bt_b|x_at_a) = e^{i\mathcal{A}^N_{\rm cl}/\hbar}F^N_\omega(t_b-t_a), \tag{2.199}$$

with sliced action (2.198) and the sliced fluctuation factor (2.169).

2.4 Gelfand-Yaglom Formula

In many applications one encounters a slight generalization of the oscillator fluctuation problem: The action is harmonic but contains a time-dependent frequency $\Omega^2(t)$ instead of the constant oscillator frequency ω^2. The associated fluctuation factor is

$$F(t_b,t_a) = \int \mathcal{D}\delta x(t)\exp\left(\frac{i}{\hbar}\mathcal{A}\right), \tag{2.200}$$

with the action

$$\mathcal{A} = \int_{t_a}^{t_b} dt\frac{M}{2}[(\delta\dot{x})^2 - \Omega^2(t)(\delta x)^2]. \tag{2.201}$$

Since $\Omega(t)$ may not be translationally invariant in time, the fluctuation factor depends now in general on both the initial and final times. The ratio formula (2.186) holds also in this more general case, i.e.,

$$F^N(t_b,t_a) = \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}}\left[\frac{\det_N(-\epsilon^2\nabla\overline{\nabla}-\epsilon^2\Omega^2)}{\det_N(-\epsilon^2\nabla\overline{\nabla})}\right]^{-1/2}. \tag{2.202}$$

Here $\Omega^2(t)$ denotes the diagonal matrix

$$\Omega^2(t) = \begin{pmatrix} \Omega_N^2 & & \\ & \ddots & \\ & & \Omega_1^2 \end{pmatrix}, \tag{2.203}$$

with the matrix elements $\Omega_n^2 = \Omega^2(t_n)$.

2.4.1 Recursive Calculation of Fluctuation Determinant

In general, the full set of eigenvalues of the matrix $-\nabla\overline{\nabla} - \Omega^2(t)$ is quite difficult to find, even in the continuum limit. It is, however, possible to derive a powerful difference equation for the fluctuation determinant which can often be used to find its value without knowing all eigenvalues. The method is due to Gelfand and Yaglom.[11]

Let us denote the determinant of the $N \times N$ fluctuation matrix by D_N, i.e.,

$$D_N \equiv \det_N\left(-\epsilon^2\overline{\nabla}\nabla - \epsilon^2\Omega^2\right) \tag{2.204}$$

$$\equiv \begin{vmatrix} 2-\epsilon^2\Omega_N^2 & -1 & 0 & \dots & 0 & 0 & 0 \\ -1 & 2-\epsilon^2\Omega_{N-1}^2 & -1 & \dots & 0 & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & \dots & -1 & 2-\epsilon^2\Omega_2^2 & -1 \\ 0 & 0 & 0 & \dots & 0 & -1 & 2-\epsilon^2\Omega_1^2 \end{vmatrix}.$$

By expanding this along the first column, we obtain the recursion relation

$$D_N = (2-\epsilon^2\Omega_N^2)D_{N-1} - D_{N-2}, \tag{2.205}$$

which may be rewritten as

$$\epsilon^2\left[\frac{1}{\epsilon}\left(\frac{D_N - D_{N-1}}{\epsilon} - \frac{D_{N-1} - D_{N-2}}{\epsilon}\right) + \Omega_N^2 D_{N-1}\right] = 0. \tag{2.206}$$

Since the equation is valid for all N, it implies that the determinant D_N satisfies the difference equation

$$(\nabla\overline{\nabla} + \Omega_{N+1}^2)D_N = 0. \tag{2.207}$$

In this notation, the operator $-\nabla\overline{\nabla}$ is understood to act on the dimensional label N of the determinant. The determinant D_N may be viewed as the discrete values of a function of $D(t)$ evaluated on the sliced time axis. Equation (2.207) is called the *Gelfand-Yaglom formula*. Thus the determinant as a function of N is the solution of the classical difference equation of motion and the desired result for a given N is obtained from the final value $D_N = D(t_{N+1})$. The initial conditions are

$$\begin{aligned} D_1 &= (2-\epsilon^2\Omega_1^2), \\ D_2 &= (2-\epsilon^2\Omega_1^2)(2-\epsilon^2\Omega_2^2) - 1. \end{aligned} \tag{2.208}$$

2.4.2 Examples

As an illustration of the power of the Gelfand-Yaglom formula, consider the known case of a constant $\Omega^2(t) \equiv \omega^2$ where the Gelfand-Yaglom formula reads

$$(\nabla\overline{\nabla} + \omega^2)D_N = 0. \tag{2.209}$$

This is solved by a linear combination of $\sin(N\tilde{\omega}\epsilon)$ and $\cos(N\tilde{\omega}\epsilon)$, where $\tilde{\omega}$ is given by (2.163). The solution satisfying the correct boundary condition is obviously

$$D_N = \frac{\sin(N+1)\epsilon\tilde{\omega}}{\sin\epsilon\tilde{\omega}}. \tag{2.210}$$

[11] I.M. Gelfand and A.M. Yaglom, J. Math. Phys. *1*, 48 (1960).

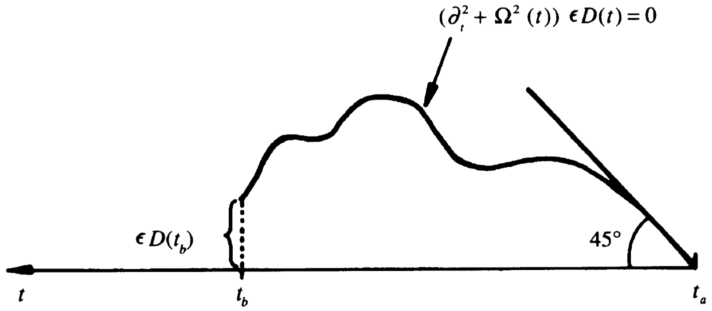

Figure 2.2 Solution of equation of motion with zero initial value and unit initial slope. Its value at the final time is equal to ϵ times the discrete fluctuation determinant $D_N = D(t_b)$.

Indeed, the two lowest elements are

$$\begin{aligned} D_1 &= 2\cos\epsilon\tilde{\omega}, \\ D_2 &= 4\cos^2\epsilon\tilde{\omega} - 1, \end{aligned} \tag{2.211}$$

which are the same as (2.208), since $\epsilon^2\Omega^2 \equiv \epsilon^2\omega^2{=}2(1-\cos\tilde{\omega}\epsilon)$.

The Gelfand-Yaglom formula becomes especially easy to handle in the continuum limit $\epsilon \to 0$. Then, by considering the renormalized function

$$D_{\rm ren}(t_N) = \epsilon D_N, \tag{2.212}$$

the initial conditions $D_1 = 2$ and $D_2 = 3$ can be re-expressed as

$$(\epsilon D)_1 = D_{\rm ren}(t_a) = 0, \tag{2.213}$$

$$\frac{\epsilon D_2 - \epsilon D_1}{\epsilon} = (\nabla\epsilon D)_1 \xrightarrow{\epsilon\to 0} \dot{D}_{\rm ren}(t_a) = 1. \tag{2.214}$$

The difference equation for D_N turns into the differential equation for $D_{\rm ren}(t)$:

$$[\partial_t^2 + \Omega^2(t)]D_{\rm ren}(t) = 0. \tag{2.215}$$

The situation is pictured in Fig. 2.2. The determinant D_N is $1/\epsilon$ times the value of the function $D_{\rm ren}(t)$ at t_b. This value is found by solving the differential equation starting from t_a with zero value and unit slope.

As an example, consider once more the harmonic oscillator with a fixed frequency ω. The equation of motion in the continuum limit is solved by

$$D_{\rm ren}(t) = \frac{1}{\omega}\sin\omega(t - t_a), \tag{2.216}$$

which satisfies the initial conditions (2.214). Thus we find the fluctuation determinant to become, for small ϵ,

$$\det(-\epsilon^2\nabla\overline{\nabla} - \epsilon^2\omega^2) \xrightarrow{\epsilon\to 0} \frac{1}{\epsilon}\frac{\sin\omega(t_b - t_a)}{\omega}, \tag{2.217}$$

in agreement with the earlier result (2.210). For the free particle, the solution is $D_{\rm ren}(t) = t - t_a$ and we obtain directly the determinant $\det_N(-\epsilon^2\nabla\overline{\nabla}) = (t_b - t_a)/\epsilon$.

For time-dependent frequencies $\Omega(t)$, an analytic solution of the Gelfand-Yaglom initial-value problem (2.213), (2.214), and (2.215) can be found only for special classes of functions $\Omega(t)$. In fact, (2.215) has the form of a Schrödinger equation of a point particle in a potential $\Omega^2(t)$, and the classes of potentials for which the Schrödinger equation can be solved are well-known.

2.4.3 Calculation on Unsliced Time Axis

In general, the most explicit way of expressing the solution is by linearly combining $D_{\rm ren}{=}\epsilon D_N$ from any two independent solutions $\xi(t)$ and $\eta(t)$ of the homogeneous differential equation

$$[\partial_t^2 + \Omega^2(t)]x(t) = 0. \tag{2.218}$$

The solution of (2.215) is found from a linear combination

$$D_{\rm ren}(t) = \alpha\xi(t) + \beta\eta(t). \tag{2.219}$$

The coefficients are determined from the initial condition (2.214), which imply

$$\begin{aligned} \alpha\xi(t_a) + \beta\eta(t_a) &= 0, \\ \alpha\dot\xi(t_a) + \beta\dot\eta(t_a) &= 1, \end{aligned} \tag{2.220}$$

and thus

$$D_{\rm ren}(t) = \frac{\xi(t)\eta(t_a) - \xi(t_a)\eta(t)}{\dot\xi(t_a)\eta(t_a) - \xi(t_a)\dot\eta(t_a)}. \tag{2.221}$$

The denominator is recognized as the time-independent *Wronski determinant* of the two solutions

$$W \equiv \xi(t) \overset{\leftrightarrow}{\partial}_t \eta(t) \equiv \xi(t)\dot\eta(t) - \dot\xi(t)\eta(t) \tag{2.222}$$

at the initial point t_a. The right-hand side is independent of t.

The Wronskian is an important quantity in the theory of second-order differential equations. It is defined for all equations of the Sturm-Liouville type

$$\frac{d}{dt}\left[a(t)\frac{dy(t)}{dt}\right] + b(t)y(t) = 0, \tag{2.223}$$

for which it is proportional to $1/a(t)$. The Wronskian is used to construct the Green function for all such equations.[12]

In terms of the Wronskian, Eq. (2.221) has the general form

$$D_{\rm ren}(t) = -\frac{1}{W}\left[\xi(t)\eta(t_a) - \xi(t_a)\eta(t)\right]. \tag{2.224}$$

Inserting $t = t_b$ gives the desired determinant

$$D_{\rm ren} = -\frac{1}{W}\left[\xi(t_b)\eta(t_a) - \xi(t_a)\eta(t_b)\right]. \tag{2.225}$$

Note that the same functional determinant can be found from by evaluating the function

$$\tilde D_{\rm ren}(t) = -\frac{1}{W}\left[\xi(t_b)\eta(t) - \xi(t)\eta(t_b)\right] \tag{2.226}$$

[12]For its typical use in classical electrodynamics, see J.D. Jackson, *Classical Electrodynamics*, John Wiley & Sons, New York, 1975, Section 3.11.

at t_a. This also satisfies the homogenous differential equation (2.215), but with the initial conditions

$$\tilde{D}_{\rm ren}(t_b) = 0, \qquad \dot{\tilde{D}}_{\rm ren}(t_b) = -1. \tag{2.227}$$

It will be useful to emphasize at which ends the Gelfand-Yaglom boundary conditions are satisfied by denoting $D_{\rm ren}(t)$ and $\tilde{D}_{\rm ren}(t)$ by $D_a(t)$ and $D_b(t)$, respectively, summarizing their symmetric properties as

$$[\partial_t^2 + \Omega^2(t)]D_a(t) = 0\ ; \quad D_a(t_a) = 0, \quad \dot{D}_a(t_a) = 1, \tag{2.228}$$

$$[\partial_t^2 + \Omega^2(t)]D_b(t) = 0\ ; \quad D_b(t_b) = 0, \quad \dot{D}_b(t_b) = -1, \tag{2.229}$$

with the determinant being obtained from either function as

$$D_{\rm ren} = D_a(t_b) = D_b(t_a). \tag{2.230}$$

In contrast to this we see from the explicit equations (2.224) and (2.226) that the time derivatives of two functions at opposite endpoints are in general not related. Only for frequencies $\Omega(t)$ with time reversal invariance, one has

$$\dot{D}_a(t_b) = -\dot{D}_b(t_a), \qquad \text{for} \quad \Omega(t) = \Omega(-t). \tag{2.231}$$

For arbitrary $\Omega(t)$, one can derive a relation

$$\dot{D}_a(t_b) + \dot{D}_b(t_a) = -2\int_{t_a}^{t_b} dt\, \Omega(t)\dot{\Omega}(t)D_a(t)D_b(t). \tag{2.232}$$

As an application of these formulas, consider once more the linear oscillator, for which two independent solutions are

$$\xi(t) = \cos\omega t, \qquad \eta(t) = \sin\omega t. \tag{2.233}$$

Hence

$$W = \omega, \tag{2.234}$$

and the fluctuation determinant becomes

$$D_{\rm ren} = -\frac{1}{\omega}(\cos\omega t_b \sin\omega t_a - \cos\omega t_a \sin\omega t_b) = \frac{1}{\omega}\sin\omega(t_b - t_a). \tag{2.235}$$

2.4.4 D'Alembert's Construction

It is important to realize that the construction of the solutions of Eqs. (2.228) and (2.229) requires only the knowledge of one solution of the homogenous differential equation (2.218), say $\xi(t)$. A second linearly independent solution $\eta(t)$ can always be found with the help of a formula due to d'Alembert,

$$\eta(t) = w\,\xi(t)\int^t \frac{dt'}{\xi^2(t')}, \tag{2.236}$$

where w is some constant. Differentiation yields

$$\dot{\eta} = \frac{\dot{\xi}\eta}{\xi} + \frac{w}{\xi}, \qquad \ddot{\eta} = \frac{\ddot{\xi}\eta}{\xi}. \tag{2.237}$$

The second equation shows that with $\xi(t)$, also $\eta(t)$ is a solution of the homogenous differential equation (2.218). From the first equation we find that the Wronski determinant of the two functions is equal to w:

$$W = \xi(t)\dot{\eta}(t) - \dot{\xi}(t)\eta(t) = w. \tag{2.238}$$

Inserting the solution (2.236) into the formulas (2.224) and (2.226), we obtain explicit expressions for the Gelfand-Yaglom functions in terms of one arbitrary solution of the homogenous differential equation (2.218):

$$D_{\rm ren}(t) = D_a(t) = \xi(t)\xi(t_a)\int_{t_a}^{t}\frac{dt'}{\xi^2(t')}, \qquad \tilde{D}_{\rm ren}(t) = D_b(t) = \xi(t_b)\xi(t)\int_{t}^{t_b}\frac{dt'}{\xi^2(t')}. \tag{2.239}$$

The desired functional determinant is

$$D_{\rm ren} = \xi(t_b)\xi(t_a)\int_{t_a}^{t_b}\frac{dt'}{\xi^2(t')}. \tag{2.240}$$

2.4.5 Another Simple Formula

There exists yet another useful formula for the functional determinant. For this we solve the homogenous differential equation (2.218) for an arbitrary initial position x_a and initial velocity $\dot{x}_a$ at the time t_a. The result may be expressed as the following linear combination of $D_a(t)$ and $D_b(t)$:

$$x(x_a, \dot{x}_a; t) = \frac{1}{D_b(t_a)}\left[D_b(t) - D_a(t)\dot{D}_b(t_a)\right] x_a + D_a(t)\dot{x}_a \,. \tag{2.241}$$

We then see that the Gelfand-Yaglom function $D_{\rm ren}(t) = D_a(t)$ can be obtained from the partial derivative

$$D_{\rm ren}(t) = \frac{\partial x(x_a, \dot{x}_a; t)}{\partial \dot{x}_a}. \tag{2.242}$$

This function obviously satisfies the Gelfand-Yaglom initial conditions $D_{\rm ren}(t_a) = 0$ and $\dot{D}_{\rm ren}(t_a) = 1$ of (2.213) and (2.214), which are a direct consequence of the fact that x_a and $\dot{x}_a$ are independent variables in the function $x(x_a, \dot{x}_a; t)$, for which $\partial x_a/\partial \dot{x}_a = 0$ and $\partial \dot{x}_a/\partial \dot{x}_a = 1$.

The fluctuation determinant $D_{\rm ren} = D_a(t_b)$ is then given by

$$D_{\rm ren} = \frac{\partial x_b}{\partial \dot{x}_a}, \tag{2.243}$$

where x_b abbreviates the function $x(x_a, \dot{x}_a; t_b)$. It is now obvious that the analogous equations (2.229) are satisfied by the partial derivative $D_b(t) = -\partial x(t)/\partial \dot{x}_b$, where $x(t)$ is expressed in terms of the final position x_b and velocity $\dot{x}_b$ as $x(t) = x(x_b, \dot{x}_b; t)$

$$x(x_b, \dot{x}_b; t) = \frac{1}{D_a(t_b)}\left[D_a(t) + D_b(t)\dot{D}_a(t_b)\right] x_b - D_b(t)\dot{x}_b \,, \tag{2.244}$$

so that we obtain the alternative formula

$$D_{\rm ren} = -\frac{\partial x_a}{\partial \dot{x}_b}. \tag{2.245}$$

These results can immediately be generalized to functional determinants of differential operators of the form $-\partial_t^2\delta_{ij} - \Omega_{ij}^2(t)$ where the time-dependent frequency is a $D\times D$-dimensional matrix $\Omega_{ij}^2(t)$, $(i,j=1,\dots,D)$. Then the associated Gelfand-Yaglom function $D_a(t)$ becomes a matrix $D_{ij}(t)$ satisfying the initial conditions $D_{ij}(t_a) = 0$, $\dot{D}_{ij}(t_b) = \delta_{ij}$, and the desired functional determinant $D_{\rm ren}$ is equal to the ordinary determinant of $D_{ij}(t_b)$:

$$D_{\rm ren} = {\rm Det}\left[-\partial_t^2\delta_{ij} - \Omega_{ij}^2(t)\right] = \det D_{ij}(t_b). \tag{2.246}$$

The homogeneous differential equation and the initial conditions are obviously satisfied by the partial derivative matrix $D_{ij}(t) = \partial x^i(t)/\partial \dot{x}_a^j$, so that the explicit representations of $D_{ij}(t)$ in terms of the general solution of the classical equations of motion $\left[-\partial_t^2\delta_{ij} - \Omega_{ij}^2(t)\right] x_j(t) = 0$ become

$$D_{\rm ren} = \det \frac{\partial x_b^i}{\partial \dot{x}_a^j} = \det\left(-\frac{\partial x_a^i}{\partial \dot{x}_b^j}\right). \tag{2.247}$$

A further couple of formulas for functional determinants can be found by constructing a solution of the homogeneous differential equation (2.218) which passes through specific initial and final points x_a and x_b at t_a and t_b, respectively:

$$x(x_b, x_a; t) = \frac{D_b(t)}{D_b(t_a)} x_a + \frac{D_a(t)}{D_a(t_b)} x_b. \tag{2.248}$$

The Gelfand-Yaglom functions $D_a(t)$ and $D_b(t)$ can therefore be obtained from the partial derivatives

$$\frac{D_a(t)}{D_a(t_b)} = \frac{\partial x(x_b,x_a;t)}{\partial x_b}, \qquad \frac{D_b(t)}{D_b(t_a)} = \frac{\partial x(x_b,x_a;t)}{\partial x_a}. \tag{2.249}$$

At the endpoints, Eqs. (2.248) yield

$$\dot{x}_a = \frac{\dot{D}_b(t_a)}{D_b(t_a)} x_a + \frac{1}{D_a(t_b)} x_b, \tag{2.250}$$

$$\dot{x}_b = -\frac{1}{D_b(t_a)} x_a + \frac{\dot{D}_a(t_b)}{D_a(t_b)} x_b, \tag{2.251}$$

so that the fluctuation determinant $D_{\rm ren} = D_a(t_b) = D_b(t_a)$ is given by the formulas

$$D_{\rm ren} = \left(\frac{\partial \dot{x}_a}{\partial x_b}\right)^{-1} = -\left(\frac{\partial \dot{x}_b}{\partial x_a}\right)^{-1}, \tag{2.252}$$

where $\dot{x}_a$ and $\dot{x}_b$ are functions of the independent variables x_a and x_b. The equality of these expressions with the previous ones in (2.243) and (2.245) is a direct consequence of the mathematical identity for partial derivatives

$$\left.\frac{\partial x_b}{\partial \dot{x}_a}\right|_{x_a} = \left(\left.\frac{\partial \dot{x}_a}{\partial x_b}\right|_{x_a}\right)^{-1}. \tag{2.253}$$

Let us emphasize that all functional determinants calculated in this Chapter apply to the fluctuation factor of paths with fixed endpoints. In mathematics, this property is referred to as Dirichlet boundary conditions. In the context of quantum statistics, we shall also need such determinants for fluctuations with periodic boundary conditions, for which the Gelfand-Yaglom method must be modified. We shall see in Section 2.11 that this causes considerable complications in the lattice derivation, which will make it desirable to find a simpler derivation of both functional determinants. This will be found in Section 3.27 in a continuum formulation.

In general, the homogenous differential equation (2.218) with time-dependent frequency $\Omega(t)$ cannot be solved analytically. The equation has the same form as a Schrödinger equation for a point particle in one dimension moving in a one dimensional potential $\Omega^2(t)$, and there are only a few classes of potentials for which the solutions are known in closed form. Fortunately, however, the functional determinant will usually arise in the context of quadratic fluctuations around classical solutions in time-independent potentials (see in Section 4.3). If such a classical solution is known analytically, it will provide us automatically with a solution of the homogeneous differential equation (2.218). Some important examples will be discussed in Sections 17.4 and 17.11.

2.4.6 Generalization to D Dimensions

The above formulas have an obvious generalization to a D-dimensional version of the fluctuation action (2.201)

$$\mathcal{A} = \int_{t_a}^{t_b} dt \frac{M}{2} [(\delta\dot{\mathbf{x}})^2 - \delta\mathbf{x}^T \, \mathbf{\Omega}^2(t) \delta\mathbf{x}], \tag{2.254}$$

where $\mathbf{\Omega}^2(t)$ is a $D \times D$ matrix with elements $\Omega^2_{ij}(t)$. The fluctuation factor (2.202) generalizes to

$$F^N(t_b, t_a) = \frac{1}{\sqrt{2\pi\hbar i(t_b - t_a)/M}^D} \left[\frac{\det_N(-\epsilon^2 \nabla\overline{\nabla} - \epsilon^2 \mathbf{\Omega}^2)}{\det_N(-\epsilon^2 \nabla\overline{\nabla})} \right]^{-1/2}. \tag{2.255}$$

The fluctuation determinant is found by Gelfand-Yaglom's construction from a formula

$$D_{\rm ren} = \det \mathbf{D}_a(t_b) = \det \mathbf{D}_b(t_a), \tag{2.256}$$

with the matrices $\mathbf{D}_a(t)$ and $\mathbf{D}_b(t)$ satisfying the classical equations of motion and initial conditions corresponding to (2.228) and (2.229):

$$[\partial_t^2 + \mathbf{\Omega}^2(t)] \mathbf{D}_a(t) = 0 \; ; \quad \mathbf{D}_a(t_a) = 0, \quad \dot{\mathbf{D}}_a(t_a) = \mathbf{1}, \tag{2.257}$$

$$[\partial_t^2 + \mathbf{\Omega}^2(t)] \mathbf{D}_b(t) = 0 \; ; \quad \mathbf{D}_b(t_b) = 0, \quad \dot{\mathbf{D}}_b(t_b) = -\mathbf{1}, \tag{2.258}$$

where $\mathbf{1}$ is the unit matrix in D dimensions. We can then repeat all steps in the last section and find the D-dimensional generalization of formulas (2.252):

$$D_{\rm ren} = \left(\det \frac{\partial \dot{x}_a^i}{\partial x_b^j} \right)^{-1} = \left[\det \left(-\frac{\partial \dot{x}_b^i}{\partial x_a^j} \right) \right]^{-1}. \tag{2.259}$$

2.5 Harmonic Oscillator with Time-Dependent Frequency

The results of the last section put us in a position to solve exactly the path integral of a harmonic oscillator with arbitrary time-dependent frequency $\Omega(t)$. We shall first do this in coordinate space, later in momentum space.

2.5.1 Coordinate Space

Consider the path integral

$$(x_b t_b|x_a t_a) \quad = \quad \int \mathcal{D}x \exp\left\{\frac{i}{\hbar}\mathcal{A}[x]\right\}, \tag{2.260}$$

with the Lagrangian action

$$\mathcal{A}[x] = \frac{M}{2}\int_{t_a}^{t_b} dt \, \left[\dot{x}^2(t) - \Omega^2(t)x^2(t)\right], \tag{2.261}$$

which is harmonic with a time-dependent frequency. As in Eq. (2.14), the result can be written as a product of a fluctuation factor and an exponential containing the classical action:

$$(x_b t_b|x_a t_a) = \int \mathcal{D}x \, e^{i\mathcal{A}[x]/\hbar} = F_\Omega(t_b, t_a) e^{i\mathcal{A}_{\rm cl}/\hbar}. \tag{2.262}$$

From the discussion in the last section we know that the fluctuation factor is, by analogy with (2.171), and recalling (2.243),

$$F_\Omega(t_b, t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}}\frac{1}{\sqrt{D_a(t_b)}}. \tag{2.263}$$

The determinant $D_a(t_b) = D_{\rm ren}$ may be expressed in terms of partial derivatives according to formulas (2.243) and (2.252):

$$F_\Omega(t_b, t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}}\left(\frac{\partial x_b}{\partial \dot{x}_a}\right)^{-1/2} = \frac{1}{\sqrt{2\pi i\hbar/M}}\left(\frac{\partial \dot{x}_a}{\partial x_b}\right)^{1/2}, \tag{2.264}$$

where the first partial derivative is calculated from the function $x(x_a, \dot{x}_a; t)$, the second from $\dot{x}(x_b, x_a; t)$. Equivalently we may use (2.245) and the right-hand part of Eq. (2.252) to write

$$F_\Omega(t_b, t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}}\left(-\frac{\partial x_a}{\partial \dot{x}_b}\right)^{-1/2} = \frac{1}{\sqrt{2\pi i\hbar/M}}\left(-\frac{\partial \dot{x}_b}{\partial x_a}\right)^{1/2}. \tag{2.265}$$

It remains to calculate the classical action $\mathcal{A}_{\rm cl}$. This can be done in the same way as in Eqs. (2.155) to (2.159). After a partial integration, we have as before

$$\mathcal{A}_{\rm cl} = \frac{M}{2}(x_b\dot{x}_b - x_a\dot{x}_a). \tag{2.266}$$

Exploiting the linear dependence of $\dot{x}_b$ and $\dot{x}_a$ on the endpoints x_b and x_a, we may rewrite this as

$$\mathcal{A}_{\rm cl} = \frac{M}{2}\left(x_b\frac{\partial \dot{x}_b}{\partial x_b}x_b - x_a\frac{\partial \dot{x}_a}{\partial x_a}x_a + x_b\frac{\partial \dot{x}_b}{\partial x_a}x_a - x_a\frac{\partial \dot{x}_a}{\partial x_b}x_b\right). \tag{2.267}$$

Inserting the partial derivatives from (2.250) and (2.251) and using the equality of $D_a(t_b)$ and $D_b(t_a)$, we obtain the classical action

$$\mathcal{A}_{\rm cl} = \frac{M}{2D_a(t_b)}\left[x_b^2\dot{D}_a(t_b) - x_a^2\dot{D}_b(t_a) - 2x_bx_a\right]. \tag{2.268}$$

Note that there exists another simple formula for the fluctuation determinant $D_{\rm ren}$:

$$D_{\rm ren} = D_a(t_b) = D_b(t_a) = -M\left(\frac{\partial^2}{\partial x_b \partial x_a}\mathcal{A}_{\rm cl}\right)^{-1}. \tag{2.269}$$

For the harmonic oscillator with time-independent frequency ω, the Gelfand-Yaglom function $D_a(t)$ of Eq. (2.235) has the property (2.231) due to time reversal invariance, and (2.268) reproduces the known result (2.159).

The expressions containing partial derivatives are easily extended to D dimensions: We simply have to replace the partial derivatives $\partial x_b/\partial \dot{x}_a$, $\partial \dot{x}_b/\partial \dot{x}_a, \dots$ by the corresponding $D \times D$ matrices, and write the action as the associated quadratic form.

The D-dimensional versions of the fluctuation factors (2.264) are

$$F_\Omega(t_b,t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}^D}\left[\det\frac{\partial x_b^i}{\partial \dot{x}_a^j}\right]^{-1/2} = \frac{1}{\sqrt{2\pi i\hbar/M}^D}\left[\det\frac{\partial \dot{x}_a^i}{\partial x_b^j}\right]^{1/2}. \tag{2.270}$$

All formulas for fluctuation factors hold initially only for sufficiently short times $t_b - t_a$. For larger times, they carry phase factors determined as before in (2.169). The fully defined expression may be written as

$$F_\Omega(t_b,t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}^D}\left|\det\frac{\partial x_b^i}{\partial \dot{x}_a^j}\right|^{-1/2} e^{-i\nu\pi/2} = \frac{1}{\sqrt{2\pi i\hbar/M}^D}\left|\det\frac{\partial \dot{x}_a^i}{\partial x_b^j}\right|^{1/2} e^{-i\nu\pi/2}, \tag{2.271}$$

where ν is the Maslov-Morse index. In the one-dimensional case it counts the turning points of the trajectory, in the multidimensional case the number of zeros in determinant $\det \partial x_b^i/\partial \dot{x}_a^j$ along the trajectory, if the zero is caused by a reduction of the rank of the matrix $\partial x_b^i/\partial \dot{x}_a^j$ by one unit. If it is reduced by more than one unit, ν increases accordingly. In this context, the number ν is also called the *Morse index* of the trajectory.

The zeros of the functional determinant are also called *conjugate points*. They are generalizations of the turning points in one-dimensional systems. The surfaces in $\mathbf{x}$-space, on which the determinant vanishes, are called *caustics*. The conjugate points are the places where the orbits touch the caustics.[13]

Note that for infinitesimally short times, all fluctuation factors and classical actions coincide with those of a free particle. This is obvious for the time-independent harmonic oscillator, where the amplitude (2.177) reduces to that of a free particle

[13]See M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Springer, Berlin, 1990.

in Eq. (2.74) in the limit $t_b \to t_a$. Since a time-dependent frequency is constant over an infinitesimal time, this same result holds also here. Expanding the solution of the equations of motion for infinitesimally short times as

$$\mathbf{x}_b \approx (t_b - t_a)\dot{\mathbf{x}}_a + \mathbf{x}_a, \qquad \mathbf{x}_a \approx -(t_b - t_a)\dot{\mathbf{x}}_b + \mathbf{x}_b, \tag{2.272}$$

we have immediately

$$\frac{\partial x_b^i}{\partial \dot{x}_a^j} = \delta_{ij}(t_b - t_a), \qquad \frac{\partial x_a}{\partial \dot{x}_b^j} = -\delta_{ij}(t_b - t_a). \tag{2.273}$$

Similarly, the expansions

$$\dot{\mathbf{x}}_b \approx \dot{\mathbf{x}}_a \approx \frac{\mathbf{x}_b - \mathbf{x}_a}{t_b - t_a} \tag{2.274}$$

lead to

$$\frac{\partial \dot{x}_b^i}{\partial x_a^j} = -\delta_{ij}\frac{1}{t_b - t_a}, \qquad \frac{\partial \dot{x}_a^i}{\partial x_b^j} = \delta_{ij}\frac{1}{t_b - t_a}. \tag{2.275}$$

Inserting the expansions (2.273) or (2.274) into (2.266) (in D dimensions), the action reduces approximately to the free-particle action

$$\mathcal{A}_{\rm cl} \approx \frac{M}{2}\frac{(\mathbf{x}_b - \mathbf{x}_a)^2}{t_b - t_a}. \tag{2.276}$$

2.5.2 Momentum Space

Let us also find the time evolution amplitude in momentum space. For this we write the classical action (2.267) as a quadratic form

$$\mathcal{A}_{\rm cl} = \frac{M}{2}\,(x_b, x_a)\,A\begin{pmatrix} x_b \\ x_a \end{pmatrix} \tag{2.277}$$

with a matrix

$$A = \begin{pmatrix} \dfrac{\partial \dot{x}_b}{\partial x_b} & \dfrac{\partial \dot{x}_b}{\partial x_a} \\ -\dfrac{\partial \dot{x}_a}{\partial x_b} & -\dfrac{\partial \dot{x}_a}{\partial x_a} \end{pmatrix}. \tag{2.278}$$

The inverse of this matrix is

$$A^{-1} = \begin{pmatrix} \dfrac{\partial x_b}{\partial \dot{x}_b} & -\dfrac{\partial x_b}{\partial \dot{x}_a} \\ \dfrac{\partial x_a}{\partial \dot{x}_b} & -\dfrac{\partial x_a}{\partial \dot{x}_a} \end{pmatrix}. \tag{2.279}$$

The partial derivatives of x_b and x_a are calculated from the solution of the homogeneous differential equation (2.218) specified in terms of the final and initial velocities $\dot{x}_b$ and $\dot{x}_a$:

$$x(\dot{x}_b, \dot{x}_a; t) = \frac{1}{\dot{D}_a(t_b)\dot{D}_b(t_a) + 1} \times \left\{\left[D_a(t) + D_b(t)\dot{D}_a(t_b)\right]\dot{x}_a + \left[-D_b(t) + D_a(t)\dot{D}_b(t_a)\right]\dot{x}_b\right\}, \tag{2.280}$$

which yields

$$x_a = \frac{1}{\dot{D}_a(t_b)\dot{D}_b(t_a)+1}\left[D_b(t_a)\dot{D}_a(t_a)\dot{x}_b - D_b(t_a)\dot{x}_b\right], \tag{2.281}$$

$$x_b = \frac{1}{\dot{D}_a(t_b)\dot{D}_b(t_a)+1}\left[D_a(t_b)\dot{x}_a + D_a(t_b)\dot{D}_b(t_a)\dot{x}_b\right], \tag{2.282}$$

so that

$$A^{-1} = \frac{D_a(t_b)}{\dot{D}_a(t_b)\dot{D}_b(t_a)+1}\begin{pmatrix} \dot{D}_b(t_a) & -1 \\ -1 & -\dot{D}_a(t_b)\end{pmatrix}. \tag{2.283}$$

The determinant of A is the Jacobian

$$\det A = -\frac{\partial(\dot{x}_b,\dot{x}_a)}{\partial(x_b,x_a)} = -\frac{\dot{D}_a(t_b)\dot{D}_b(t_a)+1}{D_a(t_b)D_b(t_a)}. \tag{2.284}$$

We can now perform the Fourier transform of the time evolution amplitude and find, via a quadratic completion,

$$\begin{aligned}(p_bt_b|p_at_a) &= \int dx_b\, e^{-ip_bx_b/\hbar}\int dx_a\, e^{ip_ax_a/\hbar}(x_bt_b|x_at_a) \\ &= \sqrt{\frac{2\pi\hbar}{iM}}\sqrt{\frac{D_a(t_b)}{\dot{D}_a(t_b)\dot{D}_b(t_a)+1}} \\ &\times\ \exp\left\{\frac{i}{\hbar}\frac{1}{2M}\frac{D_a(t_b)}{\dot{D}_a(t_b)\dot{D}_b(t_a)+1}\left[-\dot{D}_b(t_a)p_b^2+\dot{D}_a(t_b)p_a^2-2p_bp_a\right]\right\}.\end{aligned} \tag{2.285}$$

Inserting here $D_a(t_b) = \sin\omega(t_b-t_a)/\omega$ and $\dot{D}_a(t_b) = \cos\omega(t_b-t_a)$, we recover the oscillator result (2.189).

In D dimensions, the classical action has the same quadratic form as in (2.277)

$$\mathcal{A}_{\rm cl} = \frac{M}{2}\left(\mathbf{x}_b^T,\mathbf{x}_a^T\right)\mathbf{A}\begin{pmatrix}\mathbf{x}_b\\ \mathbf{x}_a\end{pmatrix} \tag{2.286}$$

with a matrix $\mathbf{A}$ generalizing (2.278) by having the partial derivatives replaced by the corresponding $D\times D$-matrices. The inverse is the $2D\times 2D$-version of (2.279), i.e.

$$\mathbf{A} = \begin{pmatrix} \dfrac{\partial\dot{\mathbf{x}}_b}{\partial\mathbf{x}_b} & \dfrac{\partial\dot{\mathbf{x}}_b}{\partial\mathbf{x}_a} \\ -\dfrac{\partial\dot{\mathbf{x}}_a}{\partial\mathbf{x}_b} & -\dfrac{\partial\dot{\mathbf{x}}_a}{\partial\mathbf{x}_a}\end{pmatrix}, \qquad \mathbf{A}^{-1} = \begin{pmatrix} \dfrac{\partial\mathbf{x}_b}{\partial\dot{\mathbf{x}}_b} & -\dfrac{\partial\mathbf{x}_b}{\partial\dot{\mathbf{x}}_a} \\ \dfrac{\partial\mathbf{x}_a}{\partial\dot{\mathbf{x}}_b} & -\dfrac{\partial\mathbf{x}_a}{\partial\dot{\mathbf{x}}_a}\end{pmatrix}. \tag{2.287}$$

The determinant of such a block matrix

$$\mathbf{A} = \begin{pmatrix} a & b\\ c & d\end{pmatrix} \tag{2.288}$$

is calculated after a triangular decomposition

$$\mathbf{A} = \begin{pmatrix} a & b\\ c & d\end{pmatrix} = \begin{pmatrix} a & 0\\ c & 1\end{pmatrix}\begin{pmatrix} 1 & a^{-1}b\\ 0 & d-ca^{-1}b\end{pmatrix} = \begin{pmatrix} 1 & b\\ 0 & d\end{pmatrix}\begin{pmatrix} a-bd^{-1}c & 0\\ d^{-1}c & 1\end{pmatrix} \tag{2.289}$$

in two possible ways as

$$\det\begin{pmatrix} a & b\\ c & d\end{pmatrix} = \det a\,\cdot\det\left(d-ca^{-1}b\right) = \det\left(a-bd^{-1}c\right)\,\cdot\det d, \tag{2.290}$$

depending whether $\det a$ or $\det b$ is nonzero. The inverse is in the first case

$$\mathbf{A}=\begin{pmatrix}1 & -a^{-1}bx\\ 0 & x\end{pmatrix}\begin{pmatrix}a^{-1} & 0\\ -ca^{-1} & 1\end{pmatrix}=\begin{pmatrix}a^{-1}+a^{-1}bxca^{-1} & -a^{-1}bx\\ -xca^{-1} & x\end{pmatrix},\quad x\equiv(d-ca^{-1}b)^{-1}. \tag{2.291}$$

The resulting amplitude in momentum space is

$$\begin{aligned}(\mathbf{p}_bt_b|\mathbf{p}_at_a) &= \int dx_b\, e^{-i\mathbf{p}_b\mathbf{x}_b/\hbar}\int dx_a\, e^{i\mathbf{p}_a\mathbf{x}_a/\hbar}(\mathbf{x}_bt_b|\mathbf{x}_at_a)\\ &= \frac{2\pi}{\sqrt{2\pi i\hbar M}}\frac{1}{\sqrt{D_{\rm ren}\det\mathbf{A}}}\exp\left\{\frac{i}{\hbar}\frac{1}{2M}\left[\left(\mathbf{p}_b^T,\mathbf{p}_a^T\right)\mathbf{A}^{-1}\begin{pmatrix}\mathbf{p}_b\\ \mathbf{p}_a\end{pmatrix}\right]\right\}.\end{aligned} \tag{2.292}$$

Also in momentum space, the amplitude (2.292) reduces to the free-particle one in Eq. (2.73) in the limit of infinitesimally short time t_b-t_a: For the time-independent harmonic oscillator, this was shown in Eq. (2.191), and the time-dependence of $\Omega(t)$ becomes irrelevant in the limit of small $t_b-t_a\to 0$.

2.6 Free-Particle and Oscillator Wave Functions

In Eq. (1.335) we have expressed the time evolution amplitude of the free particle (2.72) as a Fourier integral

$$(x_bt_b|x_at_a) \;=\; \int\frac{dp}{(2\pi\hbar)}e^{ip(x_b-x_a)/\hbar}e^{-ip^2(t_b-t_a)/2M\hbar}. \tag{2.293}$$

This expression contains the information on all stationary states of the system. To find these states we have to perform a spectral analysis of the amplitude. Recall that according to Section 1.7, the amplitude of an arbitrary time-independent system possesses a spectral representation of the form

$$(x_bt_b|x_at_a)=\sum_{n=0}^{\infty}\psi_n(x_b)\psi_n^*(x_a)e^{-iE_n(t_b-t_a)/\hbar}, \tag{2.294}$$

where E_n are the eigenvalues and $\psi_n(x)$ the wave functions of the stationary states. In the free-particle case the spectrum is continuous and the spectral sum is an integral. Comparing (2.294) with (2.293) we see that the Fourier decomposition itself happens to be the spectral representation. If the sum over n is written as an integral over the momenta, we can identify the wave functions as

$$\psi_p(x)=\frac{1}{\sqrt{2\pi\hbar}}e^{ipx}. \tag{2.295}$$

For the time evolution amplitude of the harmonic oscillator

$$\begin{aligned}(x_bt_b|x_at_a) \;&=\; \frac{1}{\sqrt{2\pi i\hbar\sin\left[\omega(t_b-t_a)\right]/M\omega}}\\ &\quad\times\exp\left\{\frac{iM\omega}{2\hbar\sin\left[\omega(t_b-t_a)\right]}\left[(x_b^2+x_a^2)\cos\omega(t_b-t_a)-2x_bx_a\right]\right\},\end{aligned} \tag{2.296}$$

the procedure is not as straight-forward. Here we must make use of a summation formula for *Hermite polynomials* (see Appendix 2C) $H_n(x)$ due to Mehler:[14]

$$\frac{1}{\sqrt{1-a^2}}\exp\left\{-\frac{1}{2(1-a^2)}[(x^2+x'^2)(1+a^2)-4xx'a]\right\}$$
$$=\exp(-x^2/2-x'^2/2)\sum_{n=0}^{\infty}\frac{a^n}{2^n n!}H_n(x)H_n(x'), \qquad (2.297)$$

with

$$H_0(x)=1,\ H_1(x)=2x,\ H_2(x)=4x^2-2,\ldots,H_n(x)=(-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}. \qquad (2.298)$$

Identifying

$$x\equiv\sqrt{M\omega/\hbar}\,x_b, \qquad x'\equiv\sqrt{M\omega/\hbar}\,x_a, \qquad a\equiv e^{-i\omega(t_b-t_a)}, \qquad (2.299)$$

so that

$$\frac{a}{1-a^2}=\frac{1}{2i\sin[\omega(t_b-t_a)]}, \qquad \frac{1+a^2}{1-a^2}=\frac{1+e^{-2i\omega(t_b-t_a)}}{1-e^{-2i\omega(t_b-t_a)}}=\frac{\cos[\omega(t_b-t_a)]}{i\sin[\omega(t_b-t_a)]}$$

we arrive at the spectral representation

$$(x_bt_b|x_at_a)=\sum_{n=0}^{\infty}\psi_n(x_b)\psi_n(x_a)e^{-i(n+1/2)\omega(t_b-t_a)}. \qquad (2.300)$$

From this we deduce that the harmonic oscillator has the energy eigenvalues

$$E_n=\hbar\omega(n+1/2) \qquad (2.301)$$

and the wave functions

$$\psi_n(x)=N_n\lambda_\omega^{-1/2}e^{-x^2/2\lambda_\omega^2}H_n(x/\lambda_\omega). \qquad (2.302)$$

Here, λ_ω is the natural length scale of the oscillator

$$\lambda_\omega\equiv\sqrt{\frac{\hbar}{M\omega}}, \qquad (2.303)$$

and N_n the normalization constant

$$N_n=(1/2^n n!\sqrt{\pi})^{1/2}. \qquad (2.304)$$

It is easy to check that the wave functions satisfy the orthonormality relation

$$\int_{-\infty}^{\infty}dx\,\psi_n(x)\psi_{n'}(x)^*=\delta_{nn'}, \qquad (2.305)$$

using the well-known orthogonality relation of Hermite polynomials[15]

$$\frac{1}{2^n n!\sqrt{\pi}}\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)H_{n'}(x)=\delta_{n,n'}. \qquad (2.306)$$

[14] See P.M. Morse and H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill, New York, Vol. I, p. 781 (1953).
[15] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formula 7.374.1.

2.7 General Time-Dependent Harmonic Action

A simple generalization of the harmonic oscillator with time-dependent frequency allows also for a time-dependent mass, so that the action (2.307) becomes

$$\mathcal{A}[x] = \int_{t_a}^{t_b} dt \frac{M}{2}\left[g(t)\dot{x}^2(t) - \Omega^2(t)x^2(t)\right], \tag{2.307}$$

with some dimensionless time-dependent factor $g(t)$. This factor changes the measure of path integration so that the time evolution amplitude can no longer be calculated from (2.260). To find the correct measure we must return to the canonical path integral (2.29) which now reads

$$(x_bt_b|x_at_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{i\mathcal{A}[p,x]/\hbar}, \tag{2.308}$$

with the canonical action

$$\mathcal{A}[p,x] = \int_{t_a}^{t_b} dt \left[p\dot{x} - \frac{p^2}{2Mg(t)} - \frac{M}{2}\Omega^2(t)x^2(t)\right]. \tag{2.309}$$

Integrating the momentum variables out in the sliced form of this path integral as in Eqs. (2.51)–(2.53) yields

$$(x_bt_b|x_at_a) \approx \frac{1}{\sqrt{2\pi\hbar i\epsilon/Mg(t_{N+1})}} \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{2\pi\hbar i\epsilon/Mg(t_n)}}\right] \exp\left(\frac{i}{\hbar}\mathcal{A}^N\right). \tag{2.310}$$

The continuum limit of this path integral is written as

$$(x_bt_b|x_at_a) \;=\; \int \mathcal{D}x\sqrt{g}\exp\left\{\frac{i}{\hbar}\mathcal{A}[x]\right\}, \tag{2.311}$$

with the action (2.307).

The classical orbits solve the equation of motion

$$\left[-\partial_t g(t)\partial_t - \Omega^2(t)\right]x(t) = 0, \tag{2.312}$$

which, by the transformation

$$\tilde{x}(t) = \sqrt{g(t)}x(t), \quad \tilde{\Omega}^2(t) = \frac{1}{g(t)}\left[\Omega^2(t) + \frac{\dot{g}^2(t)}{4g(t)} - \frac{\ddot{g}(t)}{2}\right], \tag{2.313}$$

can be reduced to the previous form

$$\sqrt{g(t)}\left[-\partial_t^2 - \tilde{\Omega}^2(t)\right]\tilde{x}(t) = 0. \tag{2.314}$$

The result of the path integration is therefore

$$(x_bt_b|x_at_a) = \int \mathcal{D}x\sqrt{g}\, e^{i\mathcal{A}[x]/\hbar} = F(x_b,t_b;x_a,t_a)e^{i\mathcal{A}_{\rm cl}/\hbar}, \tag{2.315}$$

with a fluctuation factor [compare (2.263)]

$$F(x_b,t_b;x_a,t_a) = \frac{1}{\sqrt{2\pi i\hbar/M}}\frac{1}{\sqrt{D_a(t_b)}}, \tag{2.316}$$

where $D_a(t_b)$ is found from a generalization of the formulas (2.264)–(2.269). The classical action is

$$\mathcal{A}_{\rm cl} = \frac{M}{2}(g_bx_b\dot{x}_b - g_ax_a\dot{x}_a), \tag{2.317}$$

where $g_b \equiv g(t_b)$, $g_a \equiv g(t_a)$. The solutions of the equation of motion can be expressed in terms of modified Gelfand-Yaglom functions (2.228) and (2.229) with the properties

$$[\partial_t g(t)\partial_t + \Omega^2(t)]D_a(t) = 0\ ; \quad D_a(t_a) = 0, \quad \dot{D}_a(t_a) = 1/g_a, \tag{2.318}$$
$$[\partial_t g(t)\partial_t + \Omega^2(t)]D_b(t) = 0\ ; \quad D_b(t_b) = 0, \quad \dot{D}_b(t_b) = -1/g_b, \tag{2.319}$$

as in (2.248):

$$x(x_b, x_a; t) = \frac{D_b(t)}{D_b(t_a)} x_a + \frac{D_a(t)}{D_a(t_b)} x_b. \tag{2.320}$$

This allows us to write the classical action (2.317) in the form

$$\mathcal{A}_{\rm cl} = \frac{M}{2D_a(t_b)} \left[g_b x_b^2 \dot{D}_a(t_b) - g_a x_a^2 \dot{D}_b(t_a) - 2x_b x_a \right]. \tag{2.321}$$

From this we find, as in (2.269),

$$D_{\rm ren} = D_a(t_b) = D_b(t_a) = -M \left(\frac{\partial^2 \mathcal{A}_{\rm cl}}{\partial x_b \partial x_a} \right)^{-1}, \tag{2.322}$$

so that the fluctuation factor becomes

$$F(x_b, t_b; x_a, t_a) = \frac{1}{\sqrt{2\pi i\hbar}} \sqrt{-\frac{\partial^2 \mathcal{A}_{\rm cl}}{\partial x_b \partial x_a}}. \tag{2.323}$$

As an example take a free particle with a time-dependent mass term, where

$$D_a(t) = \int_{t_a}^{t} dt'\, g^{-1}(t'),\ D_b(t) = \int_{t}^{t_b} dt'\, g^{-1}(t'),\ D_{\rm ren} = D_a(t_b) = D_b(t_a) = \int_{t_a}^{t_b} dt'\, g^{-1}(t'), \tag{2.324}$$

and the classical action reads

$$\mathcal{A}_{\rm cl} = \frac{M}{2} \frac{(x_b - x_a)^2}{D_a(t_b)}. \tag{2.325}$$

The result can easily be generalized to an arbitrary harmonic action

$$\mathcal{A} = \int_{t_a}^{t_b} dt\, \frac{M}{2} \left[g(t)\dot{x}^2 + 2b(t)x\dot{x} - \Omega^2(t)x^2 \right], \tag{2.326}$$

which is extremized by the Euler-Lagrange equation [recall (1.8)]

$$\left[\partial_t g(t)\partial_t + \dot{b}(t) + \Omega^2(t) \right] x = 0. \tag{2.327}$$

The solution of the path integral (2.315) is again given by (2.315), with the fluctuation factor (2.323), where $\mathcal{A}_{\rm cl}$ is the action (2.326) along the classical path connecting the endpoints.

A further generalization to D dimensions is obvious by adapting the procedure in Subsection 2.4.6, which makes Eqs. (2.318)–(2.320). matrix equations.

2.8 Path Integrals and Quantum Statistics

The path integral approach is useful to also understand the thermal equilibrium properties of a system. We assume the system to have a *time-independent* Hamiltonian and to be in contact with a reservoir of temperature T. As explained in Section 1.7, the bulk thermodynamic quantities can be determined from the quantum-statistical partition function

$$Z = \mathrm{Tr}\left(e^{-\hat{H}/k_BT} \right) = \sum_n e^{-E_n/k_BT}. \tag{2.328}$$

This, in turn, may be viewed as an analytic continuation of the quantum-mechanical partition function

$$Z_{\rm QM} = {\rm Tr}\left(e^{-i(t_b-t_a)\hat{H}/\hbar}\right) \tag{2.329}$$

to the imaginary time

$$t_b - t_a = -\frac{i\hbar}{k_B T} \equiv -i\hbar\beta. \tag{2.330}$$

In the local particle basis $|x\rangle$, the quantum-mechanical trace corresponds to an integral over all positions so that the quantum-statistical partition function can be obtained by integrating the time evolution amplitude over $x_b = x_a$ and evaluating it at the analytically continued time:

$$Z \equiv \int_{-\infty}^{\infty} dx\, z(x) = \int_{-\infty}^{\infty} dx\, \langle x|e^{-\beta\hat{H}}|x\rangle = \int_{-\infty}^{\infty} dx\, (x\, t_b|x\, t_a)|_{t_b-t_a=-i\hbar\beta}. \tag{2.331}$$

The diagonal elements

$$z(x) \equiv \langle x|e^{-\beta\hat{H}}|x\rangle = (x\, t_b|x\, t_a)|_{t_b-t_a=-i\hbar\beta} \tag{2.332}$$

play the role of a *partition function density*. For a harmonic oscillator, this quantity has the explicit form [recall (2.175)]

$$z_\omega(x) = \frac{1}{\sqrt{2\pi\hbar/M}}\sqrt{\frac{\omega}{\sinh\hbar\beta\omega}}\exp\left(-\frac{M\omega}{\hbar}\tanh\frac{\hbar\beta\omega}{2}\; x^2\right). \tag{2.333}$$

By splitting the Boltzmann factor $e^{-\beta\hat{H}}$ into a product of $N+1$ factors $e^{-\epsilon\hat{H}/\hbar}$ with $\epsilon = \hbar/k_B T(N+1)$, we can derive for Z a similar path integral representation just as for the corresponding quantum-mechanical partition function in (2.42), (2.48):

$$\begin{aligned} Z \equiv & \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} dx_n\right] \\ \times\; & \langle x_{N+1}|e^{-\epsilon\hat{H}/\hbar}|x_N\rangle\langle x_N|e^{-\epsilon\hat{H}/\hbar}|x_{N-1}\rangle \times \ldots \times \langle x_2|e^{-\epsilon\hat{H}/\hbar}|x_1\rangle\langle x_1|e^{-\epsilon\hat{H}/\hbar}|x_{N+1}\rangle. \end{aligned} \tag{2.334}$$

As in the quantum-mechanical case, the matrix elements $\langle x_n|e^{-\epsilon\hat{H}/\hbar}|x_{n-1}\rangle$ are re-expressed in the form

$$\langle x_n|e^{-\epsilon\hat{H}/\hbar}|x_{n-1}\rangle \approx \int_{-\infty}^{\infty}\frac{dp_n}{2\pi\hbar}e^{ip_n(x_n-x_{n-1})/\hbar-\epsilon H(p_n,x_n)/\hbar}, \tag{2.335}$$

with the only difference that there is now no imaginary factor i in front of the Hamiltonian. The product (2.334) can thus be written as

$$Z \approx \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} dx_n \int_{-\infty}^{\infty}\frac{dp_n}{2\pi\hbar}\right]\exp\left(-\frac{1}{\hbar}\mathcal{A}_{\rm e}^N\right), \tag{2.336}$$

where $\mathcal{A}_{\rm e}^N$ denotes the sum

$$\mathcal{A}_{\rm e}^N = \sum_{n=1}^{N+1} \left[-ip_n(x_n - x_{n-1}) + \epsilon H(p_n, x_n)\right]. \tag{2.337}$$

In the continuum limit $\epsilon \to 0$, the sum goes over into the integral

$$\mathcal{A}_{\rm e}[p,x] = \int_0^{\hbar\beta} d\tau[-ip(\tau)\dot{x}(\tau) + H(p(\tau), x(\tau))], \tag{2.338}$$

and the partition function is given by the path integral

$$Z = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{-\mathcal{A}_{\rm e}[p,x]/\hbar}. \tag{2.339}$$

In this expression, $p(\tau), x(\tau)$ may be considered as paths running along an "imaginary time axis" $\tau = it$. The expression $\mathcal{A}_{\rm e}[p,x]$ is very similar to the mechanical canonical action (2.27). Since it governs the quantum-statistical path integrals it is called *quantum-statistical action* or *Euclidean action*, indicated by the subscript e. The name alludes to the fact that a D-dimensional Euclidean space extended by an imaginary-time axis $\tau = it$ has the same geometric properties as a $D+1$-dimensional Euclidean space. For instance, a four-vector in a Minkowski spacetime has a square length $dx^2 = -(cdt)^2 + (d\mathbf{x})^2$. Continued to an imaginary time, this becomes $dx^2 = (cd\tau)^2 + (d\mathbf{x})^2$ which is the square distance in a Euclidean four-dimensional space with four-vectors $(c\tau, \mathbf{x})$.

The integrand of the Euclidean action (2.339) is the *Euclidean Lagrangian* $L_{\rm e}$. It is related to the Hamiltonian by the *Euclidean Legendre transform* [compare (1.9)]

$$H = L_{\rm e} + i\frac{\partial L_{\rm e}}{\partial \dot{x}}\dot{x} = L_{\rm e} + ip\dot{x} \tag{2.340}$$

in which $\dot{x}$ is eliminated in favor of $p = \partial L_{\rm e}/\partial \dot{x}$ [compare (1.10)].

Just as in the path integral for the quantum-mechanical partition function (2.48), the measure of integration $\oint \mathcal{D}x \int \mathcal{D}p/2\pi\hbar$ in the quantum-statistical expression (2.339) is automatically symmetric in all p's and x's:

$$\oint \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} = \oint \frac{\mathcal{D}p}{2\pi\hbar} \int \mathcal{D}x = \prod_{n=1}^{N+1} \int_{-\infty}^{\infty} dx_n \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar}. \tag{2.341}$$

The symmetry is of course due to the trace integration over all initial ≡ final positions.

Most remarks made in connection with Eq. (2.48) carry over to the present case. The above path integral (2.339) is a natural extension of the rules of classical statistical mechanics. According to these, each cell in phase space $dxdp/h$ is occupied with equal statistical weight, with the probability factor e^{-E/k_BT}. In quantum statistics, the *paths* of all particles fluctuate evenly over the cells in *path phase space* $\prod_n dx(\tau_n)dp(\tau_n)/h$ $(\tau_n \equiv n\epsilon)$, each path carrying a probability factor $e^{-\mathcal{A}_{\rm e}/\hbar}$ involving the Euclidean action of the system.

2.9 Density Matrix

The partition function does not determine any local thermodynamic quantities. Important local information resides in the thermal analog of the time evolution amplitude $\langle x_b|e^{-\hat{H}/k_BT}|x_a\rangle$. Consider, for instance, the diagonal elements of this amplitude renormalized by a factor Z^{-1}:

$$\rho(x_a) \equiv Z^{-1}\langle x_a|e^{-\hat{H}/k_BT}|x_a\rangle. \tag{2.342}$$

They determine the thermal average of the particle density of a quantum-statistical system. Due to (2.334), the factor Z^{-1} makes the spatial integral over ρ equal to unity:

$$\int_{-\infty}^{\infty} dx\, \rho(x) = 1. \tag{2.343}$$

By inserting into (2.342) a complete set of eigenfunctions $\psi_n(x)$ of the Hamiltonian operator $\hat{H}$, we find the spectral decomposition

$$\rho(x_a) = \sum_n |\psi_n(x_a)|^2 e^{-\beta E_n} \Big/ \sum_n e^{-\beta E_n}. \tag{2.344}$$

Since $|\psi_n(x_a)|^2$ is the probability distribution of the system in the eigenstate $|n\rangle$, while the ratio $e^{-\beta E_n}/\sum_n e^{-\beta E_n}$ is the normalized probability to encounter the system in the state $|n\rangle$, the quantity $\rho(x_a)$ represents the normalized average particle density in space as a function of temperature.

Note the limiting properties of $\rho(x_a)$. In the limit $T \to 0$, only the lowest energy state survives and $\rho(x_a)$ tends towards the particle distribution in the ground state

$$\rho(x_a) \xrightarrow{T\to 0} |\psi_0(x_a)|^2. \tag{2.345}$$

In the opposite limit of high temperatures, quantum effects are expected to become irrelevant and the partition function should converge to the classical expression (1.538) which is the integral over the phase space of the Boltzmann distribution

$$Z \xrightarrow{T\to\infty} Z_{\rm cl} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{-H(p,x)/k_BT}. \tag{2.346}$$

We therefore expect the large-T limit of $\rho(x)$ to be equal to the *classical particle distribution*

$$\rho(x) \xrightarrow{T\to\infty} \rho_{\rm cl}(x) \quad = \quad Z_{\rm cl}^{-1} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{-H(p,x)/k_BT}. \tag{2.347}$$

Within the path integral approach, this limit will be discussed in more detail in Section 2.13. At this place we roughly argue as follows: When going in the original time-sliced path integral (2.334) to large T, i.e., small $\tau_b - \tau_a = \hbar/k_BT$, we may keep only a single time slice and write

$$Z \approx \left[\int_{-\infty}^{\infty} dx\right] \langle x|e^{-\epsilon\hat{H}/\hbar}|x\rangle, \tag{2.348}$$

with

$$\langle x|e^{-\epsilon\hat{H}}|x\rangle \approx \int_{-\infty}^{\infty}\frac{dp_n}{2\pi\hbar}e^{-\epsilon H(p_n,x)/\hbar}. \tag{2.349}$$

After substituting $\epsilon=\tau_b-\tau_a$ this gives directly (2.347). Physically speaking, the path has at high temperatures "no (imaginary) time" to fluctuate, and only one term in the product of integrals needs to be considered.

If $H(p,x)$ has the standard form

$$H(p,x)=\frac{p^2}{2M}+V(x), \tag{2.350}$$

the momentum integral is Gaussian in p and can be done using the formula

$$\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}e^{-ap^2/2\hbar}=\frac{1}{\sqrt{2\pi\hbar a}}. \tag{2.351}$$

This leads to the pure x-integral for the classical partition function

$$Z_{\rm cl}=\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi\hbar^2/Mk_BT}}e^{-V(x)/k_BT}=\int_{-\infty}^{\infty}\frac{dx}{l_{\rm e}(\hbar\beta)}e^{-\beta V(x)}. \tag{2.352}$$

In the second expression we have introduced the length

$$l_{\rm e}(\hbar\beta)\equiv\sqrt{2\pi\hbar^2\beta/M}. \tag{2.353}$$

It is the thermal (or Euclidean) analog of the characteristic length $l(t_b-t_a)$ introduced before in (2.131). It is called the *de Broglie wavelength associated with the temperature* $T=1/k_B\beta$ or, in short, the *thermal de Broglie wavelength*.

Omitting the x-integration in (2.352) renders the large-T limit $\rho(x)$, the classical particle distribution

$$\rho(x)\xrightarrow{T\to\infty}\rho_{\rm cl}(x)\;=\;Z_{\rm cl}^{-1}\frac{1}{l_{\rm e}(\hbar\beta)}e^{-\bar{V}(x)}. \tag{2.354}$$

For a free particle, the integral over x in (2.352) diverges. If we imagine the length of the x-axis to be very large but finite, say equal to L, the partition function is equal to

$$Z_{\rm cl}=\frac{L}{l_{\rm e}(\hbar\beta)}. \tag{2.355}$$

In D dimensions, this becomes

$$Z_{\rm cl}=\frac{V_D}{l_{\rm e}^D(\hbar\beta)}, \tag{2.356}$$

where V_D is the volume of the D-dimensional system. For a harmonic oscillator with potential $M\omega^2x^2/2$, the integral over x in (2.352) is finite and yields, in the D-dimensional generalization

$$Z_{\rm cl}=\frac{l_\omega^D}{l^D(\hbar\beta)}, \tag{2.357}$$

where

$$l_\omega \equiv \sqrt{\frac{2\pi}{\beta M \omega^2}} \tag{2.358}$$

denotes the classical length scale defined by the frequency of the harmonic oscillator. It is related to the quantum-mechanical one λ_ω of Eq. (2.303) by

$$l_\omega \, l_{\rm e}(\hbar\beta) = 2\pi \, \lambda_\omega^2. \tag{2.359}$$

Thus we obtain the *mnemonic rule* for going over from the partition function of a harmonic oscillator to that of a free particle: we must simply replace

$$l_\omega \xrightarrow[\omega\to 0]{} L, \tag{2.360}$$

or

$$\frac{1}{\omega} \xrightarrow[\omega\to 0]{} \sqrt{\frac{\beta M}{2\pi}} \, L. \tag{2.361}$$

The real-time version of this is, of course,

$$\frac{1}{\omega} \xrightarrow[\omega\to 0]{} \sqrt{\frac{(t_b - t_a)M}{2\pi\hbar}} \, L. \tag{2.362}$$

Let us write down a path integral representation for $\rho(x)$. Omitting in (2.339) the final trace integration over $x_b \equiv x_a$ and normalizing the expression by a factor Z^{-1}, we obtain

$$\begin{aligned} \rho(x_a) &= Z^{-1} \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{-\mathcal{A}_{\rm e}[p,x]/\hbar} \\ &= Z^{-1} \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}x e^{-\mathcal{A}_{\rm e}[x]/\hbar}. \end{aligned} \tag{2.363}$$

The thermal equilibrium expectation of an arbitrary Hermitian operator $\hat{O}$ is given by

$$\langle \hat{O} \rangle_T \equiv Z^{-1} \sum_n e^{-\beta E_n} \langle n | \hat{O} | n \rangle. \tag{2.364}$$

In the local basis $|x\rangle$, this becomes

$$\langle \hat{O} \rangle_T = Z^{-1} \iint_{-\infty}^{\infty} dx_b dx_a \langle x_b | e^{-\beta \hat{H}} | x_a \rangle \langle x_a | \hat{O} | x_b \rangle. \tag{2.365}$$

An arbitrary function of the position operator $\hat{x}$ has the expectation

$$\langle f(\hat{x}) \rangle_T = Z^{-1} \iint_{-\infty}^{\infty} dx_b dx_a \langle x_b | e^{-\beta \hat{H}} | x_a \rangle \delta(x_b - x_a) f(x_a) = \int dx \rho(x) f(x). \tag{2.366}$$

The particle density $\rho(x_a)$ determines the thermal averages of local observables.

If f depends also on the momentum operator $\hat{p}$, then the off-diagonal matrix elements $\langle x_b | e^{-\beta \hat{H}} | x_a \rangle$ are also needed. They are contained in the *density matrix* introduced for pure quantum systems in Eq. (1.221), and reads now in a thermal ensemble of temperature T:

$$\rho(x_b, x_a) \equiv Z^{-1}\langle x_b|e^{-\beta\hat{H}}|x_a\rangle, \tag{2.367}$$

whose diagonal values coincide with the above particle density $\rho(x_a)$.

It is useful to keep the analogy between quantum mechanics and quantum statistics as close as possible and to introduce the time translation operator along the imaginary time axis

$$\hat{U}_{\rm e}(\tau_b, \tau_a) \equiv e^{-(\tau_b-\tau_a)\hat{H}/\hbar}, \qquad \tau_b > \tau_a, \tag{2.368}$$

defining its local matrix elements as *imaginary* or *Euclidean* time evolution amplitudes[16]

$$(x_b\tau_b|x_a\tau_a) \equiv \langle x_b|\hat{U}_{\rm e}(\tau_b, \tau_a)|x_a\rangle, \qquad \tau_b > \tau_a. \tag{2.369}$$

As in the real-time case, we shall only consider the causal time-ordering $\tau_b > \tau_a$. Otherwise the partition function and the density matrix do not exist in systems with energies up to infinity. Given the imaginary-time amplitudes, the partition function is found by integrating over the diagonal elements

$$Z = \int_{-\infty}^{\infty} dx (x\,\hbar\beta|x\,0), \tag{2.370}$$

and the density matrix

$$\rho(x_b, x_a) = Z^{-1}(x_b\hbar\beta|x_a0). \tag{2.371}$$

For the sake of generality we may sometimes also consider the imaginary-time evolution operators for time-dependent Hamiltonians and the associated amplitudes. They are obtained by time-slicing the local matrix elements of the operator

$$\hat{U}(\tau_b, \tau_a) = T_\tau \exp\left[-\frac{1}{\hbar}\int_{\tau_a}^{\tau_b} d\tau \hat{H}(-i\tau)\right]. \tag{2.372}$$

Here T_τ is an ordering operator along the imaginary-time axis.

It must be emphasized that the usefulness of the operator (2.372) in describing thermodynamic phenomena is restricted to the Hamiltonian operator $\hat{H}(t)$ depending very weakly on the physical time t. The system has to remain close to equilibrium at all times. This is the range of validity of the so-called *linear response theory* (see Chapter 18 for more details).

The imaginary-time evolution amplitude (2.369) has a path integral representation which is obtained by dropping the final integration in (2.336) and relaxing the condition $x_b = x_a$:

$$(x_b\tau_b|x_a\tau_a) \approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} dx_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dp_n}{2\pi\hbar}\right]\exp\left(-\mathcal{A}_{\rm e}^N/\hbar\right). \tag{2.373}$$

[16]The imaginary-time amplitude $(x_b\beta|x_a\,0) = \langle x_b|e^{-\beta\hat{H}}|x_a\rangle$ is often referred to as *heat kernel*.

The time-sliced Euclidean action is

$$\mathcal{A}_{\rm e}^{N}=\sum_{n=1}^{N+1}\left[-ip_n(x_n-x_{n-1})+\epsilon H(p_n,x_n,\tau_n)\right] \tag{2.374}$$

(we have omitted the factor $-i$ in the τ-argument of H). In the continuum limit this is written as a path integral

$$(x_b\tau_b|x_a\tau_a)=\int\mathcal{D}'x\int\frac{\mathcal{D}p}{2\pi\hbar}\exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\rm e}[p,x]\right\} \tag{2.375}$$

[by analogy with (2.339)]. For a Hamiltonian of the standard form (2.7),

$$H(p,x,\tau)=\frac{p^2}{2M}+V(x,\tau),$$

with a smooth potential $V(x,\tau)$, the momenta can be integrated out, just as in (2.53), and the Euclidean version of the pure x-space path integral (2.54) leads to (2.55):

$$\begin{aligned}(x_b\tau_b|x_a\tau_a) &= \int\mathcal{D}x\,\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\left[\frac{M}{2}(\partial_\tau x)^2+V(x,\tau)\right]\right\}\\ &\approx \frac{1}{\sqrt{2\pi\hbar\epsilon/M}}\prod_{n=1}^{N}\left[\int_{-\infty}^{\infty}\frac{dx_n}{\sqrt{2\pi\beta/M}}\right]\\ &\quad\times\exp\left\{-\frac{1}{\hbar}\epsilon\sum_{n=1}^{N+1}\left[\frac{M}{2}\left(\frac{x_n-x_{n-1}}{\epsilon}\right)^2+V(x_n,\tau_n)\right]\right\}.\end{aligned} \tag{2.376}$$

From this we calculate the quantum-statistical partition function

$$\begin{aligned}Z &= \int_{-\infty}^{\infty}dx\,(x\,\hbar\beta|x\,0)\\ &= \int dx\int_{x(0)=x}^{x(\hbar\beta)=x}\mathcal{D}x\,e^{-\mathcal{A}_{\rm e}[x]/\hbar}=\oint\mathcal{D}x\,e^{-\mathcal{A}_{\rm e}[x]/\hbar},\end{aligned} \tag{2.377}$$

where $\mathcal{A}_{\rm e}[x]$ is the Euclidean version of the Lagrangian action

$$\mathcal{A}_{\rm e}[x]=\int_{\tau_a}^{\tau_b}d\tau\left[\frac{M}{2}x'^2+V(x,\tau)\right]. \tag{2.378}$$

The prime denotes differentiation with respect to the imaginary time. As in the quantum-mechanical partition function in (2.63), the path integral $\oint\mathcal{D}x$ now stands for

$$\oint\mathcal{D}x\approx\prod_{n=1}^{N+1}\int_{-\infty}^{\infty}\frac{dx_n}{\sqrt{2\pi\hbar\epsilon/M}}. \tag{2.379}$$

It contains no extra $1/\sqrt{2\pi\hbar\epsilon/M}$ factor, as in (2.376), due to the trace integration over the exterior x.

The condition $x(\hbar\beta) = x(0)$ is most easily enforced by expanding $x(\tau)$ into a Fourier series

$$x(\tau) = \sum_{m=-\infty}^{\infty} \frac{1}{\sqrt{N+1}} e^{-i\omega_m \tau} x_m, \tag{2.380}$$

with the Matsubara frequencies

$$\omega_m \equiv 2\pi m k_B T/\hbar = \frac{2\pi m}{\hbar\beta}, \quad m = 0, \pm 1, \pm 2, \dots \ . \tag{2.381}$$

When considered as functions on the entire τ-axis, the paths are periodic in $\hbar\beta$ at any τ, i.e.,

$$x(\tau) = x(\tau + \hbar\beta). \tag{2.382}$$

Thus the path integral for the quantum-statistical partition function comprises all periodic paths with a period $\hbar\beta$. In the time-sliced path integral (2.376), the coordinates $x(\tau)$ are needed only at the discrete times $\tau_n = n\epsilon$. Correspondingly, the sum over m in (2.380) can be restricted to run from $m = -N/2$ to $N/2$ for even N and from $-(N-1)/2$ to $(N+1)/2$ for odd N (see Fig. 2.3). In order to have a real $x(\tau_n)$, we must require that

$$x_m = x^*_{-m} \quad (\text{modulo } N+1). \tag{2.383}$$

Note that the Matsubara frequencies in the expansion of the paths $x(\tau)$ are now twice as big as the frequencies ν_m in the quantum fluctuations (2.115) (after analytic continuation of $t_b - t_a$ to $-i\hbar/k_BT$). Still, they have about the same total number, since they run over positive *and* negative integers. An exception is the zero frequency $\omega_m = 0$, which is *included* here, in contrast to the frequencies ν_m in (2.115) which run only over positive $m = 1, 2, 3, \dots$. This is necessary to describe paths with arbitrary nonzero endpoints $x_b = x_a = x$ (included in the trace).

2.10 Quantum Statistics of the Harmonic Oscillator

The harmonic oscillator is a good example for solving the quantum-statistical path integral. The τ-axis is sliced at $\tau_n = n\epsilon$, with $\epsilon \equiv \hbar\beta/(N+1)$ $(n = 0, \dots, N+1)$, and the partition function is given by the $N \to \infty$ -limit of the product of integrals

$$Z_\omega^N = \prod_{n=0}^{N} \left[\int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{2\pi\hbar\epsilon/M}} \right] \exp\left(-\mathcal{A}_{\rm e}^N/\hbar\right), \tag{2.384}$$

where $\mathcal{A}_{\rm e}^N$ is the time-sliced Euclidean oscillator action

$$\mathcal{A}_{\rm e}^N = \frac{M}{2\epsilon} \sum_{n=1}^{N+1} x_n(-\epsilon^2 \nabla\overline{\nabla} + \epsilon^2\omega^2) x_n. \tag{2.385}$$

Integrating out the x_n's, we find immediately

$$Z_\omega^N = \frac{1}{\sqrt{\det_{N+1}(-\epsilon^2\nabla\overline{\nabla} + \epsilon^2\omega^2)}}. \tag{2.386}$$

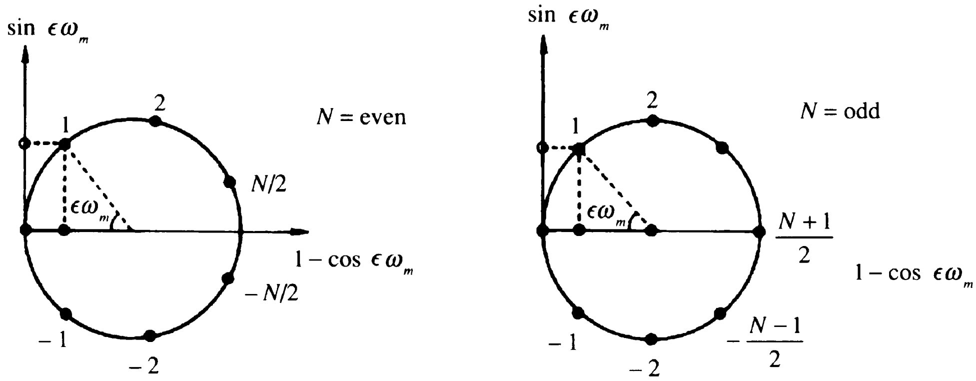

Figure 2.3 Illustration of the eigenvalues (2.387) of the fluctuation matrix in the action (2.385) for even and odd N.

Let us evaluate the fluctuation determinant via the product of eigenvalues which diagonalize the matrix $-\epsilon^2\nabla\overline{\nabla}+\epsilon^2\omega^2$ in the sliced action (2.385). They are

$$\epsilon^2\Omega_m\overline{\Omega}_m+\epsilon^2\omega^2 = 2-2\cos\omega_m\epsilon+\epsilon^2\omega^2, \tag{2.387}$$

with the Matsubara frequencies ω_m. For $\omega=0$, the eigenvalues are pictured in Fig. 2.3. The action (2.385) becomes diagonal after going to the Fourier components x_m. To do this we arrange the real and imaginary parts $\mathrm{Re}\,x_m$ and $\mathrm{Im}\,x_m$ in a row vector

$$(\mathrm{Re}\,x_1,\mathrm{Im}\,x_1;\mathrm{Re}\,x_2,\mathrm{Im}\,x_2;\ldots;\mathrm{Re}\,x_n,\mathrm{Im}\,x_n;\ldots),$$

and see that it is related to the time-sliced positions $x_n=x(\tau_n)$ by a transformation matrix with the rows

$$\begin{aligned} T_{mn}x_n &= (T_m)_n x_n \\ &= \sqrt{\frac{2}{N+1}}\Big(\frac{1}{\sqrt{2}},\cos\frac{m}{N+1}2\pi\cdot 1,\sin\frac{m}{N+1}2\pi\cdot 1, \\ &\quad \cos\frac{m}{N+1}2\pi\cdot 2,\sin\frac{m}{N+1}2\pi\cdot 2,\ldots \\ &\quad \ldots,\cos\frac{m}{N+1}2\pi\cdot n,\sin\frac{m}{N+1}2\pi\cdot n,\ldots\Big)_n x_n. \end{aligned} \tag{2.388}$$

For each row index $m=0,\ldots,N,$ the column index n runs from zero to $N/2$ for even N, and to $(N+1)/2$ for odd N. In the odd case, the last column $\sin\frac{m}{N+1}2\pi\cdot n$ with $n=(N+1)/2$ vanishes identically and must be dropped, so that the number of columns in T_{mn} is in both cases $N+1$, as it should be. For odd N, the second-last column of T_{mn} is an alternating sequence ± 1. Thus, for a proper normalization, it has to be multiplied by an extra normalization factor $1/\sqrt{2}$, just as the elements in the first column. An argument similar to (2.120), (2.121) shows that the resulting matrix is orthogonal. Thus, we can diagonalize the sliced action in (2.385) as follows

$$\mathcal{A}_{\mathrm{e}}^N=\frac{M}{2}\epsilon\left\{\begin{array}{ll} \Big[\omega^2x_0^2+2\sum_{m=1}^{N/2}(\Omega_m\overline{\Omega}_m+\omega^2)|x_m|^2\Big] & \text{for}\quad N=\text{even}, \\ \big[\omega^2x_0^2+(\Omega_{(N+1)/2}\overline{\Omega}_{(N+1)/2}+\omega^2)x_{\frac{N+1}{2}}^2 & \\ \qquad +2\sum_{m=1}^{(N-1)/2}(\Omega_m\overline{\Omega}_m+\omega^2)|x_m|^2\Big] & \text{for}\quad N=\text{odd}. \end{array}\right. \tag{2.389}$$

Thanks to the orthogonality of T_{mn}, the measure $\prod_n\int_{-\infty}^{\infty}dx(\tau_n)$ transforms simply into

$$\int_{-\infty}^{\infty}dx_0\prod_{m=1}^{N/2}\int_{-\infty}^{\infty}d\,\mathrm{Re}\,x_m\int_{-\infty}^{\infty}d\,\mathrm{Im}\,x_m\quad\text{for}\quad N=\text{even},$$

$$\int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dx_{(N+1)/2} \prod_{m=1}^{(N-1)/2} \int_{-\infty}^{\infty} d\,\mathrm{Re}\,x_m \int_{-\infty}^{\infty} d\,\mathrm{Im}\,x_m \quad \text{for} \quad N = \text{odd}. \tag{2.390}$$

By performing the Gaussian integrals we obtain the partition function

$$\begin{aligned} Z_\omega^N &= \left[\det{}_{N+1}(-\epsilon^2\nabla\overline{\nabla} + \epsilon^2\omega^2)\right]^{-1/2} = \left[\prod_{m=0}^{N}(\epsilon^2\Omega_m\overline{\Omega}_m + \epsilon^2\omega^2)\right]^{-1/2} \\ &= \left\{\prod_{m=0}^{N}\left[2(1-\cos\omega_m\epsilon) + \epsilon^2\omega^2\right]\right\}^{-1/2} = \left[\prod_{m=0}^{N}\left(4\sin^2\frac{\omega_m\epsilon}{2} + \epsilon^2\omega^2\right)\right]^{-1/2}. \end{aligned} \tag{2.391}$$

Thanks to the periodicity of the eigenvalues under the replacement $n \to n + N + 1$, the result has become a unique product expression for both even and odd N.

It is important to realize that contrary to the fluctuation factor (2.162) in the real-time amplitude, the partition function (2.391) contains the square root of only positive eigenmodes as a unique result of Gaussian integrations. There are no phase subtleties as in the Fresnel integral (1.337).

To calculate the product, we observe that upon decomposing

$$\sin^2\frac{\omega_m\epsilon}{2} = \left(1 + \cos\frac{\omega_m\epsilon}{2}\right)\left(1 - \cos\frac{\omega_m\epsilon}{2}\right), \tag{2.392}$$

the sequence of first factors

$$1 + \cos\frac{\omega_m\epsilon}{2} \equiv 1 + \cos\frac{\pi m}{N+1} \tag{2.393}$$

runs for $m = 1, \dots N$ through the same values as the sequence of second factors

$$1 - \cos\frac{\omega_m\epsilon}{2} = 1 - \cos\frac{\pi m}{N+1} \equiv 1 + \cos\pi\frac{N+1-m}{N+1}, \tag{2.394}$$

except in an opposite order. Thus, separating out the $m = 0$ -term, we rewrite (2.391) in the form

$$Z_\omega^N = \frac{1}{\epsilon\omega}\left[\prod_{m=1}^{N} 2\left(1 - \cos\frac{\omega_m\epsilon}{2}\right)\right]^{-1}\left[\prod_{m=1}^{N}\left(1 + \frac{\epsilon^2\omega^2}{4\sin^2\frac{\omega_m\epsilon}{2}}\right)\right]^{-1/2}. \tag{2.395}$$

The first factor on the right-hand side is the quantum-mechanical fluctuation determinant of the free-particle determinant $\det_N(-\epsilon^2\nabla\overline{\nabla}) = N+1$ [see (2.128)], so that we obtain for both even and odd N

$$Z_\omega^N = \frac{k_BT}{\hbar\omega}\left[\prod_{m=1}^{N}\left(1 + \frac{\epsilon^2\omega^2}{4\sin^2\frac{\omega_m\epsilon}{2}}\right)\right]^{-1/2}. \tag{2.396}$$

To evaluate the remaining product, we must distinguish again between even and odd cases of N. For even N, where every eigenvalue occurs twice (see Fig. 2.3), we obtain

$$Z_\omega^N = \frac{k_BT}{\hbar\omega}\left[\prod_{m=1}^{N/2}\left(1 + \frac{\epsilon^2\omega^2}{4\sin^2\frac{m\pi}{N+1}}\right)\right]^{-1}. \tag{2.397}$$

For odd N, the term with $m = (N+1)/2$ occurs only once and must be treated separately so that

$$Z_\omega^N = \frac{k_BT}{\hbar\omega}\left[\left(1 + \frac{\epsilon^2\omega^2}{4}\right)^{1/2}\prod_{m=1}^{(N-1)/2}\left(1 + \frac{\epsilon^2\omega^2}{4\sin^2\frac{\pi m}{N+1}}\right)\right]^{-1}. \tag{2.398}$$

We now introduce the parameter $\tilde{\omega}_{\rm e}$, the Euclidean analog of (2.163), via the equations

$$\sin i\frac{\tilde{\omega}_{\rm e}\epsilon}{2} \equiv i\frac{\omega\epsilon}{2}, \quad \sinh\frac{\tilde{\omega}_{\rm e}\epsilon}{2} \equiv \frac{\omega\epsilon}{2}. \tag{2.399}$$

In the odd case, the product formula[17]

$$\prod_{m=1}^{(N-1)/2}\left[1-\frac{\sin^2 x}{\sin^2\frac{m\pi}{(N+1)}}\right] = \frac{2}{\sin 2x}\frac{\sin[(N+1)x]}{(N+1)} \tag{2.400}$$

[similar to (2.165)] yields, with $x = \tilde{\omega}_{\rm e}\epsilon/2$,

$$Z_\omega^N = \frac{k_BT}{\hbar\omega}\left[\frac{1}{\sinh(\tilde{\omega}_{\rm e}\epsilon/2)}\frac{\sinh[(N+1)\tilde{\omega}_{\rm e}\epsilon/2]}{N+1}\right]^{-1}. \tag{2.401}$$

In the even case, the formula[18]

$$\prod_{m=1}^{N/2}\left[1-\frac{\sin^2 x}{\sin^2\frac{m\pi}{(N+1)}}\right] = \frac{1}{\sin x}\frac{\sin[(N+1)x]}{(N+1)}, \tag{2.402}$$

produces once more the same result as in Eq. (2.401). Inserting Eq. (2.399) leads to the partition function on the sliced imaginary time axis:

$$Z_\omega^N = \frac{1}{2\sinh(\hbar\tilde{\omega}_{\rm e}\beta/2)}. \tag{2.403}$$

The partition function can be expanded into the following series

$$Z_\omega^N = e^{-\hbar\tilde{\omega}_{\rm e}/2k_BT} + e^{-3\hbar\tilde{\omega}_{\rm e}/2k_BT} + e^{-5\hbar\tilde{\omega}_{\rm e}/2k_BT} + \dots \ . \tag{2.404}$$

By comparison with the general spectral expansion (2.328), we display the energy eigenvalues of the system:

$$E_n = \left(n+\frac{1}{2}\right)\hbar\tilde{\omega}_{\rm e}. \tag{2.405}$$

They show the typical linearly rising oscillator sequence with

$$\tilde{\omega}_{\rm e} = \frac{2}{\epsilon}\text{arsinh}\frac{\omega\epsilon}{2} \tag{2.406}$$

playing the role of the frequency on the sliced time axis, and $\hbar\tilde{\omega}_{\rm e}/2$ being the zero-point energy.

In the continuum limit $\epsilon \to 0$, the time-sliced partition function Z_ω^N goes over into the usual oscillator partition function

$$Z_\omega = \frac{1}{2\sinh(\beta\hbar\omega/2)}. \tag{2.407}$$

In D dimensions this becomes, of course, $[2\sinh(\beta\hbar\omega/2)]^{-D}$, due to the additivity of the action in each component of $\mathbf{x}$.

Note that the continuum limit of the product in (2.396) can also be taken factor by factor. Then Z_ω becomes

$$Z_\omega = \frac{k_BT}{\hbar\omega}\left[\prod_{m=1}^{\infty}\left(1+\frac{\omega^2}{\omega_m^2}\right)\right]^{-1}. \tag{2.408}$$

[17] I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 1.391.1.

[18] *ibid.*, formula 1.391.3.

According to formula (2.173), the product $\prod_{m=1}^{\infty}\left(1+\frac{x^2}{m^2\pi^2}\right)$ converges rapidly against $\sinh x/x$ and we find with $x = \hbar\omega\beta/2$

$$Z_\omega = \frac{k_BT}{\hbar\omega}\frac{\hbar\omega/2k_BT}{\sinh(\hbar\omega/2k_BT)} = \frac{1}{2\sinh(\beta\hbar\omega/2)}. \tag{2.409}$$

As discussed after Eq. (2.183), the continuum limit can be taken in each factor since the product in (2.396) contains only ratios of frequencies.

Just as in the quantum-mechanical case, this procedure of obtaining the continuum limit can be summarized in the sequence of equations arriving at a ratio of differential operators

$$\begin{aligned} Z_\omega^N &= \left[\det{}_{N+1}(-\epsilon^2\nabla\overline{\nabla}+\epsilon^2\omega^2)\right]^{-1/2} \\ &= \left[\det{}'_{N+1}(-\epsilon^2\nabla\overline{\nabla})\right]^{-1/2}\left[\frac{\det_{N+1}(-\epsilon^2\nabla\overline{\nabla}+\epsilon^2\omega^2)}{\det'_{N+1}(-\epsilon^2\nabla\overline{\nabla})}\right]^{-1/2} \\ &\xrightarrow{\epsilon\to 0} \frac{k_BT}{\hbar}\left[\frac{\det(-\partial_\tau^2+\omega^2)}{\det'(-\partial_\tau^2)}\right]^{-1/2} = \frac{k_BT}{\hbar\omega}\prod_{m=1}^{\infty}\left[\frac{\omega_m^2+\omega^2}{\omega_m^2}\right]^{-1}. \end{aligned} \tag{2.410}$$

In the $\omega = 0$ -determinants, the zero Matsubara frequency is excluded to obtain a finite expression. This is indicated by a prime. The differential operator $-\partial_\tau^2$ acts on real functions which are periodic under the replacement $\tau \to \tau+\hbar\beta$. Remember that each eigenvalue ω_m^2 of $-\partial_\tau^2$ occurs twice, except for the zero frequency $\omega_0 = 0$, which appears only once.

Let us finally mention that the results of this section could also have been obtained directly from the quantum-mechanical amplitude (2.175) [or with the discrete times from (2.199)] by an analytic continuation of the time difference $t_b - t_a$ to imaginary values $-i(\tau_b - \tau_a)$:

$$\begin{aligned} (x_b\tau_b|x_a\tau_a) &= \frac{1}{\sqrt{2\pi\hbar/M}}\sqrt{\frac{\omega}{\sinh\omega(\tau_b-\tau_a)}} \\ &\times \exp\left\{-\frac{1}{2\hbar}\frac{M\omega}{\sinh\omega(\tau_b-\tau_a)}[(x_b^2+x_a^2)\cosh\omega(\tau_b-\tau_a)-2x_bx_a]\right\}. \end{aligned} \tag{2.411}$$

By setting $x = x_b = x_a$ and integrating over x, we obtain [compare (2.333)]

$$\begin{aligned} Z_\omega = \int_{-\infty}^{\infty} dx\,(x\,\tau_b|x\,\tau_a) &= \frac{1}{\sqrt{2\pi\hbar(\tau_b-\tau_a)/M}}\sqrt{\frac{\omega(\tau_b-\tau_a)}{\sinh[\omega(\tau_b-\tau_a)]}} \\ &\times \frac{\sqrt{2\pi\hbar\sinh[\omega(\tau_b-\tau_a)]/\omega M}}{2\sinh[\omega(\tau_b-\tau_a)/2]} = \frac{1}{2\sinh[\omega(\tau_b-\tau_a)/2]}. \end{aligned} \tag{2.412}$$

Upon equating $\tau_b - \tau_a = \hbar\beta$, we retrieve the partition function (2.407). A similar treatment of the discrete-time version (2.199) would have led to (2.403). The main reason for presenting an independent direct evaluation in the space of real periodic functions was to display the frequency structure of periodic paths and to see the difference with respect to the quantum-mechanical paths with fixed ends. We also wanted to show how to handle the ensuing product expressions.

For applications in polymer physics (see Chapter 15) one also needs the partition function of all path fluctuations with open ends

$$\begin{aligned} Z_\omega^{\text{open}} &= \int_{-\infty}^{\infty} dx_b \int_{-\infty}^{\infty} dx_a\,(x_b\tau_b|x_a\tau_a) = \frac{1}{\sqrt{2\pi\hbar(\tau_b-\tau_a)/M}}\sqrt{\frac{\omega(\tau_b-\tau_a)}{\sinh[\omega(\tau_b-\tau_a)]}\frac{2\pi\hbar}{M\omega}} \\ &= \sqrt{\frac{2\pi\hbar}{M\omega}}\frac{1}{\sqrt{\sinh[\omega(\tau_b-\tau_a)]}}. \end{aligned} \tag{2.413}$$

The prefactor is $\sqrt{2\pi}$ times the length scale λ_ω of Eq. (2.303).

2.11 Time-Dependent Harmonic Potential

It is often necessary to calculate thermal fluctuation determinants for the case of a time-dependent frequency $\Omega(\tau)$ which is periodic under $\tau \to \tau + \hbar\beta$. As in Section 2.3.6, we consider the amplitude

$$
\begin{aligned}
(x_b\tau_b|x_a\tau_a) &= \int \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{-\int_{\tau_a}^{\tau_b} d\tau[-ip\dot{x}+p^2/2M+M\Omega^2(\tau)x^2/2]/\hbar} \\
&= \int \mathcal{D}x e^{-\int_{\tau_a}^{\tau_b} d\tau[M\dot{x}^2+\Omega^2(\tau)x^2]/2\hbar}.
\end{aligned} \tag{2.414}
$$

The time-sliced fluctuation factor is [compare (2.202)]

$$
F^N(\tau_a - \tau_b) = \det{}_{N+1}[-\epsilon^2\nabla\overline{\nabla} + \epsilon\Omega^2(\tau)]^{-1/2}, \tag{2.415}
$$

with the continuum limit

$$
F(\tau_a - \tau_b) = \frac{k_BT}{\hbar}\left[\frac{\det(-\partial_\tau^2 + \Omega^2(\tau))}{\det'(-\partial_\tau^2)}\right]^{-1/2}. \tag{2.416}
$$

Actually, in the thermal case it is preferable to use the oscillator result for normalizing the fluctuation factor, rather than the free-particle result, and to work with the formula

$$
F(\tau_b, \tau_a) = \frac{1}{2\sinh(\beta\hbar\omega/2)}\left[\frac{\det(-\partial_\tau^2 + \Omega^2(\tau))}{\det(-\partial_\tau^2 + \omega^2)}\right]^{-1/2}. \tag{2.417}
$$

This has the advantage that the determinant in the denominator contains no zero eigenvalue which would require a special treatment as in (2.410); the operator $-\partial_\tau^2 + \omega^2$ is positive.

As in the quantum-mechanical case, the spectrum of eigenvalues is not known for general $\Omega(\tau)$. It is, however, possible to find a differential equation for the entire determinant, analogous to the Gelfand-Yaglom formula (2.209), with the initial condition (2.214), although the derivation is now much more tedious. The origin of the additional difficulties lies in the periodic boundary condition which introduces additional nonvanishing elements -1 in the upper right and lower left corners of the matrix $-\epsilon^2\nabla\overline{\nabla}$ [compare (2.107)]:

$$
-\epsilon^2\nabla\overline{\nabla} = \begin{pmatrix}
2 & -1 & 0 & & \dots & 0 & 0 & -1 \\
-1 & 2 & -1 & & \dots & 0 & 0 & 0 \\
\vdots & & & & & & & \vdots \\
0 & 0 & & 0 & \dots & -1 & 2 & -1 \\
-1 & 0 & 0 & & \dots & 0 & -1 & 2
\end{pmatrix}. \tag{2.418}
$$

To better understand the relation with the previous result we shall replace the corner elements -1 by $-\alpha$ which can be set equal to zero at the end, for a comparison. Adding to $-\epsilon^2\nabla\overline{\nabla}$ a time-dependent frequency matrix we then consider the fluctuation matrix

$$
-\epsilon^2\nabla\overline{\nabla} + \epsilon^2\Omega^2 = \begin{pmatrix}
2+\epsilon^2\Omega_{N+1}^2 & -1 & 0 & \dots & 0 & -\alpha \\
-1 & 2+\epsilon^2\Omega_N^2 & -1 & \dots & 0 & 0 \\
\vdots & & & & & \vdots \\
-\alpha & 0 & 0 & \dots & -1 & 2+\epsilon^2\Omega_1^2
\end{pmatrix}. \tag{2.419}
$$

Let us denote the determinant of this $(N+1)\times(N+1)$ matrix by $\tilde{D}_{N+1}$. Expanding it along the first column, it is found to satisfy the equation

$$
\begin{aligned}
\tilde{D}_{N+1} = (2+\epsilon^2\Omega_{N+1}^2) \\
\times\det{}_N \begin{pmatrix}
2+\epsilon^2\Omega_N^2 & -1 & 0 & \dots & 0 & 0 \\
\vdots & & & & & \vdots \\
0 & 0 & 0 & \dots & -1 & 2+\epsilon^2\Omega_1^2
\end{pmatrix}
\end{aligned} \tag{2.420}
$$

$$+\det_N\begin{pmatrix} -1 & 0 & 0 & 0 & \dots & 0 & -\alpha \\ -1 & 2+\epsilon^2\Omega_{N-1}^2 & -1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 2+\epsilon^2\Omega_{N-2}^2 & -1 & \dots & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & \dots & -1 & 2+\epsilon^2\Omega_1^2 \end{pmatrix}$$

$$+(-1)^{N+1}\alpha\det_N\begin{pmatrix} -1 & 0 & 0 & \dots & 0 & -\alpha \\ 2+\epsilon^2\Omega_N^2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2+\epsilon^2\Omega_{N-1}^2 & -1 & \dots & 0 & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & \dots & 2+\epsilon^2\Omega_2^2 & -1 \end{pmatrix}.$$

The first determinant was encountered before in Eq. (2.204) (except that there it appeared with $-\epsilon^2\Omega^2$ instead of $\epsilon^2\Omega^2$). There it was denoted by D_N, satisfying the difference equation

$$\left(-\epsilon^2\overline{\nabla}\nabla + \epsilon^2\Omega_{N+1}^2\right) D_N = 0, \tag{2.421}$$

with the initial conditions

$$\begin{aligned} D_1 &= 2+\epsilon^2\Omega_1^2, \\ D_2 &= (2+\epsilon^2\Omega_1^2)(2+\epsilon^2\Omega_2^2) - 1. \end{aligned} \tag{2.422}$$

The second determinant in (2.420) can be expanded with respect to its first column yielding

$$-D_{N-1} - \alpha. \tag{2.423}$$

The third determinant is more involved. When expanded along the first column it gives

$$(-1)^N\left[1 + (2+\epsilon^2\Omega_N^2)H_{N-1} - H_{N-2}\right], \tag{2.424}$$

with the $(N-1)\times(N-1)$ determinant

$$H_{N-1} \equiv (-1)^{N-1} \tag{2.425}$$

$$\times\det_{N-1}\begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 & -\alpha \\ 2+\epsilon^2\Omega_{N-1}^2 & -1 & 0 & \dots & 0 & 0 & 0 \\ -1 & 2+\epsilon^2\Omega_{N-2}^2 & -1 & \dots & 0 & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & \dots & -1 & 2+\epsilon^2\Omega_2^2 & -1 \end{pmatrix}.$$

By expanding this along the first column, we find that H_N satisfies the same difference equation as D_N:

$$(-\epsilon^2\overline{\nabla}\nabla + \epsilon^2\Omega_{N+1}^2)H_N = 0. \tag{2.426}$$

However, the initial conditions for H_N are different:

$$H_2 = \begin{vmatrix} 0 & -\alpha \\ 2+\epsilon^2\Omega_2^2 & -1 \end{vmatrix} = \alpha(2+\epsilon^2\Omega_2^2), \tag{2.427}$$

$$\begin{aligned} H_3 &= -\begin{vmatrix} 0 & 0 & -\alpha \\ 2+\epsilon^2\Omega_3^2 & -1 & 0 \\ -1 & 2+\epsilon^2\Omega_2^2 & -1 \end{vmatrix} \\ &= \alpha\left[(2+\epsilon^2\Omega_2^2)(2+\epsilon^2\Omega_3^2) - 1\right]. \end{aligned} \tag{2.428}$$

They show that H_N is in fact equal to αD_{N-1}, provided we shift Ω_N^2 by one lattice unit upwards to Ω_{N+1}^2. Let us indicate this by a superscript $+$, i.e., we write

$$H_N = \alpha D_{N-1}^+. \tag{2.429}$$

Thus we arrive at the equation

$$\begin{aligned}\tilde{D}_{N+1} &= (2+\epsilon^2\Omega_N^2)D_N - D_{N-1} - \alpha \\ &\quad -\alpha[1+(2+\epsilon^2\Omega_N^2)\alpha D_{N-2}^+ - \alpha D_{N-3}^+].\end{aligned} \tag{2.430}$$

Using the difference equations for D_N and D_N^+, this can be brought to the convenient form

$$\tilde{D}_{N+1} = D_{N+1} - \alpha^2 D_{N-1}^+ - 2\alpha. \tag{2.431}$$

For quantum-mechanical fluctuations with $\alpha = 0$, this reduces to the earlier result in Section 2.3.6. For periodic fluctuations with $\alpha = 1$, the result is

$$\tilde{D}_{N+1} = D_{N+1} - D_{N-1}^+ - 2. \tag{2.432}$$

In the continuum limit, $D_{N+1} - D_{N-1}^+$ tends towards $2\dot{D}_{\rm ren}$, where $D_{\rm ren}(\tau) = D_a(t)$ is the imaginary-time version of the Gelfand-Yaglom function in Section 2.4 solving the homogenous differential equation (2.215), with the initial conditions (2.213) and (2.214), or Eqs. (2.228). The corresponding properties are now:

$$\left[-\partial_\tau^2 + \Omega^2(\tau)\right] D_{\rm ren}(\tau) = 0, \qquad D_{\rm ren}(0) = 0, \qquad \dot{D}_{\rm ren}(0) = 1. \tag{2.433}$$

In terms of $D_{\rm ren}(\tau)$, the determinant is given by the *Gelfand-Yaglom-like* formula

$$\det(-\epsilon^2\overline{\nabla}\nabla + \epsilon\Omega^2)_T \xrightarrow{\epsilon\to 0} 2[\dot{D}_{\rm ren}(\hbar\beta) - 1], \tag{2.434}$$

and the partition function reads

$$Z_\Omega = \frac{1}{\sqrt{2\left[\dot{D}_{\rm ren}(\hbar\beta) - 1\right]}}. \tag{2.435}$$

The result may be checked by going back to the amplitude $(x_b t_b|x_a t_a)$ of Eq. (2.262), continuing it to imaginary times $t = i\tau$, setting $x_b = x_a = x$, and integrating over all x. The result is

$$Z_\Omega = \frac{1}{2\sqrt{\dot{D}_a(t_b) - 1}}, \qquad t_b = i\hbar\beta, \tag{2.436}$$

in agreement with (2.435).

As an example, take the harmonic oscillator for which the solution of (2.433) is

$$D_{\rm ren}(\tau) = \frac{1}{\omega}\sinh\omega\tau \tag{2.437}$$

[the analytically continued (2.216)]. Then

$$2[\dot{D}_{\rm ren}(\tau) - 1] = 2(\cosh\beta\hbar\omega - 1) = 4\sinh^2(\beta\hbar\omega/2), \tag{2.438}$$

and we find the correct partition function:

$$\begin{aligned}Z_\omega &= \left\{2[\dot{D}_{\rm ren}(\tau) - 1]\right\}^{-1/2}\Big|_{\tau=\hbar\beta} \\ &= \frac{1}{2\sinh(\beta\hbar\omega/2)}.\end{aligned} \tag{2.439}$$

On a sliced imaginary-time axis, the case of a constant frequency $\Omega^2 \equiv \omega^2$ is solved as follows. From Eq. (2.210) we take the ordinary Gelfand-Yaglom function D_N, and continue it to Euclidean $\tilde{\omega}_{\rm e}$, yielding the imaginary-time version

$$D_N = \frac{\sinh(N+1)\tilde{\omega}_{\rm e}\epsilon}{\sinh\tilde{\omega}_{\rm e}\epsilon}. \tag{2.440}$$

Then we use formula (2.432), which simplifies for a constant $\Omega^2 \equiv \omega^2$ for which $D^+_{N-1} = D_{N-1}$, and calculate

$$\begin{aligned}\tilde{D}_{N+1} &= \frac{1}{\sinh\tilde{\omega}_{\rm e}\epsilon}\left[\sinh(N+2)\tilde{\omega}_{\rm e}\epsilon - \sinh N\tilde{\omega}_{\rm e}\epsilon\right] - 2\\ &= 2\left[\cosh(N+1)\tilde{\omega}_{\rm e}\epsilon - 1\right] = 4\sinh^2[(N+1)\tilde{\omega}_{\rm e}\epsilon/2].\end{aligned} \tag{2.441}$$

Inserting this into Eq. (2.386) yields the partition function

$$Z_\omega = \frac{1}{\sqrt{\tilde{D}_{N+1}}} = \frac{1}{2\sinh(\hbar\tilde{\omega}_{\rm e}\beta/2)}, \tag{2.442}$$

in agreement with (2.403).

2.12 Functional Measure in Fourier Space

There exists an alternative definition for the quantum-statistical path integral which is useful for some applications (for example in Section 2.13 and in Chapter 5). The limiting product formula (2.410) suggests that instead of summing over all zigzag configurations of paths on a sliced time axis, a path integral may be defined with the help of the Fourier components of the paths on a continuous time axis. As in (2.380), but with a slightly different normalization of the coefficients, we expand these paths here as

$$x(\tau) = x_0 + \eta(\tau) \equiv x_0 + \sum_{m=1}^{\infty}\left(x_m e^{i\omega_m\tau} + \text{c.c.}\right), \qquad x_0 = \text{real}, \qquad x_{-m} \equiv x_m^*. \tag{2.443}$$

Note that the temporal integral over the time-dependent fluctuations $\eta(\tau)$ is zero, $\int_0^{\hbar/k_BT} d\tau\,\eta(\tau) = 0$, so that the zero-frequency component x_0 is the temporal average of the fluctuating paths:

$$x_0 = \bar{x} \equiv \frac{k_BT}{\hbar}\int_0^{\hbar/k_BT} d\tau\, x(\tau). \tag{2.444}$$

In contrast to (2.380) which was valid on a sliced time axis and was therefore subject to a restriction on the range of the m-sum, the present sum is unrestricted and runs over *all* Matsubara frequencies $\omega_m = 2\pi m k_BT/\hbar = 2\pi m/\hbar\beta$. In terms of x_m, the Euclidean action of the linear oscillator is

$$\begin{aligned}\mathcal{A}_{\rm e} &= \frac{M}{2}\int_0^{\hbar/k_BT} d\tau\,(\dot{x}^2 + \omega^2 x^2)\\ &= \frac{M\hbar}{k_BT}\left[\frac{\omega^2}{2}x_0^2 + \sum_{m=1}^{\infty}(\omega_m^2 + \omega^2)|x_m|^2\right].\end{aligned} \tag{2.445}$$

The integration variables of the time-sliced path integral were transformed to the Fourier components x_m in Eq. (2.388). The product of integrals $\prod_n \int_{-\infty}^{\infty} dx(\tau_n)$ turned into the product (2.390) of integrals over real and imaginary parts of x_m. In the continuum limit, the result is

$$\int_{-\infty}^{\infty} dx_0 \prod_{m=1}^{\infty} \int_{-\infty}^{\infty} d\,\mathrm{Re}\, x_m \int_{-\infty}^{\infty} d\,\mathrm{Im}\, x_m. \tag{2.446}$$

Placing the exponential $e^{-\mathcal{A}_e/\hbar}$ with the frequency sum (2.445) into the integrand, the product of Gaussian integrals renders a product of inverse eigenvalues $(\omega_m^2+\omega^2)^{-1}$ for $m = 1, \ldots, \infty$, with some infinite factor. This may be determined by comparison with the known continuous result (2.410) for the harmonic partition function. The infinity is of the type encountered in Eq. (2.183), and must be divided out of the measure (2.446). The correct result (2.408) is obtained from the following measure of integration in Fourier space

$$\oint \mathcal{D}x \equiv \int_{-\infty}^{\infty} \frac{dx_0}{l_e(\hbar\beta)} \prod_{m=1}^{\infty} \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\,\mathrm{Re}\, x_m d\,\mathrm{Im}\, x_m}{\pi k_B T / M\omega_m^2} \right]. \tag{2.447}$$

The divergences in the product over the factors $(\omega_m^2 + \omega^2)^{-1}$ discussed after Eq. (2.183) are canceled by the factors ω_m^2 in the measure. It will be convenient to introduce a short-hand notation for the measure on the right-hand side, writing it as

$$\oint \mathcal{D}x \equiv \int_{-\infty}^{\infty} \frac{dx_0}{l_e(\hbar\beta)} \oint \mathcal{D}'x. \tag{2.448}$$

The denominator of the x_0-integral is the length scale $l_e(\hbar\beta)$ associated with β defined in Eq. (2.353).

Then we calculate

$$\begin{aligned} Z_\omega^{x_0} \equiv \oint \mathcal{D}'x\, e^{-\mathcal{A}_e/\hbar} &= \prod_{m=1}^{\infty} \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\,\mathrm{Re}\, x_m d\,\mathrm{Im}\, x_m}{\pi k_B T / M\omega_m^2} \right] e^{-M\hbar\left[\omega^2 x_0^2/2 + \sum_{m=1}^{\infty}(\omega_m^2+\omega^2)|x_m|^2\right]/k_B T} \\ &= e^{-M\omega^2 x_0^2/2k_B T} \prod_{m=1}^{\infty} \left[\frac{\omega_m^2 + \omega^2}{\omega_m^2} \right]^{-1}. \end{aligned} \tag{2.449}$$

The final integral over the zero-frequency component x_0 yields the partition function

$$Z_\omega = \oint \mathcal{D}x\, e^{-\mathcal{A}_e/\hbar} = \int_{-\infty}^{\infty} \frac{dx_0}{l_e(\hbar\beta)} Z_\omega^{x_0} = \frac{k_B T}{\hbar\omega} \prod_{m=1}^{\infty} \left[\frac{\omega_m^2 + \omega^2}{\omega_m^2} \right]^{-1}, \tag{2.450}$$

as in (2.410).

The same measure can be used for the more general amplitude (2.414), as is obvious from (2.416). With the predominance of the kinetic term in the measure of path integrals [the divergencies discussed after (2.183) stem only from it], it can easily be shown that the same measure is applicable to any system with the standard kinetic term.

It is also possible to find a Fourier decomposition of the paths and an associated integration measure for the open-end partition function in Eq. (2.413). We begin by considering the slightly reduced set of all paths satisfying the Neumann boundary conditions

$$\dot{x}(\tau_a) = v_a = 0, \qquad \dot{x}(\tau_b) = v_b = 0. \tag{2.451}$$

They have the Fourier expansion

$$x(\tau) = x_0 + \eta(\tau) = x_0 + \sum_{n=1}^{\infty} x_n \cos \nu_n(\tau - \tau_a), \qquad \nu_n = n\pi/\beta. \tag{2.452}$$

The frequencies ν_n are the Euclidean version of the frequencies (3.64) for Dirichlet boundary conditions. Let us calculate the partition function for such paths by analogy with the above periodic case by a Fourier decomposition of the action

$$\mathcal{A}_{\rm e} = \frac{M}{2}\int_0^{\hbar/k_BT} d\tau\,(\dot{x}^2 + \omega^2 x^2) = \frac{M\hbar}{k_BT}\left[\frac{\omega^2}{2}x_0^2 + \frac{1}{2}\sum_{n=1}^{\infty}(\nu_n^2+\omega^2)x_n^2\right], \tag{2.453}$$

and of the measure

$$\begin{aligned}\oint \mathcal{D}x \;&\equiv\; \int_{-\infty}^{\infty}\frac{dx_0}{l_{\rm e}(\hbar\beta)}\prod_{n=1}^{\infty}\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\,x_n}{\pi k_BT/2M\nu_n^2}\right] \\ &\equiv\; \int_{-\infty}^{\infty}\frac{dx_0}{l_{\rm e}(\hbar\beta)}\oint \mathcal{D}'x. \end{aligned}\tag{2.454}$$

We now perform the path integral over all fluctuations at fixed x_0 as in (2.449):

$$\begin{aligned} Z_\omega^{{\rm N},x_0} \equiv \oint \mathcal{D}'x\, e^{-\mathcal{A}_{\rm e}/\hbar} &= \prod_{n=1}^{\infty}\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\,x_n}{\pi k_BT/2M\nu_n^2}\right] e^{-M\hbar\left[\omega^2x_0^2/2+\sum_{n=1}^{\infty}(\nu_n^2+\omega^2)|x_n|^2\right]/k_BT} \\ &= e^{-M\omega^2x_0^2/2k_BT}\prod_{n=1}^{\infty}\left[\frac{\nu_n^2+\omega^2}{\nu_n^2}\right]^{-1}. \end{aligned}\tag{2.455}$$

Using the product formula (2.183), this becomes

$$Z_\omega^{{\rm N},x_0} = \sqrt{\frac{\omega\hbar\beta}{\sinh\omega\hbar\beta}}\exp\left(-\beta\frac{M}{2}\omega^2x_0^2\right). \tag{2.456}$$

The final integral over the zero-frequency component x_0 yields the partition function

$$Z_\omega^{\rm N} = \frac{1}{l_{\rm e}(\hbar\beta)}\sqrt{\frac{2\pi\hbar}{M\omega}}\frac{1}{\sqrt{\sinh\omega\hbar\beta}}. \tag{2.457}$$

We have replaced the denominator in the prefactor $1/l_{\rm e}(\hbar\beta)$ by the length scale $1/l_{\rm e}(\hbar\beta)$ of Eq. (2.353). Apart from this prefactor, the Neumann partition function coincides precisely with the open-end partition function $Z_\omega^{\rm open}$ in Eq. (2.413).

What is the reason for this coincidence up to a trivial factor, even though the paths satisfying Neumann boundary conditions do *not* comprise all paths with open ends? Moreover, the integrals over the endpoints in the defining equation (2.413) do not force the endpoint *velocities*, but rather endpoint *momenta* to vanish. Indeed, recalling Eq. (2.189) for the time evolution amplitude in momentum space we can see immediately that the partition function with open ends Z_ω^{open} in Eq. (2.413) is identical to the imaginary-time amplitude with vanishing endpoint momenta:

$$Z_\omega^{\text{open}} = (p_b\,\hbar\beta|p_a\,0)|_{p_b=p_a=0}. \tag{2.458}$$

Thus, the sum over all paths with arbitrary open ends is equal to the sum of all paths satisfying Dirichlet boundary conditions in momentum space. Only classically, the vanishing of the endpoint momenta implies the vanishing of the endpoint velocities. From the general discussion of the time-sliced path integral in phase space in Section 2.1 we know that fluctuating paths have $M\dot{x} \neq p$. The fluctuations of the difference are controlled by a Gaussian exponential of the type (2.53). This leads to the explanation of the trivial factor between Z_ω^{open} and Z_ω^{N}. The difference between $M\dot{x}$ and p appears only in the last short-time intervals at the ends. But at short time, the potential does not influence the fluctuations in (2.53). This is the reason why the fluctuations at the endpoints contribute only a trivial overall factor $l_{\text{e}}(\hbar\beta)$ to the partition function Z_ω^{N}.

2.13 Classical Limit

The alternative measure of the last section serves to show, somewhat more convincingly than before, that in the high-temperature limit the path integral representation of any quantum-statistical partition function reduces to the classical partition function as stated in Eq. (2.346). We start out with the Lagrangian formulation (2.376). Inserting the Fourier decomposition (2.443), the kinetic term becomes

$$\int_0^{\hbar\beta} d\tau\, \frac{M}{2}\dot{x}^2 = \frac{M\hbar}{k_BT}\sum_{m=1}^{\infty}\omega_m^2|x_m|^2, \tag{2.459}$$

and the partition function reads

$$Z = \oint \mathcal{D}x \, \exp\left[-\frac{M}{k_BT}\sum_{m=1}^{\infty}\omega_m^2|x_m|^2 - \frac{1}{\hbar}\int_0^{\hbar/k_BT} d\tau\, V(x_0 + {\sum_{m=-\infty}^{\infty}}' x_m e^{-i\omega_m\tau})\right]. \tag{2.460}$$

The summation symbol with a prime implies the absence of the $m = 0$ -term. The measure is the product (2.447) of integrals of all Fourier components.

We now observe that for large temperatures, the Matsubara frequencies for $m \neq 0$ diverge like $2\pi m k_BT/\hbar$. This has the consequence that the Boltzmann factor for the $x_{m\neq 0}$ fluctuations becomes sharply peaked around $x_m = 0$. The average size of x_m is $\sqrt{k_BT/M}/\omega_m = \hbar/2\pi m\sqrt{Mk_BT}$. If the potential $V\left(x_0 + \sum{}'^{\,\infty}_{m=-\infty}{}' x_m e^{-i\omega_m\tau}\right)$ is a smooth function of its arguments, we can approximate it by $V(x_0)$ plus terms containing higher powers of x_m. For large temperatures, these are small on the average and can be ignored. The leading term $V(x_0)$ is time-independent. Hence we obtain in the high-temperature limit

$$Z \xrightarrow{T\to\infty} \oint \mathcal{D}x \exp\left[-\frac{M}{k_BT}\sum_{m=1}^{\infty}\omega_m^2|x_m|^2 - \frac{1}{k_BT}V(x_0)\right]. \tag{2.461}$$

The right-hand side is quadratic in the Fourier components x_m. With the measure of integration (2.447), we perform the integrals over x_m and obtain

$$Z \xrightarrow{T\to\infty} Z_{\rm cl} = \int_{-\infty}^{\infty}\frac{dx_0}{l_{\rm e}(\hbar\beta)}e^{-V(x_0)/k_BT}. \tag{2.462}$$

This agrees with the classical statistical partition function (2.352).

The derivation reveals an important prerequisite for the validity of the classical limit: It holds only for sufficiently smooth potentials. We shall see in Chapter 8 that for singular potentials such as $-1/|x|$ (Coulomb), $1/|x|^2$ (centrifugal barrier), $1/\sin^2\theta$ (angular barrier), this condition is not fulfilled and the classical limit is no longer given by (2.462). The particle distribution $\rho(x)$ at a fixed x does not have this problem. It always tends towards the naively expected classical limit (2.354):

$$\rho(x) \xrightarrow{T\to\infty} Z_{\rm cl}^{-1}e^{-V(x)/k_BT}. \tag{2.463}$$

The convergence is nonuniform in x, which is the reason why the limit does not always carry over to the integral (2.462). This will be an important point in deriving in Chapter 12 a new path integral formula valid for singular potentials. At first, we shall ignore such subtleties and continue with the conventional discussion valid for smooth potentials.

2.14 Calculation Techniques on Sliced Time Axis via the Poisson Formula

In the previous sections we have used tabulated product formulas such as (2.127), (2.165), (2.173), (2.400), (2.402) to find fluctuation determinants on a finite sliced time axis. With the recent interest in lattice models of quantum field theories, it is useful to possess an efficient calculational technique to derive such product formulas (and related sums). Consider, as a typical example, the quantum-statistical partition function for a harmonic oscillator of frequency ω on a time axis with $N+1$ slices of thickness ϵ,

$$Z = \prod_{m=0}^{N}[2(1-\cos\omega_m\epsilon)+\epsilon^2\omega^2]^{-1/2}, \tag{2.464}$$

with the product running over all Matsubara frequencies $\omega_m = 2\pi m k_BT/\hbar$. Instead of dealing with this product it is advantageous to consider the free energy

$$F = -k_BT\log Z = \frac{1}{2}k_BT\sum_{m=0}^{N}\log[2(1-\cos\omega_m\epsilon)+\epsilon^2\omega^2]. \tag{2.465}$$

We now observe that by virtue of Poisson's summation formula (1.205), the sum can be rewritten as the following combination of a sum and an integral:

$$F = \frac{1}{2}k_BT(N+1)\sum_{n=-\infty}^{\infty}\int_0^{2\pi}\frac{d\lambda}{2\pi}e^{i\lambda n(N+1)}\log[2(1-\cos\lambda)+\epsilon^2\omega^2]. \tag{2.466}$$

The sum over n squeezes λ to integer multiples of $2\pi/(N+1)=\omega_m\epsilon$ which is precisely what we want.

We now calculate the integrals in (2.466):

$$\int_0^{2\pi}\frac{d\lambda}{2\pi}e^{i\lambda n(N+1)}\log[2(1-\cos\lambda)+\epsilon^2\omega^2]. \tag{2.467}$$

For this we rewrite the logarithm of an arbitrary positive argument as the limit

$$\log a = \lim_{\delta\to 0}\left[-\int_\delta^\infty \frac{d\tau}{\tau}e^{-\tau a/2}\right]+\log(2\delta)+\gamma, \tag{2.468}$$

where

$$\gamma \equiv -\Gamma'(1)/\Gamma(1) = \lim_{N\to\infty}\left(\sum_{n=1}^{N}\frac{1}{n}-\log N\right)\approx 0.5773156649\ldots \tag{2.469}$$

is the Euler-Mascheroni constant. Indeed, the function

$$E_1(x) = \int_x^\infty \frac{dt}{t}e^{-t} \tag{2.470}$$

is known as the *exponential integral* with the small-x expansion[19]

$$E_1(x) = -\gamma - \log x - \sum_{k=1}^{\infty}\frac{(-x)^k}{kk!}. \tag{2.471}$$

With the representation (2.468) for the logarithm, the free energy can be rewritten as

$$F = \frac{1}{2\epsilon}\sum_{n=-\infty}^{\infty}\lim_{\delta\to 0}\left\{-\int_\delta^\infty\frac{d\tau}{\tau}\int_0^{2\pi}\frac{d\lambda}{2\pi}e^{i\lambda n(N+1)-\tau[2(1-\cos\lambda)+\epsilon^2\omega^2]/2}-\delta_{n0}\left[\log(2\delta)+\gamma\right]\right\}. \tag{2.472}$$

The integral over λ is now performed[20] giving rise to a modified Bessel function $I_{n(N+1)}(\tau)$:

$$F = \frac{1}{2\epsilon}\sum_{n=-\infty}^{\infty}\lim_{\delta\to 0}\left\{-\int_\delta^\infty\frac{d\tau}{\tau}I_{n(N+1)}(\tau)e^{-\tau(2+\epsilon^2\omega^2)/2}-\delta_{n0}\left[\log(2\delta)+\gamma\right]\right\}. \tag{2.473}$$

If we differentiate this with respect to $\epsilon^2\omega^2\equiv m^2$, we obtain

$$\frac{\partial F}{\partial m^2} = \frac{1}{4\epsilon}\sum_{n=-\infty}^{\infty}\int_0^\infty d\tau I_{n(N+1)}(\tau)e^{-\tau(2+m^2)/2} \tag{2.474}$$

and perform the τ-integral, using the formula valid for Re $\nu>-1$, Re $\alpha>$ Re μ

$$\int_0^\infty d\tau\, I_\nu(\mu\tau)e^{-\tau\alpha} = \mu^\nu\frac{(\alpha-\sqrt{\alpha^2-\mu^2})^{-\nu},}{\sqrt{\alpha^2-\mu^2}} = \mu^{-\nu}\frac{(\alpha-\sqrt{\alpha^2-\mu^2})^{\nu}}{\sqrt{\alpha^2-\mu^2}}, \tag{2.475}$$

[19]I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 8.214.2.
[20]I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formulas 8.411.1 and 8.406.1.

to find

$$\frac{\partial F}{\partial m^2} = \frac{1}{2\epsilon}\sum_{n=-\infty}^{\infty}\frac{1}{\sqrt{(m^2+2)^2-4}}\left[\frac{m^2+2-\sqrt{(m^2+2)^2-4}}{2}\right]^{|n|(N+1)}. \tag{2.476}$$

From this we obtain F by integration over m^2+1. The $n=0$ -term under the sum gives

$$\log[(m^2+2+\sqrt{(m^2+2)^2-4}\ )/2] + \text{const} \tag{2.477}$$

and the $n \neq 0$ -terms:

$$-\frac{1}{|n|(N+1)}[(m^2+2+\sqrt{(m^2+2)^2-4}\ )/2]^{-|n|(N+1)} + \text{const}\,, \tag{2.478}$$

where the constants of integration can depend on $n(N+1)$. They are adjusted by going to the limit $m^2 \to \infty$ in (2.473). There the integral is dominated by the small-τ regime of the Bessel functions

$$I_\alpha(z) \sim \frac{1}{|\alpha|!}\left(\frac{z}{2}\right)^\alpha [1+O(z^2)], \tag{2.479}$$

and the first term in (2.473) becomes

$$\begin{aligned} -\frac{1}{(|n|(N+1))!}&\int_\delta^\infty \frac{d\tau}{\tau}\left(\frac{\tau}{2}\right)^{|n|(N+1)} e^{-\tau m^2/2} \\ &\approx \left\{ \begin{array}{ll} \log m^2+\gamma+\log(2\delta) & n=0 \\ -(m^2)^{-|n|(N+1)}/|n|(N+1) & n\neq 0 \end{array}\right\}. \end{aligned} \tag{2.480}$$

The limit $m^2 \to \infty$ in (2.477), (2.478) gives, on the other hand, $\log m^2 + \text{const}$ and $-(m^2)^{-|n|(N+1)}/|n|(N+1) + \text{const}$, respectively. Hence the constants of integration must be zero. We can therefore write down the free energy for $N+1$ time steps as

$$\begin{aligned} F &= \frac{1}{2\beta}\sum_{m=0}^{N}\log[2(1-\cos(\omega_m\epsilon))+\epsilon^2\omega^2] \\ &= \frac{1}{2\epsilon}\left\{ \log\left[\left(\epsilon^2\omega^2+2+\sqrt{(\epsilon^2\omega^2+2)^2-4}\right)/2\right]\right. \\ &\quad \left. -\frac{2}{N+1}\sum_{n=1}^{\infty}\frac{1}{n}\left[\left(\epsilon^2\omega^2+2+\sqrt{(\epsilon^2\omega^2+2)^2-4}\right)/2\right]^{-|n|(N+1)}\right\}. \end{aligned} \tag{2.481}$$

Here it is convenient to introduce the parameter

$$\epsilon\tilde{\omega}_{\rm e} \equiv \log\left\{\left[\epsilon^2\omega^2+2+\sqrt{(\epsilon^2\omega^2+2)^2-4}\right]/2\right\}, \tag{2.482}$$

which satisfies

$$\cosh(\epsilon\tilde{\omega}_{\rm e}) = (\epsilon^2\omega^2+2)/2, \qquad \sinh(\epsilon\tilde{\omega}_{\rm e}) = \sqrt{(\epsilon^2\omega^2+2)^2-4}/2, \tag{2.483}$$

or

$$\sinh(\epsilon\tilde{\omega}_{\rm e}/2) \;=\; \epsilon\omega/2.$$

Thus it coincides with the parameter introduced in (2.399), which brings the free energy (2.481) to the simple form

$$\begin{aligned} F &= \frac{\hbar}{2}\left[\tilde{\omega}_{\rm e} - \frac{2}{\epsilon(N+1)}\sum_{n=1}^{\infty}\frac{1}{n}e^{-\epsilon\tilde{\omega}_{\rm e}n(N+1)}\right] \\ &= \frac{1}{2}\left[\hbar\tilde{\omega}_{\rm e} + 2k_BT\log(1-e^{-\beta\hbar\tilde{\omega}_{\rm e}})\right] \\ &= \frac{1}{\beta}\log\left[2\sinh(\beta\hbar\tilde{\omega}_{\rm e}/2)\right], \end{aligned} \tag{2.484}$$

whose continuum limit is

$$F \stackrel{\epsilon\to 0}{=} \frac{1}{\beta}\log\left[2\sinh\left(\beta\hbar\omega/2\right)\right] = \frac{\hbar\omega}{2} + \frac{1}{\beta}\log(1-e^{-\beta\hbar\omega}). \tag{2.485}$$

2.15 Field-Theoretic Definition of Harmonic Path Integrals by Analytic Regularization

A slight modification of the calculational techniques developed in the last section for the quantum partition function of a harmonic oscillator can be used to define the harmonic path integral in a way which neither requires time slicing, as in the original Feynman expression (2.66), nor a precise specification of the integration measure in terms of Fourier components, as in Section 2.12. The path integral for the partition function

$$Z_\omega = \oint \mathcal{D}x e^{-\int_0^{\hbar\beta} M[\dot{x}^2(\tau)+\omega^2 x^2(\tau)]/2} = \oint \mathcal{D}x e^{-\int_0^{\hbar\beta} Mx(\tau)[-\partial_\tau^2+\omega^2]x(\tau)/2} \tag{2.486}$$

is formally evaluated as

$$Z_\omega = \frac{1}{\sqrt{\mathrm{Det}(-\partial_\tau^2+\omega^2)}} = e^{-\frac{1}{2}\mathrm{Tr}\log(-\partial_\tau^2+\omega^2)}. \tag{2.487}$$

Since the determinant of an operator is the product of all its eigenvalues, we may write, again formally,

$$Z_\omega = \prod_{\omega'} \frac{1}{\sqrt{\omega'^2+\omega^2}}. \tag{2.488}$$

The product runs over an infinite set of quantities which grow with ω'^2, thus being certainly divergent. It may be turned into a divergent sum by rewriting Z_ω as

$$Z_\omega \equiv e^{-F_\omega/k_BT} = e^{-\frac{1}{2}\sum_{\omega'}\log(\omega'^2+\omega^2)}. \tag{2.489}$$

This expression has two unsatisfactory features. First, it requires a proper definition of the formal sum over a continuous set of frequencies. Second, the logarithm of the dimensionful arguments $\omega_m^2+\omega^2$ must be turned into a meaningful expression. The latter problem would be removed if we were able to exchange the logarithm by $\log[(\omega'^2+\omega^2)/\omega^2]$. This would require the formal sum $\sum_{\omega'}\log\omega^2$ to vanish. We shall see below in Eq. (2.514) that this is indeed one of the pleasant properties of analytic regularization.

At finite temperatures, the periodic boundary conditions along the imaginary-time axis make the frequencies ω' in the spectrum of the differential operator $-\partial_\tau^2+\omega^2$ discrete, and the sum in the exponent of (2.489) becomes a sum over all Matsubara frequencies $\omega_m = 2\pi k_BT/\hbar$ $(m=0,\pm1,\pm2,\ldots)$:

$$Z_\omega = \exp\left[-\frac{1}{2}\sum_{m=-\infty}^{\infty}\log(\omega_m^2+\omega^2)\right]. \tag{2.490}$$

For the free energy $F_\omega \equiv (1/\beta)\log Z_\omega$, this implies

$$F_\omega = \frac{1}{2\beta}\mathrm{Tr}\log(-\partial_\tau^2+\omega^2)\Big|_{\rm per} = \frac{1}{2\beta}\sum_{m=-\infty}^{\infty}\log(\omega_m^2+\omega^2). \qquad (2.491)$$

where the subscript per emphasizes the periodic boundary conditions in the τ-interval $(0,\hbar\beta)$.

2.15.1 Zero-Temperature Evaluation of the Frequency Sum

In the limit $T\to 0$, the sum in (2.491) goes over into an integral, and the free energy becomes

$$F_\omega \equiv \frac{1}{2\beta}\mathrm{Tr}\log(-\partial_\tau^2+\omega^2)\Big|_{\pm\infty} = \frac{\hbar}{2}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\log(\omega'^2+\omega^2), \qquad (2.492)$$

where the subscript $\pm\infty$ indicates the vanishing boundary conditions of the eigenfunctions at $\tau=\pm\infty$. Thus, at low temperature, we can replace the frequency sum in the exponent of (2.489) by

$$\sum_{\omega'} \xrightarrow[T\to 0]{} \hbar\beta\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}. \qquad (2.493)$$

This could have been expected on the basis of Planck's rules for the phase space invoked earlier on p. 97 to explain the measure of path integration. According to these rules, the volume element in the phase space of energy and time has the measure $\int dt\, dE/h = \int dt\, d\omega/2\pi$. If the integrand is independent of time, the temporal integral produces an overall factor , which for the imaginary-time interval $(0,\hbar\beta)$ of statistical mechanics is equal to $\hbar\beta=\hbar/k_BT$, thus explaining the integral version of the sum (2.493).

The integral on the right-hand side of (2.492) diverges at large ω'. This is called an *ultraviolet divergence* (UV-divergence), alluding to the fact that the ultraviolet regime of light waves contains the high frequencies of the spectrum.

The important observation is now that the divergent integral (2.492) can be made finite by a mathematical technique called *analytic regularization*.[21] This is based on rewriting the logarithm $\log(\omega'^2+\omega^2)$ in the derivative form:

$$\log(\omega'^2+\omega^2) = -\frac{d}{d\epsilon}(\omega'^2+\omega^2)^{-\epsilon}\Big|_{\epsilon=0}. \qquad (2.494)$$

Equivalently, we may obtain the logarithm from an $\epsilon\to 0$ -limit of the function

$$l_{\rm MS}(\epsilon) = -\frac{1}{\epsilon}(\omega'^2+\omega^2)^{-\epsilon}+\frac{1}{\epsilon}. \qquad (2.495)$$

[21]G. 't Hooft and M. Veltman, Nucl. Phys. B *44*, 189 (1972). Analytic regularization is at present the only method that allows to renormalize nonabelian gauge theories without destroying gauge invariance. See also the review by G. Leibbrandt, Rev. Mod. Phys. *74*, 843 (1975).

The subtraction of the pole term $1/\epsilon$ is commonly referred to a *minimal subtraction*. Indicating this process by a subscript MS, we may write

$$l_{\rm MS}(\epsilon) = -\frac{1}{\epsilon}(\omega'^2 + \omega^2)^{-\epsilon}\Big|_{\rm MS,\ \epsilon\to 0}. \tag{2.496}$$

Using the derivative formula (2.494), the trace of the logarithm in the free energy (2.492) takes the form

$$\frac{1}{\hbar\beta}{\rm Tr}\log(-\partial_\tau^2 + \omega^2) = -\frac{d}{d\epsilon}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,(\omega'^2 + \omega^2)^{-\epsilon}\Big|_{\epsilon=0}. \tag{2.497}$$

We now set up a useful integral representation, due to Schwinger, for a power $a^{-\epsilon}$ generalizing (2.468). Using the defining integral representation for the Gamma function

$$\int_0^\infty \frac{d\tau}{\tau}\tau^\mu e^{-\tau\omega^2} = \omega^{-\mu/2}\Gamma(\mu), \tag{2.498}$$

the desired generalization is

$$a^{-\epsilon} = \frac{1}{\Gamma(\epsilon)}\int_0^\infty \frac{d\tau}{\tau}\tau^\epsilon e^{-\tau a}. \tag{2.499}$$

This allows us to re-express (2.497) as

$$\frac{1}{\hbar\beta}{\rm Tr}\log(-\partial_\tau^2 + \omega^2) = -\frac{d}{d\epsilon}\frac{1}{\Gamma(\epsilon)}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\int_0^\infty\frac{d\tau}{\tau}\tau^\epsilon e^{-\tau(\omega'^2+\omega^2)}\Big|_{\epsilon=0}. \tag{2.500}$$

As long as ϵ is larger than zero, the τ-integral converges absolutely, so that we can interchange the τ- and ω'-integrations, and obtain

$$\frac{1}{\hbar\beta}{\rm Tr}\log(-\partial_\tau^2 + \omega^2) = -\frac{d}{d\epsilon}\frac{1}{\Gamma(\epsilon)}\int_0^\infty\frac{d\tau}{\tau}\tau^\epsilon\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}e^{-\tau(\omega'^2+\omega^2)}\Big|_{\epsilon=0}. \tag{2.501}$$

At this point we can perform the Gaussian integral over ω' using formula (1.338), and find

$$\frac{1}{\hbar\beta}{\rm Tr}\log(-\partial_\tau^2 + \omega^2) = -\frac{d}{d\epsilon}\frac{1}{\Gamma(\epsilon)}\int_0^\infty\frac{d\tau}{\tau}\tau^\epsilon\frac{1}{2\sqrt{\tau\pi}}e^{-\tau\omega^2}\Big|_{\epsilon=0}. \tag{2.502}$$

For small ϵ, the τ-integral is divergent at the origin. It can, however, be defined by an analytic continuation of the integral starting from the regime $\epsilon > 1/2$, where it converges absolutely, to $\epsilon = 0$. The continuation must avoid the pole at $\epsilon = 1/2$. Fortunately, this continuation is trivial since the integral can be expressed in terms of the Gamma function, whose analytic properties are well-known. Using the integral formula (2.498), we obtain

$$\frac{1}{\hbar\beta}{\rm Tr}\log(-\partial_\tau^2 + \omega^2) = -\frac{1}{2\sqrt{\pi}}\omega^{1-2\epsilon}\frac{d}{d\epsilon}\frac{1}{\Gamma(\epsilon)}\Gamma(\epsilon - 1/2)\Big|_{\epsilon=0}. \tag{2.503}$$

The right-hand side has to be continued analytically from $\epsilon > 1/2$ to $\epsilon = 0$. This is easily done using the defining property of the Gamma function $\Gamma(x) = \Gamma(1+x)/x$, from which we find $\Gamma(-1/2) = -2\Gamma(1/2) = -2\sqrt{\pi}$, and $1/\Gamma(\epsilon) \approx \epsilon/\Gamma(1+\epsilon) \approx \epsilon$. The derivative with respect to ϵ leads to the free energy of the harmonic oscillator at low temperature via analytic regularization:

$$\frac{1}{\hbar\beta}\mathrm{Tr}\log(-\partial_\tau^2+\omega^2) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\log(\omega'^2+\omega^2) = \omega, \tag{2.504}$$

so that the free energy of the oscillator at zero-temperature becomes

$$F_\omega = \frac{\hbar\omega}{2}. \tag{2.505}$$

This agrees precisely with the result obtained from the lattice definition of the path integral in Eq. (2.407), or from the path integral (3.808) with the Fourier measure (2.447).

With the above procedure in mind, we shall often use the sloppy formula expressing the derivative of Eq. (2.499) at $\epsilon = 0$:

$$\log a = -\int_0^\infty \frac{d\tau}{\tau}e^{-\tau a}. \tag{2.506}$$

This formula differs from the correct one by a minimal subtraction and can be used in all calculations with analytic regularization. Its applicability is based on the possibility of dropping the frequency integral over $1/\epsilon$ in the alternative correct expression

$$\frac{1}{\hbar\beta}\mathrm{Tr}\log(-\partial_\tau^2+\omega^2) = -\frac{1}{\epsilon}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left[\frac{1}{\epsilon}(\omega'^2+\omega^2)^{-\epsilon}-\frac{1}{\epsilon}\right]_{\epsilon\to 0}. \tag{2.507}$$

In fact, within analytic regularization one may set all integrals over arbitrary pure powers of the frequency equal to zero:

$$\int_0^\infty d\omega'\,(\omega')^\alpha = 0 \quad \text{for all } \alpha. \tag{2.508}$$

This is known as *Veltman's rule*.[22] It is a special limit of a frequency integral which is a generalization of the integral in (2.497):

$$\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{(\omega'^2)^\gamma}{(\omega'^2+\omega^2)^\epsilon} = \frac{\Gamma(\gamma+1/2)}{2\pi\Gamma(\epsilon)}(\omega^2)^{\gamma+1/2-\epsilon}. \tag{2.509}$$

This equation may be derived by rewriting the left-hand side as

$$\frac{1}{\Gamma(\epsilon)}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}(\omega'^2)^\gamma\int_0^\infty\frac{d\tau}{\tau}\tau^\epsilon e^{-\tau(\omega'^2+\omega^2)}. \tag{2.510}$$

[22] See the textbook H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of ϕ^4-Theories*, World Scientific, Singapore, 2001 (`http://www.physik.fu-berlin.de/~kleinert/b8`).

The integral over ω' is performed as follows:

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}(\omega'^2)^\gamma e^{-\tau(\omega'^2+\omega^2)} = \frac{1}{2\pi}\int_0^\infty \frac{d\omega'^2}{\omega'^2}(\omega'^2)^{\gamma+1/2} e^{-\tau(\omega'^2+\omega^2)} = \frac{\tau^{-\gamma-1/2}}{2\pi}\Gamma(\gamma+1/2), \tag{2.511}$$

leading to a τ-integral in (2.510)

$$\int_0^\infty \frac{d\tau}{\tau}\tau^{\epsilon-\gamma-1/2}e^{-\tau\omega^2} = (\omega^2)^{\gamma+1/2+\epsilon}, \tag{2.512}$$

and thus to the formula (2.509). The Veltman rule (2.508) follows from this directly in the limit $\epsilon \to 0$, since $1/\Gamma(\epsilon) \to 0$ on the right-hand side. This implies that the subtracted $1/\epsilon$ term in (2.507) gives no contribution.

The vanishing of all integrals over pure powers by Veltman's rule (2.508) was initially postulated in the process of developing a finite quantum field theory of weak and electromagnetic interactions. It has turned out to be extremely useful for the calculation of critical exponents of second-order phase transitions from field theories.[22]

An important consequence of Veltman's rule is to make the logarithms of dimensionful arguments in the partition functions (2.489) and the free energy (2.491) meaningful quantities. First, since $\int d(\omega'/2\pi)\log\omega^2 = 0$, we can divide the argument of the logarithm in (2.492) by ω^2 without harm, and make them dimensionless. At finite temperatures, we use the equality of the sum and the integral over an ω_m-independent quantity c

$$k_BT\sum_{m=-\infty}^{\infty} c = \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\,c \tag{2.513}$$

to show that also

$$k_BT\sum_{m=-\infty}^{\infty}\log\omega^2 = 0, \tag{2.514}$$

so that we have, as a consequence of Veltman's rule, that the Matsubara frequency sum over the constant $\log\omega^2$ vanishes for all temperatures. For this reason, also the argument of the logarithm in the free energy (2.491) can be divided by ω^2 without change, thus becoming dimensionless.

2.15.2 Finite-Temperature Evaluation of the Frequency Sum

At finite temperature, the free energy contains an additional term consisting of the difference between the Matsubara sum and the frequency integral

$$\Delta F_\omega = \frac{k_BT}{2}\sum_{m=-\infty}^{\infty}\log\left(\frac{\omega_m^2}{\omega^2}+1\right) - \frac{\hbar}{2}\int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\log\left(\frac{\omega_m^2}{\omega^2}+1\right), \tag{2.515}$$

where we have used dimensionless logarithms as discussed at the end of the last subsection. The sum is conveniently split into a subtracted, manifestly convergent expression

$$\Delta_1 F_\omega = k_BT \sum_{m=1}^{\infty} \left[\log\left(\frac{\omega_m^2}{\omega^2} + 1 \right) - \log \frac{\omega_m^2}{\omega^2} \right] = k_BT \sum_{m=1}^{\infty} \log \left(1 + \frac{\omega^2}{\omega_m^2} \right), \quad (2.516)$$

and a divergent sum

$$\Delta_2 F_\omega = k_BT \sum_{m=1}^{\infty} \log \frac{\omega_m^2}{\omega^2}. \quad (2.517)$$

The convergent part is most easily evaluated. Taking the logarithm of the product in Eq. (2.408) and recalling (2.409), we find

$$\prod_{m=1}^{\infty} \left(1 + \frac{\omega^2}{\omega_m^2} \right) = \frac{\sinh(\beta\hbar\omega/2)}{\beta\hbar\omega/2}, \quad (2.518)$$

and therefore

$$\Delta F_1 = \frac{1}{\beta} \log \frac{\sinh(\beta\hbar\omega/2)}{\beta\hbar\omega/2}. \quad (2.519)$$

The divergent sum (2.517) is calculated by analytic regularization as follows: We rewrite

$$\sum_{m=1}^{\infty} \log \frac{\omega_m^2}{\omega^2} = - \left[2\frac{d}{d\epsilon} \sum_{m=1}^{\infty} \left(\frac{\omega_m}{\omega} \right)^{-\epsilon} \right]_{\epsilon\to 0} = - \left[2\frac{d}{d\epsilon} \left(\frac{2\pi}{\beta\hbar\omega} \right)^{-\epsilon} \sum_{m=1}^{\infty} m^{-\epsilon} \right]_{\epsilon\to 0}, \quad (2.520)$$

and express the sum over $m^{-\epsilon}$ in terms of Riemann's zeta function

$$\zeta(z) = \sum_{m=1}^{\infty} m^{-z}. \quad (2.521)$$

This sum is well defined for $z > 1$, and can be continued analytically into the entire complex z-plane. The only singularity of this function lies at $z = 1$, where in the neighborhood $\zeta(z) \approx 1/z$. At the origin, $\zeta(z)$ is regular, and satisfies[23]

$$\zeta(0) = -1/2, \qquad \zeta'(0) = -\frac{1}{2} \log 2\pi, \quad (2.522)$$

such that we may approximate

$$\zeta(z) \approx -\frac{1}{2}(2\pi)^z, \qquad z \approx 0. \quad (2.523)$$

Hence we find

$$\sum_{m=1}^{\infty} \log \frac{\omega_m^2}{\omega^2} = - \left[2\frac{d}{d\epsilon} \left(\frac{2\pi}{\beta\hbar\omega} \right)^{-\epsilon} \zeta(\epsilon) \right]_{\epsilon\to 0} = \frac{d}{d\epsilon} (\beta\hbar\omega)^{\epsilon} \Big|_{\epsilon\to 0} = \log \hbar\omega\beta. \quad (2.524)$$

[23] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formula 9.541.4.

thus determining $\Delta_2 F_\omega$ in Eq. (2.517).

By combining this with (2.519) and the contribution $-\hbar\omega/2$ from the integral (2.515), the finite-temperature part (2.491) of the free energy becomes

$$\Delta F_\omega = \frac{1}{\beta}\log(1 - e^{-\hbar\beta\omega}). \tag{2.525}$$

Together with the zero-temperature free energy (2.505), this yields the dimensionally regularized sum formula

$$\begin{aligned} F_\omega &= \frac{1}{2\beta}\mathrm{Tr}\log(-\partial_\tau^2 + \omega^2) = \frac{1}{2\beta}\sum_{m=-\infty}^{\infty}\log(\omega_m^2 + \omega^2) = \frac{\hbar\omega}{2} + \frac{1}{\beta}\log(1 - e^{-\hbar\omega/k_BT}) \\ &= \frac{1}{\beta}\log\left(2\sinh\frac{\hbar\omega\beta}{2}\right), \end{aligned} \tag{2.526}$$

in agreement with the properly normalized free energy (2.485) at all temperatures.

Note that the property of the zeta function $\zeta(0) = -1/2$ in Eq. (2.522) leads once more to our earlier result (2.514) that the Matsubara sum of a constant c vanishes:

$$\sum_{m=-\infty}^{\infty} c = \sum_{m=-\infty}^{-1} c + c + \sum_{m=1}^{\infty} c = 0, \tag{2.527}$$

since

$$\sum_{m=1}^{\infty} 1 = \sum_{m=-1}^{-\infty} 1 = \zeta(0) = -1/2. \tag{2.528}$$

As mentioned before, this allows us to divide ω^2 out of the logarithms in the sum in Eq. (2.526) and rewrite this sum as

$$\frac{1}{2\beta}\sum_{m=-\infty}^{\infty}\log\left(\frac{\omega_m^2}{\omega^2} + 1\right) = \frac{1}{\beta}\sum_{m=1}^{\infty}\log\left(\frac{\omega_m^2}{\omega^2} + 1\right) \tag{2.529}$$

2.15.3 Quantum-Mechanical Harmonic Oscillator

This observation leads us directly to the analogous quantum-mechanical discussion. Starting from the fluctuation factor (2.91) of the free particle which can formally be written as

$$F_0(\Delta t) = \int \mathcal{D}\delta x(t) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt \frac{M}{2}\delta x(-\partial_t^2)\delta x\right] = \frac{1}{\sqrt{2\pi\hbar i\Delta t/M}}, \tag{2.530}$$

where $\Delta t \equiv t_b - t_a$ [recall (2.130)]. The path integral of the harmonic oscillator has the fluctuation factor [compare (2.188)]

$$F_\omega(\Delta t) = F_0(\Delta t)\left[\frac{\mathrm{Det}(-\partial_t^2 - \omega^2)}{\mathrm{Det}(-\partial_t^2)}\right]^{-1/2}. \tag{2.531}$$

The ratio of the determinants has the Fourier decomposition

$$\frac{\mathrm{Det}(-\partial_t^2-\omega^2)}{\mathrm{Det}(-\partial_t^2)}=\exp\left\{\sum_{n=1}^{\infty}\left[\log(\nu_n^2-\omega^2)-\log\nu_n^2\right]\right\}, \tag{2.532}$$

where $\nu_n=n\pi/\Delta t$ [recall (2.115)], and was calculated in Eq. (2.188) to be

$$\frac{\mathrm{Det}(-\partial_t^2-\omega^2)}{\mathrm{Det}(-\partial_t^2)}=\frac{\sin\omega\Delta t}{\omega\Delta t}. \tag{2.533}$$

This result can be reproduced with the help of formulas (2.529) and (2.526). We raplace β by $2\Delta t$, and use again $\Sigma_n 1=\zeta(0)=-1/2$ to obtain

$$\begin{aligned}\mathrm{Det}(-\partial_t^2-\omega^2) &= \sum_{n=1}^{\infty}\log(\nu_n^2+\omega^2)\Big|_{\omega\to i\omega}=\sum_{n=1}^{\infty}\left[\log\left(\frac{\nu_n^2}{\omega^2}+1\right)+\log\omega^2\right]_{\omega\to i\omega}\\ &=\left[\sum_{n=1}^{\infty}\log\left(\frac{\nu_n^2}{\omega^2}+1\right)-\frac{1}{2}\log\omega^2\right]_{\omega\to i\omega}=\log\left(2\frac{\sin\omega\Delta t}{\omega}\right).\end{aligned} \tag{2.534}$$

For $\omega=0$ this reproduces Formula (2.524). Inserting this and (2.534) into (2.532), we recover the result (2.533). Thus we find the amplitude

$$(x_bt_b|x_at_a)=\frac{1}{\sqrt{\pi i/M}}\mathrm{Det}^{-1/2}(-\partial_t^2-\omega^2)e^{i\mathcal{A}_{\rm cl}/\hbar}=\frac{1}{\sqrt{\pi i/M}}\sqrt{\frac{\omega}{2\sin\omega\Delta t}}e^{i\mathcal{A}_{\rm cl}/\hbar}, \tag{2.535}$$

in agreement with (2.175).

2.15.4 Tracelog of the First-Order Differential Operator

The trace of the logarithm in the free energy (2.492) can obviously be split into two terms

$$\mathrm{Tr}\log(-\partial_\tau^2+\omega^2)=\mathrm{Tr}\log(\partial_\tau+\omega)+\mathrm{Tr}\log(-\partial_\tau+\omega). \tag{2.536}$$

Since the left-hand side is equal to $\beta\hbar\omega$ by (2.504), and the two integrals must be the same, we obtain the low-temperature result

$$\begin{aligned}\mathrm{Tr}\log(\partial_\tau+\omega)=\mathrm{Tr}\log(-\partial_\tau+\omega)&=\hbar\beta\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\log(-i\omega'+\omega)=\hbar\beta\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\log(i\omega'+\omega)\\ &=\frac{\hbar\beta\omega}{2}.\end{aligned} \tag{2.537}$$

The same result could be obtained from analytic continuation of the integrals over $\partial_\epsilon(\pm i\omega'+\omega)^\epsilon$ to $\epsilon=0$.

For a finite temperature, we may use Eq. (2.526) to find

$$\mathrm{Tr}\log(\partial_\tau+\omega)=\mathrm{Tr}\log(-\partial_\tau+\omega)=\frac{1}{2}\mathrm{Tr}\log(-\partial_\tau^2+\omega^2)=\log\left(2\sinh\frac{\beta\hbar\omega}{2}\right), \tag{2.538}$$

which reduces to (2.537) for $T \to 0$.

The result is also the same if there is an extra factor i in the argument of the tracelog. To see this we consider the case of time-independent frequency where Veltman's rule (2.508) tells us that it does not matter whether one evaluates integrals over $\log(i\omega' \mp \omega)$ or over $\log(\omega' \pm i\omega)$.

Let us also replace ω' by $i\omega'$ in the zero-temperature tracelog (2.504) of the second-order differential operator $(-\partial_\tau^2 + \omega^2)$. Then we rotate the contour of integration clockwise in the complex plane to find

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log(-\omega'^2 + \omega^2 - i\eta) = \omega, \quad \omega \geq 0, \tag{2.539}$$

where an infinitesimal positive η prescribes how to bypass the singularities at $\omega' = \pm\omega \mp i\eta$ along the rotated contour of integration. Recall the discussion of the $i\eta$-prescription in Section 3.3. The integral (2.539) can be split into the integrals

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log[\omega' \pm (\omega - i\eta)] = i\,\frac{\omega}{2}, \quad \omega \geq 0. \tag{2.540}$$

Hence formula (2.537) can be generalized to arbitrary complex frequencies $\omega = \omega_R + i\omega_I$ as follows:

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log(\omega' \pm i\omega) = \mp\epsilon(\omega_R)\,\frac{\omega}{2}, \tag{2.541}$$

and

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log(\omega' \pm \omega) = -i\epsilon(\omega_I)\,\frac{\omega}{2}, \tag{2.542}$$

where $\epsilon(x) = \Theta(x) - \Theta(-x) = x/|x|$ is the antisymmetric Heaviside function (1.315), which yields the sign of its argument. The formulas (2.541) and (2.542) are the large-time limit of the more complicated sums

$$\frac{k_BT}{\hbar} \sum_{m=-\infty}^{\infty} \log(\omega_m \pm i\omega) = \frac{k_BT}{\hbar} \log\left[2\epsilon(\omega_R)\sinh\frac{\hbar\omega}{2k_BT}\right], \tag{2.543}$$

and

$$\frac{k_BT}{\hbar} \sum_{m=-\infty}^{\infty} \log(\omega_m \pm \omega) = \frac{k_BT}{\hbar} \log\left[-2i\epsilon(\omega_I)\sin\frac{\hbar\omega}{2k_BT}\right]. \tag{2.544}$$

The first expression is periodic in the imaginary part of ω, with period $2\pi k_BT$, the second in the real part. The determinants possess a meaningful large-time limit only if the periodic parts of ω vanish. In many applications, however, the fluctuations will involve sums of logarithms (2.544) and (2.543) with different complex frequencies ω, and only the sum of the imaginary or real parts will have to vanish to obtain a meaningful large-time limit. On these occasions we may use the simplified formulas (2.541) and (2.542). Important examples will be encountered in Section 18.9.2.

In Subsection 3.3.2, Formula (2.538) will be generalized to arbitrary positive time-dependent frequencies $\Omega(\tau)$, where it reads [see (3.133)]

$$\begin{aligned} \text{Tr}\,\log\left[\pm\partial_\tau+\Omega(\tau)\right] &= \log\left\{2\sinh\left[\frac{1}{2}\int_0^{\hbar\beta}d\tau''\,\Omega(\tau'')\right]\right\} \\ &= \frac{1}{2}\int_0^{\hbar\beta}d\tau''\,\Omega(\tau'')+\log\left[1-e^{-\int_0^{\hbar\beta}d\tau''\,\Omega(\tau'')}\right]. \end{aligned} \tag{2.545}$$

2.15.5 Gradient Expansion of the One-Dimensional Tracelog

Formula (2.545) may be used to calculate the trace of the logarithm of a second-order differential equation with arbitrary frequency as a semiclassical expansion. We introduce the Planck constant $\hbar$ and the potential $w(\tau)\equiv\hbar\Omega(\tau)$, and factorize as in (2.536):

$$\text{Det}\left[-\hbar^2\partial_\tau^2+w^2(\tau)\right]=\text{Det}\left[-\hbar\partial_\tau-\bar{w}(\tau)\right]\times\text{Det}\left[\hbar\partial_\tau-\bar{w}(\tau)\right], \tag{2.546}$$

where the function $\bar{w}(\tau)$ satisfies the *Riccati differential equation*:[24]

$$\hbar\partial_\tau\bar{w}(\tau)+\bar{w}^2(\tau)=w^2(\tau). \tag{2.547}$$

By solving this we obtain the trace of the logarithm from (2.545):

$$\text{Tr}\log\left[-\hbar^2\partial_\tau^2+w^2(\tau)\right]=\log\left\{4\sinh^2\left[\frac{1}{2\hbar}\int_0^{\hbar\beta}d\tau'\,\bar{w}(\tau')\right]\right\}. \tag{2.548}$$

The exponential of this yields the functional determinant. For constant $\bar{w}(\tau)=\omega$ this agrees with the result (2.433) of the Gelfand-Yaglom formula for periodic boundary conditions.

This agreement is no coincidence. We can find the solution of any Riccati differential equation if we know how to solve the second-order differential equation (2.433). Imposing the Gelfand-Yaglom boundary conditions in (2.433), we find $D_{\text{ren}}(\tau)$ and from this the functional determinant $2[\dot{D}_{\text{ren}}(\hbar\beta)-1]$. Comparison with (2.548) shows that the solution of the Riccati differential equation (2.547) is given by

$$\bar{w}(\tau)=2\hbar\partial_\tau\,\text{arsinh}\sqrt{[\dot{D}_{\text{ren}}(\tau)-1]/2}. \tag{2.549}$$

For the harmonic oscillator where $\dot{D}_{\text{ren}}(\tau)$ is equal to (2.437), this leads to the constant $\bar{w}(\tau)=\hbar\omega$, as it should.

If we cannot solve the second-order differential equation (2.433), a solution to the Riccati equation (2.547) can still be found as a power series in $\hbar$:

$$\bar{w}(\tau)=\sum_{n=0}^{\infty}\bar{w}_n(\tau)\hbar^n, \tag{2.550}$$

[24]Recall the general form of the Riccati differential equation $y'=f(\tau)y+g(\tau)y^2+h(y)$, which is an inhomogeneous version of the Bernoulli differential equation $y'=f(\tau)y+g(\tau)y^n$ for $n=2$.

which provides us with a so-called *gradient expansion* of the trace of the logarithm. The lowest-order coefficient function $\bar{w}_0(\tau)$ is obviously equal to $w(\tau)$. The higher ones obey the recursion relation

$$\bar{w}_n(\tau) = -\frac{1}{2w(\tau)}\left(\dot{\bar{w}}_{n-1}(\tau) + \sum_{k=1}^{n-1}\bar{w}_{n-k}(\tau)\bar{w}_k(\tau)\right), \qquad n \geq 1. \tag{2.551}$$

These are solved for $n = 0, 1, 2, 3$ by

$$\left\{\sqrt{v(\tau)}, -\frac{v'(\tau)}{4\,v(\tau)}, \quad -\frac{5\,v'(\tau)^2}{32\,v(\tau)^{5/2}} + \frac{v''(\tau)}{8\,v(\tau)^{3/2}}, \quad -\frac{15\,v'(\tau)^3}{64\,v(\tau)^4} + \frac{9\,v'(\tau)\,v''(\tau)}{32\,v(\tau)^3} - \frac{v^{(3)}(\tau)}{16\,v(\tau)^2}, \right.$$
$$\left. -\frac{1105\,v'(\tau)^4}{2048\,v(\tau)^{11/2}} + \frac{221\,v'(\tau)^2\,v''(\tau)}{256\,v(\tau)^{9/2}} - \frac{19\,v''(\tau)^2}{128\,v(\tau)^{7/2}} - \frac{7\,v'(\tau)\,v^{(3)}(\tau)}{32\,v(\tau)^{7/2}} + \frac{v^{(4)}(\tau)}{32\,v(\tau)^{5/2}}\right\}, \tag{2.552}$$

where $v(\tau) \equiv w^2(\tau)$. The series can, of course, be trivially extended to any desired orders.

2.15.6 Duality Transformation and Low-Temperature Expansion

There exists another method of calculating the finite-temperature part of the free energy (2.491) which is worth presenting at this place, due to its broad applicability in statistical mechanics. For this we rewrite (2.515) in the form

$$\Delta F_\omega = \frac{k_BT}{2}\left(\sum_{m=-\infty}^{\infty} - \frac{\hbar}{k_BT}\int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\log(\omega_m^2 + \omega^2). \tag{2.553}$$

Changing the integration variable to m, this becomes

$$\Delta F_\omega = \frac{k_BT}{2}\left(\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}dm\right)\log\left[\left(\frac{2\pi k_BT}{\hbar}\right)^2 m^2 + \omega^2\right]. \tag{2.554}$$

Within analytic regularization, this expression is rewritten with the help of formula (2.506) as

$$\Delta F_\omega = -\frac{k_BT}{2}\int_0^\infty\frac{d\tau}{\tau}\left(\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}dm\right)e^{-\tau\left[(2\pi k_BT/\hbar)^2m^2+\omega^2\right]}. \tag{2.555}$$

The duality transformation proceeds by performing the sum over the Matsubara frequencies with the help of Poisson's formula (1.205) as an integral $\int d\mu$ plus by an extra sum over integer numbers n. This brings (2.555) to the form (expressing the temperature in terms of β),

$$\Delta F_\omega = -\frac{1}{2\beta}\int_0^\infty\frac{d\tau}{\tau}\int_{-\infty}^{\infty}d\mu\left(\sum_{n=-\infty}^{\infty}e^{2\pi\mu ni} - 1\right)e^{-\tau\left[(2\pi/\hbar\beta)^2\mu^2+\omega^2\right]}. \tag{2.556}$$

The parentheses contain the sum $2\sum_{n=1}^{\infty} e^{2\pi\mu ni}$. After a quadratic completion of the exponent

$$2\pi\mu ni - \tau\left(\frac{2\pi}{\hbar\beta}\right)^2\mu^2 = -\tau\left(\frac{2\pi}{\hbar\beta}\right)^2\left[\mu - i\frac{n\hbar^2\beta^2}{4\pi\tau}\right]^2 - \frac{1}{4\tau}(\hbar\beta n)^2, \tag{2.557}$$

the integral over μ can be performed, with the result

$$\Delta F_\omega = -\frac{\hbar}{2\sqrt{\pi}}\int_0^\infty \frac{d\tau}{\tau}\tau^{-1/2}\sum_{n=1}^{\infty} e^{-(n\hbar\beta)^2/4\tau - \tau\omega^2}. \tag{2.558}$$

Now we may use the integral formula [compare (1.347)][25]

$$\int_0^\infty \frac{d\tau}{\tau}\tau^\nu e^{-a^2/\tau - b^2\tau} = 2\left(\frac{a}{b}\right)^\nu K_\nu(2ab), \qquad K_\nu(2ab) = K_{-\nu}(2ab), \tag{2.559}$$

to obtain the sum over modified Bessel functions

$$\Delta F_\omega = -\frac{\hbar\omega}{2\sqrt{\pi}}\sum_{n=1}^{\infty} 2\,(n\beta\hbar\omega)^{-1/2}\,\sqrt{2}K_{1/2}(n\beta\hbar\omega). \tag{2.560}$$

The modified Bessel functions with index 1/2 are particularly simple:

$$K_{1/2}(z) = \sqrt{\frac{\pi}{2z}}e^{-z}. \tag{2.561}$$

Inserting this into (2.560), the sum is a simple geometric one, and may be performed as follows:

$$\Delta F_\omega = -\frac{1}{\beta}\sum_{n=1}\frac{1}{n}e^{-\beta\hbar\omega n} = \frac{1}{\beta}\log\left(1 - e^{-\beta\hbar\omega}\right), \tag{2.562}$$

in agreement with the previous result (2.525).

The effect of the duality tranformation may be rephrased in another way. It converts the sum over Matsubara frequencies ω_m in (2.516):

$$S(\beta\hbar\omega) = k_BT\sum_{m=1}^{\infty}\log\left(1 + \frac{\omega^2}{\omega_m^2}\right) \tag{2.563}$$

into a sum over the quantum numbers n of the harmonic oscillator:

$$S(\beta\hbar\omega) = \frac{\beta\hbar\omega}{2} - \log\beta\hbar\omega - \sum_{n=1}^{\infty}\frac{1}{n}e^{-n\beta\hbar\omega}. \tag{2.564}$$

The sum (2.563) converges fast at high temperatures, where it can be expanded in powers of ω^2:

$$S(\beta\hbar\omega) = -\sum_{k=1}^{\infty}\frac{(-1)^k}{k}\left(\sum_{m=1}^{\infty}\frac{1}{m^{2k}}\right)\left[\left(\frac{\beta\hbar\omega}{2\pi}\right)^2\right]^k. \tag{2.565}$$

[25] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formulas 3.471.9 and 8.486.16.

The expansion coefficients are equal to Riemann's zeta function $\zeta(z)$ of Eq. (2.521) at even arguments $z = 2k$, so that we may write

$$S(\beta\hbar\omega) = -\sum_{m=1}^{\infty} \frac{(-1)^k}{k}\zeta(2k)\left(\frac{\beta\hbar\omega}{2\pi}\right)^{2k}. \tag{2.566}$$

At even positive arguments, the values of the zeta function are related to the Bernoulli numbers by[26]

$$\zeta(2n) = \frac{(2\pi)^{2n}}{2(2n)!}|B_{2n}|. \tag{2.567}$$

The Bernoulli numbers are defined by the expansion

$$\frac{t}{e^t - 1} = \sum_{n=0}^{\infty} B_n \frac{t^n}{n!}. \tag{2.568}$$

The lowest nonzero Bernoulli numbers are $B_0 = 1$, $B_1 = -1/2$, $B_2 = 1/2$, $B_4 = -1/30, \dots$. The Bernoulli numbers determine also the values of the zeta functions at negative odd arguments:

$$\zeta(1-2n) = -\frac{B_{2n}}{2n}, \tag{2.569}$$

this being a consequence of the general identity[27]

$$\zeta(z) = 2^z\pi^{z-1}\sin(\pi z/2)\Gamma(1-z)\zeta(1-z) = 2^{z-1}\pi^z\zeta(1-z)/\Gamma(z)\cos\frac{z\pi}{2}. \tag{2.570}$$

Typical values of $\zeta(z)$ which will be needed here are[28]

$$\zeta(2) = \frac{\pi^2}{6}, \quad \zeta(4) = \frac{\pi^4}{90}, \quad \zeta(6) = \frac{\pi^6}{945}, \quad \dots \quad , \quad \zeta(\infty) = 1. \tag{2.571}$$

In contrast to the Matsubara frequency sum (2.563) and its expansion (2.566), the dually transformed sum over the quantum numbers n in (2.564) converges rapidly for low temperatures. It converges everywhere except at very large temperatures, where it diverges logarithmically. The precise behavior can be calculated as follows: For large T there exists a large number N which is still much smaller than $1/\beta\hbar\omega$, such that $e^{-\beta\hbar\omega N}$ is close to unity. Then we split the sum as

$$\sum_{n=1}^{\infty} \frac{1}{n}e^{-n\beta\hbar\omega} \approx \sum_{n=1}^{N-1}\frac{1}{n} + \sum_{n=N}^{\infty}\frac{1}{n}e^{-n\beta\hbar\omega}. \tag{2.572}$$

[26] *ibid.*, Formulas 9.542 and 9.535.

[27] *ibid.*, Formula 9.535.2.

[28] Other often-needed values are $\zeta(0) = -1/2$, $\zeta'(0) = -\log(2\pi)/2$, $\zeta(-2n) = 0$, $\zeta(3) \approx 1.202057$, $\zeta(5) \approx 1.036928, \dots$.

Since N is large, the second sum can be approximated by an integral

$$\int_N^\infty \frac{dn}{n} e^{-n\beta\hbar\omega} = \int_{N\beta\hbar\omega}^\infty \frac{dx}{x} e^{-x},$$

which is an exponential integral $E_1(N\beta\hbar\omega)$ of Eq. (2.470) with the large-argument expansion $-\gamma - \log(N\beta\hbar\omega)$ of Eq. (2.471).

The first sum in (2.572) is calculated with the help of the Digamma function

$$\psi(z) \equiv \frac{\Gamma'(z)}{\Gamma(z)}. \tag{2.573}$$

This has an expansion[29]

$$\psi(z) = -\gamma - \sum_{n=0}^\infty \left(\frac{1}{n+z} - \frac{1}{n+1} \right), \tag{2.574}$$

which reduces for integer arguments to

$$\psi(N) = -\gamma + \sum_{n=1}^{N-1} \frac{1}{n}, \tag{2.575}$$

and has the large-z expansion

$$\psi(z) \approx \log z - \frac{1}{2z} - \sum_{n=1}^\infty \frac{B_{2n}}{2nz^{2n}}. \tag{2.576}$$

Combining this with (2.471), the logarithm of N cancels, and we find for the sum in (2.572) the large-T behavior

$$\sum_{n=1}^\infty \frac{1}{n} e^{-n\beta\hbar\omega} \underset{T\to\infty}{\approx} -\log \beta\hbar\omega + \mathcal{O}(\beta). \tag{2.577}$$

This cancels the logarithm in (2.564).

The low-temperature series (2.564) can be used to illustrate the power of analytic regularization. Suppose we want to extract from it the large-T behavior, where the sum

$$g(\beta\hbar\omega) \equiv \sum_{n=1}^\infty \frac{1}{n} e^{-n\beta\hbar\omega} \tag{2.578}$$

converges slowly. We would like to expand the exponentials in the sum into powers of ω, but this gives rise to sums over positive powers of n. It is possible to make sense of these sums by analytic continuation. For this we introduce a generalization of (2.578):

$$\zeta_\nu(e^{\beta\hbar\omega}) \equiv \sum_{n=1}^\infty \frac{1}{n^\nu} e^{-n\beta\hbar\omega}, \tag{2.579}$$

[29] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formula 1.362.1.

which reduces to $g(\beta\hbar\omega)$ for $\nu = 1$. This sum is evaluated by splitting it into an integral over n and a difference between sum and integral:

$$\zeta_\nu(e^{\beta\hbar\omega}) = \int_0^\infty dn\,\frac{1}{n^\nu}e^{-n\beta\hbar\omega} + \left(\sum_{n=1}^\infty - \int_0^\infty\right)\frac{1}{n^\nu}e^{-n\beta\hbar\omega}. \tag{2.580}$$

The integral is convergent for $\nu < 1$ and yields $\Gamma(1-\nu)\,(\beta\hbar\omega)^\nu$ via the integral formula (2.498). For other ν's it is defined by analytic continuation. The remainder may be expanded sloppily in powers of ω and yields

$$\zeta_\nu(e^{\beta\hbar\omega}) = \int_0^\infty dn\frac{1}{n^\nu}e^{-n\beta\hbar\omega} + \left(\sum_{n=1}^\infty - \int_0^\infty\right)\frac{1}{n^\nu} + \sum_{k=1}^\infty\left[\left(\sum_{n=1}^\infty - \int_0^\infty\right)n^{k-\nu}\right]\frac{(-1)^k}{k!}\,(\beta\hbar\omega)^k. \tag{2.581}$$

The second term is simply the Riemann zeta function $\zeta(\nu)$ [recall (2.521)]. Since the additional integral vanishes due to Veltman' rule (2.508), the zeta function may also be defined by

$$\left(\sum_{n=1}^\infty - \int_0^\infty\right)\frac{1}{\nu^k} = \zeta(\nu), \tag{2.582}$$

If this formula is applied to the last term in (2.581), we obtain the so-called *Robinson expansion*[30]

$$\zeta_\nu(e^{\beta\hbar\omega}) = \Gamma(1-\nu)(\beta\hbar\omega)^{\nu-1} + \zeta(\nu) + \sum_{k=1}^\infty \frac{1}{k!}(-\beta\hbar\omega)^k\zeta(\nu-k). \tag{2.583}$$

This expansion will later play an important role in the discussion of Bose-Einstein condensation [see Eq. (7.38)].

For various applications it is useful to record also the auxiliary formula

$$\left(\sum_{n=1}^\infty - \int_0^\infty\right)\frac{e^{n\beta\hbar\omega}}{n^\nu} = \sum_{k=1}^\infty \frac{1}{k!}(-\beta\hbar\omega)^k\zeta(\nu-k) \equiv \bar{\zeta}_\nu(e^{\beta\hbar\omega}), \tag{2.584}$$

since in the sum minus the integral, the first Robinson terms are absent and the result can be obtained from a naive Taylor expansion of the exponents $e^{n\beta\hbar\omega}$ and the summation formula (2.582).

From (2.583) we can extract the desired sum (2.578) by going to the limit $\nu \to 1$. Close to the limit, the Gamma function has a pole $\Gamma(1-\nu) = 1/(1-\nu) - \gamma + \mathcal{O}(\nu-1)$. From the identity

$$2^z\Gamma(1-z)\zeta(1-z)\sin\frac{\pi z}{2} = \pi^{1-z}\zeta(z) \tag{2.585}$$

and (2.522) we see that $\zeta(\nu)$ behaves near $\nu = 1$ like

$$\zeta(\nu) = \frac{1}{\nu-1} + \gamma + \mathcal{O}(\nu-1) = -\Gamma(1-\nu) + \mathcal{O}(\nu-1). \tag{2.586}$$

[30] J.E. Robinson, Phys. Rev. *83*, 678 (1951).

Hence the first two terms in (2.583) can be combined to yield for $\nu \to 1$ the finite result $\lim_{\nu\to 1} \Gamma(1-\nu)\,[(\beta\hbar\omega)^{\nu-1} - 1]{=}-\log\beta\hbar\omega$. The remaining terms contain in the limit the values $\zeta(0) = -1/2$, $\zeta(-1)$, $\zeta(-2)$, etc. Here we use the property of the zeta function that it vanishes at even negative arguments, and that the function at arbitrary negative argument is related to one at positive argument by the identity (2.585). This implies for the expansion coefficients in (2.583) with $k = 1, 2, 3, \dots$ in the limit $\nu \to 1$:

$$\zeta(-2p) = 0, \qquad \zeta(1-2p) = \frac{1}{p}(-1)^p \frac{(2p)!}{(2\pi)^{2p}}\zeta(2p), \quad p = 1, 2, 3, \dots\ . \tag{2.587}$$

Hence we obtain for the expansion (2.583) in the limit $\nu \to 1$:

$$g(\beta\hbar\omega) = \zeta_1(e^{\beta\hbar\omega}) = -\log\beta\hbar\omega + \frac{\beta\hbar\omega}{2} + \sum_{k=1}^{\infty}\zeta(2k)\frac{(-1)^k}{k!}(\beta\hbar\omega)^{2k}. \tag{2.588}$$

This can now be inserted into Eq. (2.564) and we recover the previous expansion (2.566) for $S(\beta\hbar\omega)$ which was derived there by a proper duality transformation.

It is interesting to observe what goes wrong if we forget the separation (2.580) of the sum into integral plus sum-minus-integral and its regularization. For this we re-expand (2.578) directly, and illegally, in powers of ω. Then we obtain for $\nu = 1$ the formal expansion

$$\zeta_1(e^{\beta\hbar\omega}) = \sum_{p=0}^{\infty}\left(\sum_{n=1}^{\infty} n^{p-1}\right)\frac{(-1)^p}{p!}(\beta\hbar\omega)^p = -\zeta(1) + \sum_{p=1}^{\infty}\zeta(1-p)\frac{(-1)^p}{p!}(\beta\hbar\omega)^p, \tag{2.589}$$

which contains the infinite quantity $\zeta(1)$. The correct result (2.588) is obtained from this by replacing the infinite quantity $\zeta(1)$ by $-\log\beta\hbar\omega$, which may be viewed as a regularized $\zeta_{\rm reg}(1)$:

$$\zeta(1) \to \zeta_{\rm reg}(1) = -\log\beta\hbar\omega. \tag{2.590}$$

The above derivation of the Robinson expansion can be supplemented by a dual version as follows. With the help of Poisson's formula (1.197) we rewrite the sum (2.579) as an integral over n and an auxiliary sum over integer numbers m, after which the integral over n can be performed yielding

$$\begin{aligned}\zeta_\nu(e^{\beta\hbar\omega}) &\equiv \sum_{m=-\infty}^{\infty}\int_0^\infty dn\, e^{(2\pi i m+\beta\hbar\omega)n}\frac{1}{n^\nu} = \Gamma(1-\nu)(-\beta\hbar\omega)^{\nu-1}\\ &+ \Gamma(1-\nu)\,2\,{\rm Re}\sum_{m=1}^{\infty}(-\beta\hbar\omega - 2\pi i m)^{\nu-1}.\end{aligned} \tag{2.591}$$

The sum can again be expanded in powers of ω

$$\begin{aligned}&2\,{\rm Re}\sum_{m=1}^{\infty}(-2\pi i m)^{\nu-1}\left(1+\frac{\beta\hbar\omega}{2\pi i m}\right)^{\nu-1}\\ &\quad = 2\sum_{k=0}^{\infty}\binom{\nu-1}{k}\cos[(1-\nu-k)\pi/2]\,(2\pi)^{\nu-1-k}\zeta(1-\nu+k)\,(\beta\hbar\omega)^k.\end{aligned} \tag{2.592}$$

Using the relation (2.585) for zeta-functions, the expansion (2.591) is seen to coincide with (2.579).

Note that the representation (2.591) of $\zeta_\nu(e^{\beta\hbar\omega})$ is a sum over Matsubara frequencies $\omega_m = 2\pi m/\beta$ [recall Eq. (2.381)]:

$$\begin{aligned}\zeta_\nu(e^{\beta\hbar\omega}) &\equiv \sum_{m=-\infty}^{\infty} \int_0^\infty dn\, e^{(i\omega_m+\hbar\omega)\beta n} \frac{1}{n^\nu} \\ &= \Gamma(1-\nu)(-\beta\hbar\omega)^{\nu-1}\left[1+2\,\mathrm{Re}\sum_{m=1}^{\infty}(1+i\omega_m/\hbar\omega)^{\nu-1}\right]. \qquad (2.593)\end{aligned}$$

The first term coming from the integral over n in (2.580) is associated with the zero Matsubara frequency. This term represents the high-temperature or classical limit of the expansion. The remainder contains the sum over all nonzero Matsubara frequencies, and thus the effect of quantum fluctuations.

It should be mentioned that the first two terms in the low-temperature expansion (2.564) can also be found from the sum (2.563) with the help of the Euler-Maclaurin formula[31] for a sum over discrete points $t = a + (k+\kappa)\Delta$ of a function $F(t)$ from $k = 0$ to $K \equiv (b-a)/\Delta$:

$$\begin{aligned}\sum_{k=0}^{K} F(a+k\Delta) &= \frac{1}{\Delta}\int_a^b dt\, F(t) + \frac{1}{2}[F(a)+F(b)] \\ &+ \sum_{p=1}^{\infty}\frac{\Delta^{2p-1}}{(2p)!}B_{2p}\left[F^{(2p-1)}(b)-F^{(2p-1)}(a)\right], \qquad (2.594)\end{aligned}$$

or, more generally for $t = a + (k+\kappa)\Delta$,

$$\sum_{k=0}^{K-1} F(a+(k+\kappa)\Delta) = \frac{1}{\Delta}\int_a^b dt\, F(t) + \sum_{p=1}^{\infty}\frac{\Delta^{p-1}}{p!}B_p(\kappa)\left[F^{(p-1)}(b)-F^{(p-1)}(a)\right], \qquad (2.595)$$

where $B_n(\kappa)$ are the Bernoulli functions defined by a generalization of the expansion (2.568):

$$\frac{te^{\kappa t}}{e^t-1} = \sum_{n=0}^{\infty} B_n(\kappa)\frac{t^n}{n!}. \qquad (2.596)$$

At $\kappa = 0$, the Bernoulli functions start out with the Bernoulli numbers: $B_n(0) = B_n$. The function $B_0(\kappa)$ is equal to 1 everywhere.

Another way of writing formula (2.597) is

$$\sum_{k=0}^{K-1} F(a+(k+\kappa)\Delta) = \frac{1}{\Delta}\int_a^b dt\left[1+\sum_{p=0}^{\infty}\frac{\Delta^p}{p!}B_p(\kappa)\partial_t^p\right]F(t). \qquad (2.597)$$

This implies that a sum over discrete values of a function can be replaced by an integral over a gradient expansion of the function.

[31] M. Abramowitz and I. Stegun, op. cit., Formulas 23.1.30 and 23.1.32.

Using the first Euler-Maclaurin formula (2.594) with $a = \omega_1^2$, $b = \omega_M^2$, and $\Delta = \omega_1$, we find

$$\sum_{m=0}^{M}\left[\log(\omega_m^2+\omega^2)-\log(\omega_m^2)\right]=\left\{\pi\frac{\omega}{\omega_1}+\frac{\omega_m}{\omega_1}\left[\log(\omega_m^2+\omega^2)-2\right]\right\}\Bigg|_{m=1}^{m=M}-\left\{\omega=0\right\}\Bigg|_{m=1}^{m=M}$$
$$+\frac{1}{2}\left\{\log(\omega_1^2+\omega^2)+\log(\omega_M^2+\omega^2)\right\}-\left\{\omega=0\right\}. \quad (2.598)$$

For small T, the leading two terms on the right-hand side are

$$\pi\frac{\omega}{\omega_1}-\frac{1}{2}\log\frac{\omega^2}{\omega_1^2}, \quad (2.599)$$

in agreement with the first two terms in the low-temperature series (2.564). Note that the Euler-Maclaurin formula is unable to recover the exponentially small terms in (2.564), since they are not expandable in powers of T.

The transformation of high- into low-temperature expansions is an important tool for analyzing phase transitions in models of statistical mechanics.[32]

2.16 Finite-N Behavior of Thermodynamic Quantities

Thermodynamic fluctuations in Euclidean path integrals are often imitated in computer simulations. These are forced to employ a sliced time axis. It is then important to know in which way the time-sliced thermodynamic quantities converge to their continuum limit. Let us calculate the internal energy E and the specific heat at constant volume C for finite N from (2.484). Using (2.484) we have

$$\frac{\partial(\beta\tilde{\omega}_{\rm e})}{\partial\beta} = \frac{\omega}{\cosh(\epsilon\tilde{\omega}_{\rm e}/2)},$$
$$\frac{\partial(\epsilon\tilde{\omega}_{\rm e})}{\partial\beta} = \frac{2}{\beta}\tanh(\epsilon\tilde{\omega}_{\rm e}/2), \quad (2.600)$$

and find the internal energy

$$E = \frac{\partial}{\partial\beta}(\beta F)=\frac{\hbar}{2}\coth(\beta\hbar\tilde{\omega}_{\rm e}/2)\frac{\partial(\beta\tilde{\omega}_{\rm e})}{\partial\beta}$$
$$= \frac{\hbar\omega}{2}\frac{\coth(\beta\hbar\tilde{\omega}_{\rm e}/2)}{\cosh(\epsilon\tilde{\omega}_{\rm e}/2)}. \quad (2.601)$$

The specific heat at constant volume is given by

$$\frac{1}{k_B}C=-\beta^2\frac{\partial^2}{\partial\beta^2}(\beta F)=-\beta^2\frac{\partial}{\partial\beta}E \quad (2.602)$$
$$=\frac{1}{4}\beta^2\hbar^2\omega^2\left[\frac{1}{\sinh^2(\beta\hbar\tilde{\omega}_{\rm e}/2)}+\coth(\beta\hbar\tilde{\omega}_{\rm e}/2)\tanh(\epsilon\tilde{\omega}_{\rm e}/2)\frac{\epsilon}{\hbar\beta}\right]\frac{1}{\cosh^2(\epsilon\tilde{\omega}_{\rm e}/2)}.$$

Plots are shown in Fig. 2.5 for various N using natural units with $\hbar = 1$, $k_B = 1$. At high

[32] See H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I Superflow and Vortex Lines, World Scientific, Singapore, 1989, pp. 1–742 (`http://www.physik.fu-berlin.de/~kleinert/b1`).

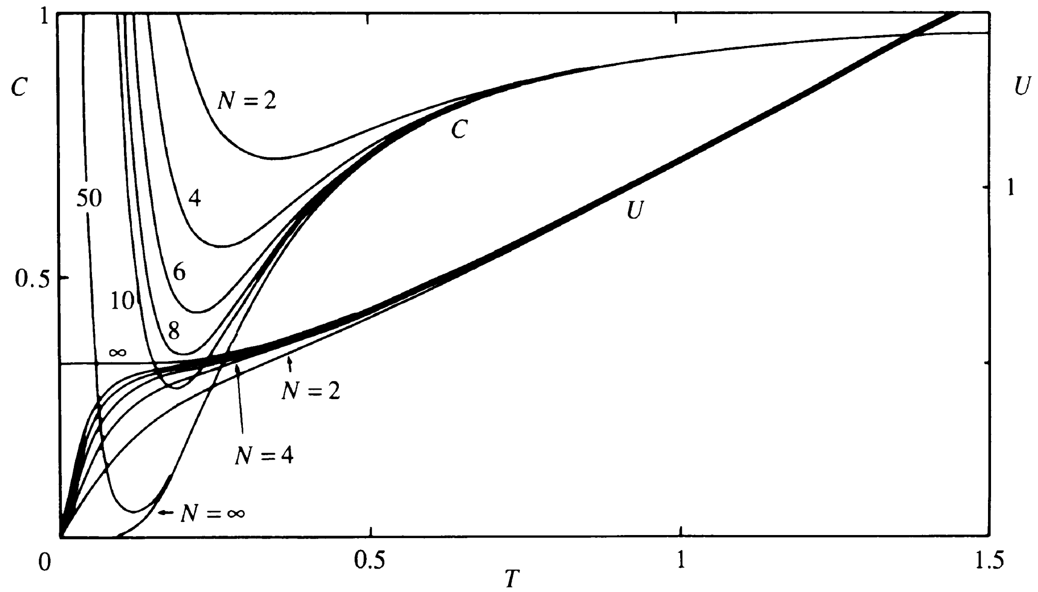

Figure 2.4 Finite-lattice effects in internal energy E and specific heat C at constant volume, as a function of the temperature for various numbers $N+1$ of time slices. Note the nonuniform way in which the exponential small-T behavior of $C \propto e^{-\omega/T}$ is approached in the limit $N \to \infty$.

temperatures, F, E, and C are independent of N:

$$F \to \frac{1}{\beta}\log\beta, \tag{2.603}$$

$$E \to \frac{1}{\beta} = T, \tag{2.604}$$

$$C \to 1. \tag{2.605}$$

These limits are a manifestation of the *Dulong-Petit law*: An oscillator has one kinetic and one potential degree of freedom, each carrying an internal energy $T/2$ and a specific heat $1/2$. At low temperatures, on the other hand, E and C are strongly N-dependent (note that since F and E are different at $T=0$, the entropy of the lattice approximation does not vanish as it must in the continuum limit). Thus, the convergence $N \to \infty$ is highly nonuniform. After reaching the limit, the specific heat goes to zero for $T \to 0$ exponentially fast, like $e^{-\omega/T}$. The quantity ω is called *activation energy*.[33] It is the energy difference between the ground state and the first excited state of the harmonic oscillator. For large but finite N, on the other hand, the specific heat has the large value $N+1$ at $T=0$. This is due to $\tilde{\omega}_{\rm e}$ and $\cosh^2(\epsilon\tilde{\omega}_{\rm e}/2)$ behaving, for a finite N and $T \to 0$ (where ϵ becomes large) like

$$\tilde{\omega}_{\rm e} \to \frac{1}{\epsilon}\log(\epsilon^2\omega^2),$$
$$\cosh(\epsilon\tilde{\omega}_{\rm e}/2) \to \epsilon\omega/2. \tag{2.606}$$

Hence

$$E \xrightarrow{T\to 0} \frac{1}{\beta}\coth[(N+1)\log(\epsilon\omega)] \xrightarrow{T\to 0} 0, \tag{2.607}$$

[33]Note that in a D-dimensional solid the lattice vibrations can be considered as an ensemble of harmonic oscillators with energies ω ranging from zero to the Debye frequency. Integrating over the corresponding specific heats with the appropriate density of states, $\int d\omega\omega^{D-1}e^{-\omega/k_BT}$, gives the well-known power law at low temperatures $C \propto T^D$.

$$C \xrightarrow{T\to 0} N+1. \tag{2.608}$$

The reason for the nonuniform approach of the $N \to \infty$ limit is obvious: If we expand (2.484) in powers of ϵ, we find

$$\tilde{\omega}_{\rm e} = \omega\left(1 - \frac{1}{24}\epsilon^2\omega^2 + \dots\right). \tag{2.609}$$

When going to low T at finite N the corrections are quite large, as can be seen by writing (2.609), with $\epsilon = \hbar\beta/(N+1)$, as

$$\tilde{\omega}_{\rm e} = \omega\left[1 - \frac{1}{24}\frac{\hbar^2\omega^2}{k_b^2 T^2 (N+1)^2} + \dots\right]. \tag{2.610}$$

Note that (2.609) contains no corrections of the order ϵ. This implies that the convergence of all thermodynamic quantities in the limit $N \to \infty, \epsilon \to 0$ at fixed T is quite fast — one order in $1/N$ faster than we might at first expect [the Trotter formula (2.26) also shows the $1/N^2$ -behavior].

2.17 Time Evolution Amplitude of Freely Falling Particle

The gravitational potential of a particle on the surface of the earth is

$$V(\mathbf{x}) = V_0 + M\,\mathbf{g}\cdot\mathbf{x}, \tag{2.611}$$

where $-\mathbf{g}$ is the earth's acceleration vector pointing towards the ground, and V_0 some constant. The equation of motion reads

$$\ddot{\mathbf{x}} = -\mathbf{g}, \tag{2.612}$$

which is solved by

$$\mathbf{x} = \mathbf{x}_a + \mathbf{v}_a(t-t_a) + \frac{\mathbf{g}}{2}(t-t_a)^2, \tag{2.613}$$

with the initial velocity

$$\mathbf{v}_a = \frac{\mathbf{x}_b - \mathbf{x}_a}{t_b - t_a} - \frac{\mathbf{g}}{2}(t_b - t_a). \tag{2.614}$$

Inserting this into the action

$$\mathcal{A} = \int_{t_a}^{t_b} dt \left(\frac{M}{2}\dot{\mathbf{x}}^2 - V_0 - \mathbf{g}\cdot\mathbf{x}\right), \tag{2.615}$$

we obtain the classical action

$$\mathcal{A}_{\rm cl} = -V_0(t_b-t_a) + \frac{M}{2}\frac{(\mathbf{x}_b-\mathbf{x}_a)^2}{t_b-t_a} - \frac{1}{2}(t_b-t_a)\mathbf{g}\cdot(\mathbf{x}_b+\mathbf{x}_a) - \frac{1}{24}(t_b-t_a)^3\mathbf{g}^2. \tag{2.616}$$

Since the quadratic part of (2.615) is the same as for a free particle, also the fluctuation factor is the same [see (2.130)], and we find the time evolution amplitude

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \frac{1}{\sqrt{2\pi i\hbar(t_b-t_a)/M}^3} e^{-\frac{i}{\hbar}V_0(t_b-t_a)}$$
$$\times \exp\left\{\frac{iM}{2\hbar}\left[\frac{(\mathbf{x}_b-\mathbf{x}_a)^2}{t_b-t_a} - (t_b-t_a)\mathbf{g}\cdot(\mathbf{x}_b+\mathbf{x}_a) - \frac{1}{12}(t_b-t_a)^3\mathbf{g}^2\right]\right\}. \tag{2.617}$$

The potential (2.611) can be considered as a limit of a harmonic potential

$$V(\mathbf{x}) = V_0 + \frac{M}{2}\omega^2(\mathbf{x}-\mathbf{x}_0)^2 \tag{2.618}$$

for

$$\omega \to 0, \quad \mathbf{x}_0 = -\mathbf{g}/\omega^2 \to -\infty \approx \hat{\mathbf{g}}, \quad V_0 = -M\mathbf{x}_0^2/2 = -Mg^2/2\omega^4 \to -\infty, \tag{2.619}$$

keeping

$$\mathbf{g} = -M\omega^2\mathbf{x}_0, \tag{2.620}$$

and

$$v_0 = V_0 + \frac{M}{2}\omega^2\mathbf{x}_0^2 \tag{2.621}$$

fixed. If we perform this limit in the amplitude (2.177), we find of course (2.617).

The wave functions can be obtained most easily by performing this limiting procedure on the wave functions of the harmonic oscillator. In one dimension, we set $n = E/\omega$ and find that the spectral representation (2.294) goes over into

$$(x_b t_b|x_a t_a) = \int dE A_E(x_b)A_E^*(x_a)e^{-i(E-v_0)(t_b-t_a)/\hbar}, \tag{2.622}$$

with the wave functions

$$A_E(x) = \frac{1}{\sqrt{l\varepsilon}}\,\mathrm{Ai}\left(\frac{x}{l}-\frac{E}{\varepsilon}\right). \tag{2.623}$$

Here $\varepsilon \equiv (\hbar^2 g^2 M/2)^{1/3}$ and $l \equiv (\hbar^2/2M^2 g)^{1/3} = \varepsilon/Mg$ are the natural units of energy and length, respectively, and $\mathrm{Ai}(z)$ is the *Airy function* solving the differential equation

$$\mathrm{Ai}''(z) = z\mathrm{Ai}(z), \tag{2.624}$$

For positive z, the Airy function can be expressed in terms of modified Bessel functions $I_\nu(\xi)$ and $K_\nu(\xi)$:[34]

$$\mathrm{Ai}(z) = \frac{\sqrt{z}}{2}[I_{-1/3}(2z^{3/2}/3) - I_{1/3}(2z^{3/2}/3)] = \frac{1}{\pi}\sqrt{\frac{z}{3}}K_{1/3}\left(2z^{3/2}/3\right). \tag{2.625}$$

For large z, this falls off exponentially:

$$\mathrm{Ai}(z) \to \frac{1}{2\sqrt{\pi}z^{1/4}}e^{-2z^{3/2}/3}, \quad z \to \infty. \tag{2.626}$$

For negative z, an analytic continuation[35]

$$\begin{aligned} I_\nu(\xi) &= e^{-\pi\nu i/2}J(e^{\pi i/2}\xi), \quad -\pi < \arg\xi \le \pi/2, \\ I_\nu(\xi) &= e^{-\pi\nu i/2}J(e^{\pi i/2}\xi), \quad \pi/2 < \arg\xi \le \pi, \end{aligned} \tag{2.627}$$

[34]A compact description of the properties of Bessel functions is found in M. Abramowitz and I. Stegun, op. cit., Chapter 10. The Airy function is expressed in Formulas 10.4.14.

[35]I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formulas 8.406.

leads to

$$\mathrm{Ai}(z) = \frac{1}{3}\sqrt{z}\left[J_{-1/3}(2(-z)^{3/2}/3) + J_{1/3}(2(-z)^{3/2}/3)\right], \tag{2.628}$$

where $J_{1/3}(\xi)$ are ordinary Bessel functions. For large arguments, these oscillate like

$$J_\nu(\xi) \to \sqrt{\frac{2}{\pi\xi}}\cos(\xi - \pi\nu/2 - \pi/4) + \mathcal{O}(\xi^{-1}), \tag{2.629}$$

from which we obtain the oscillating part of the Airy function

$$\mathrm{Ai}(z) \to \frac{1}{\sqrt{\pi}z^{1/4}}\sin\left[2(-z)^{3/2}/3 + \pi/4\right], \quad z \to -\infty. \tag{2.630}$$

The Airy function has the simple Fourier representation

$$\mathrm{Ai}(x) = \int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{i(xk+k^3/3)}. \tag{2.631}$$

In fact, the momentum space wave functions of energy E are

$$\langle p|E\rangle = \sqrt{\frac{l}{\varepsilon}}e^{-i(pE-p^3/6M)l/\varepsilon\hbar} \tag{2.632}$$

fulfilling the orthogonality and completeness relations

$$\int\frac{dp}{2\pi\hbar}\langle E'|p\rangle\langle p|E\rangle = \delta(E'-E), \qquad \int dE\,\langle p'|E\rangle\langle E|p\rangle = 2\pi\hbar\delta(p'-p). \tag{2.633}$$

The Fourier transform of (2.632) is equal to (2.623), due to (2.631).

2.18 Charged Particle in Magnetic Field

Having learned how to solve the path integral of the harmonic oscillator we are ready to study also a more involved harmonic system of physical importance: a charged particle in a magnetic field. This problem was first solved by L.D. Landau in 1930 in Schrödinger theory.[36]

2.18.1 Action

The magnetic interaction of a particle of charge e is given by

$$\mathcal{A}_{\mathrm{mag}} = \frac{e}{c}\int_{t_a}^{t_b} dt\,\dot{\mathbf{x}}(t)\cdot\mathbf{A}(\mathbf{x}(t)), \tag{2.634}$$

where $\mathbf{A}(\mathbf{x})$ is the vector potential of the magnetic field. The total action is

$$\mathcal{A}[\mathbf{x}] = \int_{t_a}^{t_b} dt\left[\frac{M}{2}\dot{\mathbf{x}}^2(t) + \frac{e}{c}\dot{\mathbf{x}}(t)\cdot\mathbf{A}(\mathbf{x}(t))\right]. \tag{2.635}$$

[36] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*, Pergamon, London, 1965.

Suppose now that the particle moves in a homogeneous magnetic field $\mathbf{B}$ pointing along the z-direction. Such a field can be described by a vector potential

$$\mathbf{A}(\mathbf{x}) = (0, Bx, 0). \tag{2.636}$$

But there are other possibilities. The magnetic field

$$\mathbf{B}(\mathbf{x}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{x}) \tag{2.637}$$

as well as the magnetic interaction (2.634) are invariant under gauge transformations

$$\mathbf{A}(\mathbf{x}) \to \mathbf{A}(\mathbf{x}) + \boldsymbol{\nabla}\Lambda(\mathbf{x}), \tag{2.638}$$

where $\Lambda(\mathbf{x})$ are arbitrary single-valued functions of $\mathbf{x}$. As such they satisfy the Schwarz integrability condition [compare (1.40)–(1.41)]

$$(\partial_i \partial_j - \partial_j \partial_i)\Lambda(\mathbf{x}) = 0. \tag{2.639}$$

For instance, the axially symmetric vector potential

$$\tilde{\mathbf{A}}(\mathbf{x}) = \frac{1}{2}\mathbf{B} \times \mathbf{x} \tag{2.640}$$

gives the same magnetic field; it differs from (2.636) by a gauge transformation

$$\tilde{\mathbf{A}}(\mathbf{x}) = \mathbf{A}(\mathbf{x}) + \boldsymbol{\nabla}\Lambda(\mathbf{x}), \tag{2.641}$$

with the gauge function

$$\Lambda(\mathbf{x}) = -\frac{1}{2}B\,xy. \tag{2.642}$$

In the canonical form, the action reads

$$\mathcal{A}[\mathbf{p}, \mathbf{x}] = \int_{t_a}^{t_b} dt \left\{ \mathbf{p} \cdot \dot{\mathbf{x}} - \frac{1}{2M}\left[\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{x})\right]^2 \right\}. \tag{2.643}$$

The magnetic interaction of a point particle is thus included in the path integral by the so-called *minimal substitution* of the momentum variable:

$$\mathbf{p} \to \mathbf{P} \equiv \mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{x}). \tag{2.644}$$

For the vector potential (2.636), the action (2.643) becomes

$$\mathcal{A}[\mathbf{p}, \mathbf{x}] = \int_{t_a}^{t_b} dt \left[\mathbf{p} \cdot \dot{\mathbf{x}} - H(\mathbf{p}, \mathbf{x})\right], \tag{2.645}$$

with the Hamiltonian

$$H(\mathbf{p}, \mathbf{x}) = \frac{\mathbf{p}^2}{2M} + \frac{1}{8}M\omega_L^2\mathbf{x}^2 - \frac{1}{2}\omega_L l_z(\mathbf{p}, \mathbf{x}), \tag{2.646}$$

where $\mathbf{x} = (x, y)$ and $\mathbf{p} = (p_x, p_y)$ and

$$l_z(\mathbf{p}, \mathbf{x}) = (\mathbf{x} \times \mathbf{p})_z = xp_y - yp_x \tag{2.647}$$

is the z-component of the orbital angular momentum. In a Schrödinger equation, the last term in $H(\mathbf{p}, \mathbf{x})$ is diagonal on states with a given angular momentum around the z-axis. We have introduced the field-dependent frequency

$$\omega_L = \frac{e}{Mc} B, \tag{2.648}$$

called *Landau frequency* or *cyclotron frequency*. This can also be written in terms of the *Bohr magneton*

$$\mu_B \equiv \frac{\hbar e}{Mc}, \tag{2.649}$$

as

$$\omega_L = \mu_B B / \hbar. \tag{2.650}$$

The first two terms in (2.646) describe a harmonic oscillator in the xy-plane with a field-dependent *magnetic frequency*

$$\omega_B \equiv \frac{\omega_L}{2}. \tag{2.651}$$

Note that in the gauge gauge (2.636), the Hamiltonian would have the rotationally noninvariant form

$$H(\mathbf{p}, \mathbf{x}) = \frac{\mathbf{p}^2}{2M} + \frac{1}{2} M \omega_L^2 x^2 - \omega_L x p_y \tag{2.652}$$

rather than (2.646), implying oscillations of frequency ω_L in the x-direction and a free motion in the y-direction.

The time-sliced form of the canonical action (2.643) reads

$$\mathcal{A}_{\mathrm{e}}^N = \sum_{n=1}^{N+1} \left\{ \mathbf{p}_n (\mathbf{x}_n - \mathbf{x}_{n-1}) - \frac{1}{2M} \left[p_{x\,n}^2 + (p_{y\,n} - B x_n)^2 + p_{zn}^2 \right] \right\}, \tag{2.653}$$

and the associated time-evolution amplitude for the particle to run from $\mathbf{x}_a$ to $\mathbf{x}_b$ is given by

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = \prod_{n=1}^{N} \left[\int d^3 x_n \right] \prod_{n=1}^{N+1} \left[\int \frac{d^3 p_n}{(2\pi\hbar)^3} \right] \exp\left(\frac{i}{\hbar} \mathcal{A}_{\mathrm{e}}^N \right), \tag{2.654}$$

with the time-sliced action

$$\mathcal{A}^N = \sum_{n=1}^{N+1} \left\{ \mathbf{p}_n (\mathbf{x}_n - \mathbf{x}_{n-1}) - \frac{1}{2M} \left[p_{x\,n}^2 + (p_{y\,n} - B x_n)^2 + p_{zn}^2 \right] \right\}. \tag{2.655}$$

2.18.2 Gauge Properties

Note that the time evolution amplitude is not gauge-invariant. If we use the vector potential in some other gauge

$$\mathbf{A}'(\mathbf{x}) = \mathbf{A}(\mathbf{x}) + \boldsymbol{\nabla}\Lambda(\mathbf{x}), \tag{2.656}$$

the action changes by a surface term

$$\Delta\mathcal{A} \;=\; \frac{e}{c}\int_{t_a}^{t_b} dt\,\dot{\mathbf{x}}\cdot\boldsymbol{\nabla}\Lambda(\mathbf{x}) = \frac{e}{c}\left[\Lambda(\mathbf{x}_b) - \Lambda(\mathbf{x}_a)\right]. \tag{2.657}$$

The amplitude is therefore multiplied by a phase factor on both ends

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a)_A \to (\mathbf{x}_b t_b|\mathbf{x}_a t_a)_{A'} = e^{ie\Lambda(\mathbf{x}_b)/c\hbar}(\mathbf{x}_b t_b|\mathbf{x}_a t_a)_A e^{-ie\Lambda(\mathbf{x}_a)/c\hbar}. \tag{2.658}$$

For the observable particle distribution $(\mathbf{x}\,t_b|\mathbf{x}\,t_a)$, the phase factors are obviously irrelevant. But all other observables of the system must also be independent of the phases $\Lambda(\mathbf{x})$ which is assured if they correspond to gauge-invariant operators.

2.18.3 Time-Sliced Path Integration

Since the action $\mathcal{A}^N$ contains the variables y_n and z_n only in the first term $\sum_{n=1}^{N+1} i\mathbf{p}_n\mathbf{x}_n$, we can perform the y_n, z_n integrations and find a product of N Δ-functions in the y- and z-components of the momenta $\mathbf{p}_n$. If the projections of $\mathbf{p}$ to the yz-plane are denoted by $\mathbf{p}'$, the product is

$$(2\pi\hbar)^2\delta^{(2)}\left(\mathbf{p}'_{N+1} - \mathbf{p}'_N\right)\cdots(2\pi\hbar)^2\delta^{(2)}\left(\mathbf{p}'_2 - \mathbf{p}'_1\right). \tag{2.659}$$

These allow performing all $p_{y\,n}, p_{z\,n}$-integrals, except for one overall $p_y,\ p_z$. The path integral reduces therefore to

$$\begin{aligned}(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = {} & \int_{-\infty}^{\infty}\frac{dp_y dp_z}{(2\pi\hbar)^2}\prod_{n=1}^{N}\left[\int_{-\infty}^{\infty}dx_n\right]\prod_{n=1}^{N+1}\left[\int\frac{dp_{x\,n}}{2\pi\hbar}\right] \\ & \times\quad \exp\left\{\frac{i}{\hbar}\left[p_y(y_b-y_a)+p_z(z_b-z_a)-(t_b-t_a)\frac{p_z^2}{2M}\right]\right\}\exp\left(\frac{i}{\hbar}\mathcal{A}_x^N\right),\end{aligned} \tag{2.660}$$

where $\mathcal{A}_x^N$ is the time-sliced action involving only a one-dimensional path integral over the x-component of the path, $x(t)$, with the sliced action

$$\mathcal{A}_x^N = \sum_{n=1}^{N+1}\left[p_{x\,n}(x_n - x_{n-1}) - \frac{p_{x\,n}^2}{2M} - \frac{1}{2M}\left(p_y - \frac{e}{c}Bx_n\right)^2\right]. \tag{2.661}$$

This is the action of a one-dimensional harmonic oscillator with field-dependent frequency ω_B whose center of oscillation depends on p_y and lies at

$$x_0 = p_y/M\omega_L. \tag{2.662}$$

The path integral over $x(t)$ is harmonic and known from (2.175):

$$(x_b t_b | x_a t_a)_{x_0} = \sqrt{\frac{M\omega_L}{2\pi i\hbar \sin\omega_L(t_b - t_a)}}$$
$$\times \exp\left(\frac{i}{\hbar}\frac{M\omega_L}{2\sin\omega_L(t_b-t_a)}\left\{\left[(x_b - x_0)^2 + (x_a - x_0)^2\right]\cos\omega_L(t_b - t_a)\right.\right.$$
$$\left.\left. - 2(x_b - x_0)(x_a - x_0)\right\}\right). \tag{2.663}$$

Doing the p_z-integral in (2.660), we arrive at the formula

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = \frac{1}{\sqrt{2\pi i\hbar(t_b - t_a)/M}} e^{i\frac{M}{2\hbar}\frac{(z_b - z_a)^2}{t_b - t_a}} (\mathbf{x}_b^{\perp} t_b | \mathbf{x}_a^{\perp} t_a), \tag{2.664}$$

with the amplitude orthogonal to the magnetic field

$$(\mathbf{x}_b^{\perp} t_b | \mathbf{x}_a^{\perp} t_a) \equiv \frac{M\omega_L}{2\pi\hbar}\int_{-\infty}^{\infty} dx_0\, e^{iM\omega_L x_0 (y_b - y_a)/\hbar} (x_b t_b | x_a t_a)_{x_0}. \tag{2.665}$$

After a quadratic completion in x_0, the total exponent in (2.665) reads

$$\frac{iM\omega_L}{2\hbar}\left[-(x_b^2 + x_a^2)\tan[\omega_L(t_b - t_a)/2] + (x_b - x_a)^2 \frac{1}{\sin\omega_L(t_b - t_a)}\right]$$
$$-i\frac{M\omega_L}{\hbar}\tan[\omega_L(t_b - t_a)/2]\left(x_0 - \frac{x_b + x_a}{2} - \frac{y_b - y_a}{2\tan[\omega_L(t_b - t_a)/2]}\right)^2$$
$$+i\frac{M\omega_L}{2\hbar}\left[\frac{(x_b + x_a)^2}{2}\tan[\omega_L(t_b - t_a)/2] + \frac{(y_b - y_a)^2}{2\tan[\omega_L(t_b - t_a)/2]}\right]$$
$$+i\frac{M\omega_L}{2\hbar}(x_b + x_a)(y_b - y_a). \tag{2.666}$$

The integration $M\omega_L \int_{-\infty}^{\infty} dx_0/2\pi\hbar$ removes the second term and results in a factor

$$\frac{M\omega_L}{2\pi\hbar}\sqrt{\frac{\pi\hbar}{iM\omega_L \tan[\omega_L(t_b - t_a)/2]}}. \tag{2.667}$$

By rearranging the remaining terms, we arrive at the amplitude

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = \sqrt{\frac{M}{2\pi i\hbar(t_b - t_a)}}^3 \frac{\omega_L(t_b - t_a)/2}{\sin[\omega_L(t_b - t_a)/2]} \exp\left[\frac{i}{\hbar}(\mathcal{A}_{\rm cl} + \mathcal{A}_{\rm sf})\right], \tag{2.668}$$

with an action

$$\mathcal{A}_{\rm cl} = \frac{M}{2}\left\{\frac{(z_b - z_a)^2}{t_b - t_a} + \frac{\omega_L}{2}\cot[\omega_L(t_b - t_a)/2]\left[(x_b - x_a)^2 + (y_b - y_a)^2\right]\right.$$
$$\left. + \ \omega_L(x_a y_b - x_b y_a)\right\}, \tag{2.669}$$

and the surface term

$$\mathcal{A}_{\rm sf} = \frac{M\omega_L}{2}(x_b y_b - x_a y_a) = \frac{e}{2c} B\, xy\Big|_a^b. \tag{2.670}$$

2.18.4 Classical Action

Since the action is harmonic, the amplitude is again a product of a phase $e^{i\mathcal{A}_{\rm cl}}$ and a fluctuation factor. A comparison with (2.641) and (2.658) shows that the surface term would be absent if the amplitude $(\mathbf{x}_b t_b|\mathbf{x}_a t_a)_{\tilde{A}}$ were calculated with the vector potential in the axially symmetric gauge (2.640). Thus $\mathcal{A}_{\rm cl}$ must be equal to the classical action in this gauge. Indeed, the orthogonal part can be rewritten as

$$\mathcal{A}_{\rm cl}^{\perp}=\int_{t_a}^{t_b}dt\left\{\frac{M}{2}\frac{d}{dt}(x\dot{x}+y\dot{y})+\frac{M}{2}\left[x(-\ddot{x}+\omega_L\dot{y})+y(-\ddot{y}-\omega_L\dot{x})\right]\right\}. \tag{2.671}$$

The equations of motion are

$$\ddot{x}=\omega_L\dot{y},\qquad \ddot{y}=-\omega_L\dot{x}, \tag{2.672}$$

reducing the action of a classical orbit to

$$\mathcal{A}_{\rm cl}^{\perp}=\frac{M}{2}(x\dot{x}+y\dot{y})\Big|_{t_a}^{t_b}=\frac{M}{2}\left([x_b\dot{x}_b-x_a\dot{x}_a]+[y_b\dot{y}_b-y_a\dot{y}_a]\right). \tag{2.673}$$

The orbits are easily determined. By inserting the two equations in (2.672) into each other we see that $\dot{x}$ and $\dot{y}$ perform independent oscillations:

$$\dddot{x}+\omega_L^2\dot{x}=0,\quad \dddot{y}+\omega_L^2\dot{y}=0. \tag{2.674}$$

The general solution of these equations is

$$x=\frac{1}{\sin\omega_L(t_b-t_a)}\left[(x_b-x_0)\sin\omega_L(t-t_a)-(x_a-x_0)\sin\omega_L(t-t_b)\right]+x_0, \tag{2.675}$$

$$y=\frac{1}{\sin\omega_L(t_b-t_a)}\left[(y_b-y_0)\sin\omega_L(t-t_a)-(y_a-y_0)\sin\omega_L(t-t_b)\right]+y_0, \tag{2.676}$$

where we have incorporated the boundary condition $x(t_{a,b})=x_{a,b}$, $y(t_{a,b})=y_{a,b}$. The constants x_0,y_0 are fixed by satisfying (2.672). This gives

$$x_0=\frac{1}{2}\left[(x_b+x_a)+(y_b-y_a)\cot\frac{\omega_L}{2}(t_b-t_a)\right], \tag{2.677}$$

$$y_0=\frac{1}{2}\left[(y_b+y_a)-(x_b-x_a)\cot\frac{\omega_L}{2}(t_b-t_a)\right]. \tag{2.678}$$

Now we calculate

$$x_b\dot{x}_b=\frac{\omega_L}{\sin\omega_L(t_b-t_a)}x_b\left[(x_0-x_a)+(x_b-x_0)\cos\omega_L(t_b-t_a)\right], \tag{2.679}$$

$$x_a\dot{x}_a=\frac{\omega_L}{\sin\omega_L(t_b-t_a)}x_a\left[(x_0-x_a)\cos\omega_L(t_b-t_a)+(x_b-x_0)\right], \tag{2.680}$$

and hence

$$\begin{aligned}x_b\dot{x}_b-x_a\dot{x}_a &= \omega_L x_0(x_b+x_a)\tan\frac{\omega_L}{2}(t_b-t_a)\\ &\quad+\frac{\omega_L}{\sin\omega_L(t_b-t_a)}\left[(x_b^2+x_a^2)\cos\omega_L(t_b-t_a)-2x_bx_a\right]\\ &= \frac{\omega_L}{2}\left[(x_b-x_a)^2\cot\frac{\omega_L}{2}(t_b-t_a)+(x_b+x_a)(y_b-y_a)\right].\end{aligned} \tag{2.681}$$

Similarly we find

$$\begin{aligned} y_b\dot{y}_b - y_a\dot{y}_a &= \omega_L y_0(y_b+y_a)\tan\frac{\omega_L}{2}(t_b-t_a) \\ &\quad + \frac{\omega_L}{\sin\omega_L(t_b-t_a)}[(y_b^2+y_a^2)\cos\omega_L(t_b-t_a)-2y_by_a] \\ &= \frac{\omega_L}{2}\left[(y_b-y_a)^2\cot\frac{\omega_L}{2}(t_b-t_a)-(x_b-x_a)(y_b+y_a)\right]. \end{aligned} \tag{2.682}$$

Inserted into (2.673), this yields the classical action for the orthogonal motion

$$\mathcal{A}_{\rm cl}^{\perp} = \frac{M}{2}\left\{\frac{\omega_L}{2}\cot[\omega_L(t_b-t_a)/2]\left[(x_b-x_a)^2+(y_b-y_a)^2\right]+\omega_L(x_ay_b-x_by_a)\right\}, \tag{2.683}$$

which is indeed the orthogonal part of the action (2.669).

2.18.5 Translational Invariance

It is interesting to see how the amplitude ensures the translational invariance of all physical observables. The first term in the classical action is trivially invariant. The last term reads

$$\Delta\mathcal{A} = \frac{M\omega_L}{2}(x_ay_b-x_by_a). \tag{2.684}$$

Under a translation by a distance $\mathbf{d}$,

$$\mathbf{x} \to \mathbf{x}+\mathbf{d}, \tag{2.685}$$

this term changes by

$$\frac{M\omega_L}{2}[d_x(y_b-y_a)+d_y(x_a-x_b)] = \frac{M\omega_L}{2}[(\mathbf{d}\times\mathbf{x})_b-(\mathbf{d}\times\mathbf{x})_a]_z \tag{2.686}$$

causing the amplitude to change by a pure gauge transformation as

$$(\mathbf{x}_bt_b|\mathbf{x}_at_a) \to e^{ie\Lambda(\mathbf{x}_b)/c\hbar}(\mathbf{x}_bt_b|\mathbf{x}_at_a)e^{-ie\Lambda(\mathbf{x}_a)/c\hbar}, \tag{2.687}$$

with the phase

$$\Lambda(\mathbf{x}) = -\frac{M\omega_L\hbar c}{2e}\left[\mathbf{d}\times\mathbf{x}\right]_z. \tag{2.688}$$

Since observables involve only gauge-invariant quantities, such transformations are irrelevant.

This will be done in 2.23.3.

2.19 Charged Particle in Magnetic Field plus Harmonic Potential

For application in Chapter 5 we generalize the above magnetic system by adding a harmonic oscillator potential, thus leaving the path integral solvable. For simplicity, we consider only the orthogonal part of the resulting system with respect to the magnetic field. Omitting orthogonality symbols, the Hamiltonian is the same as in (2.646). Without much more work we may solve the path integral of a more general system in which the harmonic potential in (2.646) has a different frequency $\omega \neq \omega_L$, and thus a Hamiltonian

$$H(\mathbf{p},\mathbf{x}) = \frac{\mathbf{p}^2}{2M} + \frac{1}{2}M\omega^2\mathbf{x}^2 - \omega_B l_z(\mathbf{p},\mathbf{x}). \tag{2.689}$$

The associated Euclidean action

$$\mathcal{A}_{\rm e}[\mathbf{p},\mathbf{x}] = \int_{\tau_a}^{\tau_b} d\tau\, [-i\mathbf{p}\cdot\dot{\mathbf{x}} + H(\mathbf{p},\mathbf{x})] \tag{2.690}$$

has the Lagrangian form

$$\mathcal{A}_{\rm e}[\mathbf{x}] = \int_0^{\hbar\beta} d\tau\, \left\{\frac{M}{2}\dot{\mathbf{x}}^2(\tau) + \frac{1}{2}M(\omega^2-\omega_B^2)\mathbf{x}^2(\tau) - iM\omega_B[\mathbf{x}(\tau)\times\dot{\mathbf{x}}(\tau)]_z\right\}. \tag{2.691}$$

At this point we observe that the system is stable only for $\omega \geq \omega_B$. The action (2.691) can be written in matrix notation as

$$\mathcal{A}_{\rm cl} = \int_0^{\hbar\beta} d\tau\, \left[\frac{M}{2}\frac{d}{d\tau}(\mathbf{x}\dot{\mathbf{x}}) + \frac{M}{2}\mathbf{x}^T\,\mathbf{D}_{\omega^2,B}\,\mathbf{x}\right], \tag{2.692}$$

where $\mathbf{D}_{\omega^2,B}$ is the 2×2 -matrix

$$\mathbf{D}_{\omega^2,B}(\tau,\tau') \equiv \begin{pmatrix} -\partial_\tau^2+\omega^2-\omega_B^2 & -2i\omega_B\partial_\tau \\ 2i\omega_B\partial_\tau & -\partial_\tau^2+\omega^2-\omega_B^2 \end{pmatrix}\delta(\tau-\tau'). \tag{2.693}$$

Since the path integral is Gaussian, we can immediately calculate the partition function

$$Z = \frac{1}{(2\pi\hbar/M)^2}\det \mathbf{D}_{\omega^2,B}^{-1/2}. \tag{2.694}$$

By expanding $\mathbf{D}_{\omega^2,B}(\tau,\tau')$ in a Fourier series

$$\mathbf{D}_{\omega^2,B}(\tau,\tau') = \frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\tilde{\mathbf{D}}_{\omega^2,B}(\omega_m)e^{-i\omega_m(\tau-\tau')}, \tag{2.695}$$

we find the Fourier components

$$\tilde{\mathbf{D}}_{\omega^2,B}(\omega_m) = \begin{pmatrix} \omega_m^2+\omega^2-\omega_B^2 & -2\omega_B\omega_m \\ 2\omega_B\omega_m & \omega_m^2+\omega^2-\omega_B^2 \end{pmatrix}, \tag{2.696}$$

with the determinants

$$\det \tilde{\mathbf{D}}_{\omega^2,B}(\omega_m) = (\omega_m^2 + \omega^2 - \omega_B^2)^2 + 4\omega_B^2\omega_m^2. \tag{2.697}$$

These can be factorized as

$$\det \tilde{\mathbf{D}}_{\omega^2,B}(\omega_m) = (\omega_m^2 + \omega_+^2)(\omega_m^2 + \omega_-^2), \tag{2.698}$$

with

$$\omega_\pm \equiv \omega \pm \omega_B. \tag{2.699}$$

The eigenvectors of $\tilde{\mathbf{D}}_{\omega^2,B}(\omega_m)$ are

$$\mathbf{e}_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \qquad \mathbf{e}_- = -\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}, \tag{2.700}$$

with eigenvalues

$$d_\pm = \omega_m^2 + \omega^2 \pm 2i\omega_m\omega_B = (\omega_m + i\omega_\pm)(\omega_m - i\omega_\mp). \tag{2.701}$$

Thus the right- and left-circular combinations $x_\pm = \pm(x \pm iy)/\sqrt{2}$ diagonalize the Lagrangian (2.692) to

$$\begin{aligned}\mathcal{A}_{\rm cl} &= \int_0^{\hbar\beta} d\tau \left\{ \frac{M}{2}\frac{d}{d\tau}\left(x_+^*\dot{x}_+ + x_-^*\dot{x}_-\right) \right. \\ &+ \left. \frac{M}{2}\left[x_+^*(-\partial_\tau - \omega_+)(-\partial_\tau + \omega_-)x_+ + x_-^*(-\partial_\tau - \omega_-)(-\partial_\tau + \omega_+)x_-\right]\right\}. \end{aligned} \tag{2.702}$$

Continued back to real times, the components $\mathrm{x}_\pm(t)$ are seen to oscillate independently with the frequencies $\omega_\pm$.

The factorization (2.698) makes (2.702) an action of two independent harmonic oscillators of frequencies $\omega_\pm$. The associated partition function has therefore the product form

$$Z = \frac{1}{2\sinh(\hbar\beta\omega_+/2)}\frac{1}{2\sinh(\hbar\beta\omega_-/2)}. \tag{2.703}$$

For the original system of a charged particle in a magnetic field discussed in Section 2.18, the partition function is obtained by going to the limit $\omega \to \omega_B$ in the Hamiltonian (2.689). Then $\omega_- \to 0$ and the partition function (2.703) diverges, since the system becomes translationally invariant in space. From the mnemonic replacement rule (2.361) we see that in this limit we must replace the relevant vanishing inverse frequency by an expression proportional to the volume of the system. The role of ω^2 in (2.361) is played here by the frequency in front of the $\mathbf{x}^2$-term of the Lagrangian (2.691). Since there are two dimensions, we must replace

$$\frac{1}{\omega^2 - \omega_B^2} \xrightarrow[\omega\to\omega_B]{} \frac{1}{2\omega\omega_-} \xrightarrow[\omega_-\to 0]{} \frac{\beta}{2\pi/M}V_2, \tag{2.704}$$

and thus

$$Z \xrightarrow[\omega_-\to 0]{} \frac{1}{2\sinh(\hbar\beta\omega)}\frac{V_2}{\lambda_\omega^2}, \tag{2.705}$$

where λ_ω is the quantum-mechanical length scale in Eqs. (2.303) and (2.359) of the harmonic oscillator.

2.20 Gauge Invariance and Alternative Path Integral Representation

The action (2.635) of a particle in an external ordinary potential $V(\mathbf{x},t)$ and a vector potential $\mathbf{A}(\mathbf{x},t)$ can be rewritten with the help of an arbitrary space- and time-dependent gauge function $\Lambda(\mathbf{x},t)$ in the following form:

$$\mathcal{A}[\mathbf{x}] = \int_{t_a}^{t_b} dt \left\{ \frac{M}{2}\dot{\mathbf{x}}^2 + \frac{e}{c}\dot{\mathbf{x}}(t)[\mathbf{A}(\mathbf{x},t) + \boldsymbol{\nabla}\Lambda(\mathbf{x},t)] - V(\mathbf{x},t) + \frac{e}{c}\partial_t\Lambda(\mathbf{x},t)\right\} - \frac{e}{c}\left[\Lambda(\mathbf{x}_b,t_b) - \Lambda(\mathbf{x}_a,t_a)\right]. \tag{2.706}$$

The $\Lambda(\mathbf{x},t)$-terms inside the integral are canceled by the last two surface terms making the action independent of $\Lambda(\mathbf{x},t)$.

We may now choose a particular function $\Lambda(\mathbf{x},t)$ equal to c/e-times the classical action $A(\mathbf{x},t)$ which solves the Hamilton-Jacobi equation (1.65), i.e.,

$$\frac{1}{2M}\left[\boldsymbol{\nabla}A(\mathbf{x},t) - \frac{e}{c}\mathbf{A}(\mathbf{x},t)\right]^2 + \partial_t A(\mathbf{x},t) + V(\mathbf{x},t) = 0. \tag{2.707}$$

Then we obtain the following alternative expression for the action:

$$\mathcal{A}[\mathbf{x}] = \int_{t_a}^{t_b} dt \frac{1}{2M}\left[M\dot{\mathbf{x}} - \boldsymbol{\nabla}A(\mathbf{x},t) + \frac{e}{c}\mathbf{A}(\mathbf{x},t)\right]^2 + A(\mathbf{x}_b,t_b) - A(\mathbf{x}_a,t_a). \tag{2.708}$$

For two infinitesimally different solutions of the Hamilton-Jacobi equation, the difference between the associated action functions δA satisfies the differential equation

$$\mathbf{v}\cdot\boldsymbol{\nabla}\delta A + \partial_t\delta A = 0, \tag{2.709}$$

where $\mathbf{v}$ is the classical velocity field

$$\mathbf{v}(\mathbf{x},t) \equiv (1/M)\left[\boldsymbol{\nabla}A(\mathbf{x},t) - \frac{e}{c}\mathbf{A}(\mathbf{x},t)\right]. \tag{2.710}$$

The differential equation (2.709) expresses the fact that two solutions $A(\mathbf{x},t)$ for which the particle energy and momenta at $\mathbf{x}$ and t differ by δE and $\delta\mathbf{p}$, respectively, satisfy the kinematic relation $\delta E = \mathbf{p}\cdot\delta\mathbf{p}/M = \dot{\mathbf{x}}_{\rm cl}\cdot\nabla\delta A$. This follows directly from $E = \mathbf{p}^2/2M$. The so-constrained variations δE and $\delta\mathbf{p}$ leave the action (2.708) invariant.

A sequence of changes δA of this type can be used to make the function $A(\mathbf{x},t)$ coincide with the action $A(\mathbf{x},t;\mathbf{x}_a,t_a)$ of paths which start out from $\mathbf{x}_a,t_a$ and arrive at $\mathbf{x},t$. In terms of this action function, the path integral representation of the time evolution amplitude takes the form

$$(\mathbf{x}_bt_b|\mathbf{x}_at_a) = e^{iA(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a)/\hbar}\int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b}\mathcal{D}\mathbf{x} \times\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\frac{1}{2M}\left[M\dot{\mathbf{x}} - \boldsymbol{\nabla}A(\mathbf{x},t;\mathbf{x}_a,t_a) + \frac{e}{c}\mathbf{A}(\mathbf{x},t)\right]^2\right\} \tag{2.711}$$

or, using $\mathbf{v}(\mathbf{x}(t),t)$,

$$(\mathbf{x}_bt_b|\mathbf{x}_at_a) = e^{iA(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a)/\hbar}\int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b}\mathcal{D}\mathbf{x}\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}dt\frac{M}{2}\left(\dot{\mathbf{x}}-\mathbf{v}\right)^2\right]. \tag{2.712}$$

The fluctuations are now controlled by the deviations of the instantaneous velocity $\dot{\mathbf{x}}(t)$ from local value of the classical velocity field $\mathbf{v}(\mathbf{x}, t)$. Since the path integral attempts to keep the deviations as small as possible, we call $\mathbf{v}(\mathbf{x}, t)$ the *desired velocity* of the particle at $\mathbf{x}$ and t. Introducing momentum variables $\mathbf{p}(t)$, the amplitude may be written as a phase space path integral

$$\begin{aligned}(\mathbf{x}_b t_b|\mathbf{x}_a t_a) &= e^{iA(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a)/\hbar}\int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b}\mathcal{D}'\mathbf{x}\int\frac{\mathcal{D}\mathbf{p}}{2\pi\hbar}\\ &\times \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left\{\mathbf{p}(t)\left[\dot{\mathbf{x}}(t)-\mathbf{v}(\mathbf{x}(t),t)\right]-\frac{1}{2M}\mathbf{p}^2(t)\right\}\right), \end{aligned} \tag{2.713}$$

which will be used in Section 18.15 to give a stochastic interpretation of quantum processes.

2.21 Velocity Path Integral

There exists yet another form of writing the path integral in which the fluctuating velocities play a fundamental role and which will later be seen to be closely related to path integrals in the so-called stochastic calculus to be introduced in Sections 18.13 and 18.640. We observe that by rewriting the path integral as

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a)=\int\mathcal{D}^3x\,\delta\left(\mathbf{x}_b-\mathbf{x}_a-\int_{t_a}^{t_b}dt\,\dot{\mathbf{x}}(t)\right)\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left[\frac{M}{2}\dot{\mathbf{x}}^2-V(\mathbf{x})\right]\right\}, \tag{2.714}$$

the δ-function allows us to include the last variable $\mathbf{x}_n$ in the integration measure of the time-sliced version of the path integral. Thus all time-sliced time derivatives $(\mathbf{x}_{n+1}-\mathbf{x}_n)/\epsilon$ for $n = 0$ to N are integrated over implying that they can be considered as independent fluctuating variables $\mathbf{v}_n$. In the potential, the dependence on the velocities can be made explicit by inserting

$$\mathbf{x}(t) = \mathbf{x}_b - \int_t^{t_b}dt\,\mathbf{v}(t), \tag{2.715}$$

$$\mathbf{x}(t) = \mathbf{x}_a + \int_{t_a}^{t}dt\,\mathbf{v}(t), \tag{2.716}$$

$$\mathbf{x}(t) = \mathbf{X} + \frac{1}{2}\int_{t_a}^{t_b}dt'\,\mathbf{v}(t')\epsilon(t'-t), \tag{2.717}$$

where

$$\mathbf{X}\equiv\frac{\mathbf{x}_b+\mathbf{x}_a}{2} \tag{2.718}$$

is the average position of the endpoints and $\epsilon(t-t')$ is the antisymmetric combination of Heaviside functions introduced in Eq. (1.315).

In the first replacement, we obtain the *velocity path integral*

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a)=\int\mathcal{D}^3v\,\delta\left(\mathbf{x}_b-\mathbf{x}_a-\int_{t_a}^{t_b}dt\,\mathbf{v}(t)\right)\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left[\frac{M}{2}\mathbf{v}^2-V\left(\mathbf{x}_b-\int_t^{t_b}dt\,\mathbf{v}(t)\right)\right]\right\}. \tag{2.719}$$

The measure of integration is normalized to make

$$\int\mathcal{D}^3v\,\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left[\frac{M}{2}\mathbf{v}^2\right]\right\}=1. \tag{2.720}$$

The correctness of this normalization can be verified by evaluating (2.719) for a free particle. Inserting the Fourier representation for the δ-function

$$\delta\left(\mathbf{x}_b-\mathbf{x}_a-\int_{t_a}^{t_b}dt\,\mathbf{v}(t)\right)=\int\frac{d^3p}{(2\pi i)^3}\exp\left[\frac{i}{\hbar}\mathbf{p}\left(\mathbf{x}_b-\mathbf{x}_a-\int_{t_a}^{t_b}dt\,\mathbf{v}(t)\right)\right], \tag{2.721}$$

we can complete the square in the exponent and integrate out the **v**-fluctuations using (2.720) to obtain

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \int \frac{d^3p}{(2\pi i)^3} \exp\left\{\frac{i}{\hbar}\left[\mathbf{p}\,(\mathbf{x}_b - \mathbf{x}_a) - \frac{\mathbf{p}^2}{2M}(t_b - t_a)\right]\right\}. \tag{2.722}$$

This is precisely the spectral representation (1.333) of the free-particle time evolution amplitude (1.335) [see also Eq. (2.53)].

A more symmetric velocity path integral is obtained by choosing the third replacement (2.717). This leads to the expression

$$\begin{aligned}(\mathbf{x}_b t_b|\mathbf{x}_a t_a) &= \int \mathcal{D}^3 v\, \delta\left(\Delta\mathbf{x} - \int_{t_a}^{t_b} dt\, \mathbf{v}(t)\right) \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt \frac{M}{2}\,\mathbf{v}^2\right\} \\ &\times\ \exp\left\{-\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, V\left(\mathbf{X} + \frac{1}{2}\int_{t_a}^{t_b} dt'\, \mathbf{v}(t')\epsilon(t'-t)\right)\right\}.\end{aligned} \tag{2.723}$$

The velocity representations are particularly useful if we want to know integrated amplitudes such as

$$\begin{aligned}\int d^3x_a\, (\mathbf{x}_b t_b|\mathbf{x}_a t_a) &= \int \mathcal{D}^3 v\, \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt \frac{M}{2}\,\mathbf{v}^2\right\}. \\ &\times\ \exp\left\{-\frac{i}{\hbar}\int_{t_a}^{t_b} dt V\left(\mathbf{x}_b - \frac{1}{2}\int_{t}^{t_b} dt'\, \mathbf{v}(t')\right)\right\},\end{aligned} \tag{2.724}$$

which will be of use in the next section.

2.22 Path Integral Representation of the Scattering Matrix

In Section 1.16 we have seen that the description of scattering processes requires several nontrivial limiting procedures on the time evolution amplitude. Let us see what these procedures yield when applied to the path integral representation of this amplitude.

2.22.1 General Development

Formula (1.474) for the scattering matrix expressed in terms of the time evolution operator in momentum space has the following path integral representation:

$$\langle \mathbf{p}_b|\hat{S}|\mathbf{p}_a\rangle \equiv \lim_{t_b - t_a \to \infty} e^{i(E_b t_b - E_a t_a)/\hbar} \int d^3x_b \int d^3x_a e^{-i(\mathbf{p}_b \mathbf{x}_b - \mathbf{p}_a \mathbf{x}_a)/\hbar} (\mathbf{x}_b t_b|\mathbf{x}_a t_a). \tag{2.725}$$

Introducing the momentum transfer $\mathbf{q} \equiv (\mathbf{p}_b - \mathbf{p}_a)$, we rewrite $e^{-i(\mathbf{p}_b\mathbf{x}_b - \mathbf{p}_a\mathbf{x}_a)/\hbar}$ as $e^{-i\mathbf{q}\mathbf{x}_b/\hbar}e^{-i\mathbf{p}_a(\mathbf{x}_b-\mathbf{x}_a)/\hbar}$, and observe that the amplitude including the exponential prefactor $e^{-i\mathbf{p}_a(\mathbf{x}_b-\mathbf{x}_a)/\hbar}$ has the path integral representation:

$$e^{-i\mathbf{p}_a(\mathbf{x}_b-\mathbf{x}_a)/\hbar}(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \int \mathcal{D}^3 x\, \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\left[\frac{M}{2}\dot{\mathbf{x}}^2 - \mathbf{p}_a\dot{\mathbf{x}} - V(\mathbf{x})\right]\right\}. \tag{2.726}$$

The linear term in $\dot{\mathbf{x}}$ is eliminated by shifting the path from $\mathbf{x}(t)$ to

$$\mathbf{y}(t) = \mathbf{x}(t) - \frac{\mathbf{p}_a}{M}\,t \tag{2.727}$$

leading to

$$e^{-i\mathbf{p}_a(\mathbf{x}_b-\mathbf{x}_b)/\hbar}(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = e^{-i\mathbf{p}_a^2(t_b-t_a)/2M\hbar}\int \mathcal{D}^3 y\, \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\left[\frac{M}{2}\dot{\mathbf{y}}^2 - V\left(\mathbf{y} + \frac{\mathbf{P}}{M}t\right)\right]\right\}. \tag{2.728}$$

Inserting everything into (2.725) we obtain

$$\begin{aligned}\langle \mathbf{p}_b|\hat{S}|\mathbf{p}_a\rangle &\equiv \lim_{t_b-t_a\to\infty} e^{i\mathbf{q}^2 t_b/2M\hbar}\int d^3y_b\, e^{-i\mathbf{q}\mathbf{y}_b/\hbar}\int d^3y_a \\ &\times \int \mathcal{D}^3y \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt \left[\frac{M}{2}\dot{\mathbf{y}}^2 - V\left(\mathbf{y}+\frac{\mathbf{p}_a}{M}t\right)\right]\right\}. \end{aligned} \tag{2.729}$$

In the absence of an interaction, the path integral over $\mathbf{y}(t)$ gives simply

$$\int d^3y_a \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\mathbf{y}_b-\mathbf{y}_a)^2}{t_b-t_a)}\right] = 1, \tag{2.730}$$

and the integral over $\mathbf{y}_a$ yields

$$\langle \mathbf{p}_b|\hat{S}|\mathbf{p}_a\rangle|_{V\equiv 0} = \lim_{t_b-t_a\to\infty} e^{i\mathbf{q}^2(t_b-t_a)/8M\hbar}(2\pi\hbar)^3\delta^{(3)}(\mathbf{q}) = (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}_b-\mathbf{p}_a), \tag{2.731}$$

which is the contribution from the unscattered beam to the scattering matrix in Eq. (1.477).

The first-order contribution from the interaction reads, after a Fourier decomposition of the potential,

$$\begin{aligned}\langle \mathbf{p}_b|\hat{S}_1|\mathbf{p}_a\rangle = -\frac{i}{\hbar}\lim_{t_b-t_a\to\infty} & e^{i\mathbf{q}^2 t_b/2M\hbar}\int d^3y_b\, e^{-i\mathbf{q}\mathbf{y}_b/\hbar}\int \frac{d^3Q}{(2\pi\hbar)^3}V(\mathbf{Q})\int d^3y_a \\ \times \int_{t_a}^{t_b} dt' \exp\left(\frac{i}{\hbar}\frac{\mathbf{p}_a\mathbf{Q}}{M}t'\right) & \int \mathcal{D}^3y \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\left[\frac{M}{2}\dot{\mathbf{y}}^2 + \delta(t'-t)\mathbf{Q}\,\mathbf{y}\right]\right\}. \end{aligned} \tag{2.732}$$

The harmonic path integral was solved in one dimension for an arbitrary source $j(t)$ in Eq. (3.168). For $\omega = 0$ and the particular source $j(t) = \delta(t'-t)Q$ the result reads, in three dimensions,

$$\begin{aligned}&\frac{1}{\sqrt{2\pi i\hbar(t_b-t_a)/M}^3}\exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\mathbf{y}_b-\mathbf{y}_a)^2}{t_b-t_a}\right] \\ &\times \exp\left(\frac{i}{\hbar}\frac{1}{t_b-t_a}\left\{[\mathbf{y}_b(t'-t_a)+\mathbf{y}_a(t_b-t')]\,\mathbf{Q} - \frac{1}{2M}(t_b-t')(t'-t_a)\mathbf{Q}^2\right\}\right). \end{aligned} \tag{2.733}$$

Performing here the integral over $\mathbf{y}_a$ yields

$$\exp\left\{\frac{i}{\hbar}\mathbf{Q}\,\mathbf{y}_b\right\}\exp\left\{-\frac{i}{\hbar}\frac{1}{2M}(t_b-t')\mathbf{Q}^2\right\}. \tag{2.734}$$

The integral over $\mathbf{y}_b$ in (2.732) leads now to a δ-function $(2\pi\hbar)^3\delta^{(3)}(\mathbf{Q}-\mathbf{q})$, such that the exponential prefactor in (2.732) is canceled by part of the second factor in (2.734).

In the limit $t_b - t_a \to \infty$, the integral over t' produces a δ-function $2\pi\hbar\delta(\mathbf{p}_b\mathbf{Q}/M + \mathbf{Q}^2/2M) = 2\pi\hbar\delta(E_b - E_a)$ which enforces the conservation of energy. Thus we find the well-known Born approximation

$$\langle \mathbf{p}_b|\hat{S}_1|\mathbf{p}_a\rangle = -2\pi i\delta(E_b-E_a)V(\mathbf{q}). \tag{2.735}$$

In general, we subtract the unscattered particle term (2.731) from (2.729), to obtain a path integral representation for the T-matrix [for the definition recall (1.477)]:

$$\begin{aligned}2\pi\hbar i\delta(E_b-E_a)\langle \mathbf{p}_b|\hat{T}|\mathbf{p}_a\rangle &\equiv -\lim_{t_b-t_a\to\infty} e^{i\mathbf{q}^2 t_b/2M\hbar}\int d^3y_b\, e^{-i\mathbf{q}\mathbf{y}_b/\hbar}\int d^3y_a \\ \times \int \mathcal{D}^3y \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\frac{M}{2}\dot{\mathbf{y}}^2\right) &\left\{\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, V\left(\mathbf{y}+\frac{\mathbf{p}_a}{M}t\right)\right] - 1\right\}. \end{aligned} \tag{2.736}$$

It is preferable to find a formula which does not contain the δ-function of energy conservation as a factor on the left-hand side. In order to remove this we observe that its origin lies in the time-translational invariance of the path integral in the limit $t_b - t_a \to \infty$. If we go over to a shifted time variable $t \to t + t_0$, and change simultaneously $\mathbf{y} \to \mathbf{y} - \mathbf{p}_a t_0/M$, then the path integral remains the same except for shifted initial and final times $t_b + t_0$ and $t_a + t_0$. In the limit $t_b - t_a \to \infty$, the integrals $\int_{t_a+t_0}^{t_b+t_0} dt$ can be replaced again by $\int_{t_a}^{t_b} dt$. The only place where a t_0-dependence remains is in the prefactor $e^{-i\mathbf{q}\mathbf{y}_b/\hbar}$ which changes to $e^{-i\mathbf{q}\mathbf{y}_b/\hbar}e^{i\mathbf{q}\mathbf{p}_a t_0/M\hbar}$. Among all path fluctuations, there exists one degree of freedom which is equivalent to a temporal shift of the path. This is equivalent to an integral over t_0 which yields a δ-function $2\pi\hbar\delta\left(\mathbf{q}\mathbf{p}_a/M\right) = 2\pi\hbar\delta\left(E_b - E_a\right)$. We only must make sure to find the relation between this temporal shift and the corresponding measure in the path integral. This is obviously a shift of the path as a whole in the direction $\hat{\mathbf{p}}_a \equiv \mathbf{p}_a/|\mathbf{p}_a|$. The formal way of isolating this degree of freedom proceeds according to a method developed by Faddeev and Popov[37] by inserting into the path integral (2.729) the following integral representation of unity:

$$1 = \frac{|\mathbf{p}_a|}{M}\int_{-\infty}^{\infty} dt_0\, \delta\left(\hat{\mathbf{p}}_a(\mathbf{y}_b + \mathbf{p}_a t_0/M)\right). \tag{2.737}$$

In the following, we shall drop the subscript a of the incoming beam, writing

$$\mathbf{p} \equiv \mathbf{p}_a, \qquad p \equiv |\mathbf{p}_a| = |\mathbf{p}_b|. \tag{2.738}$$

After the above shift in the path integral, the δ-function in (2.737) becomes $\delta\left(\hat{\mathbf{p}}_a\mathbf{y}_b\right)$ inside the path integral, with no t_0-dependence. The integral over t_0 can now be performed yielding the δ-function in the energy. Removing this from the equation we obtain the path integral representation of the T-matrix

$$\begin{aligned}\langle\mathbf{p}_b|\hat{T}|\mathbf{p}_a\rangle \equiv i\frac{p}{M}\lim_{t_b-t_a\to\infty} e^{i\mathbf{q}^2(t_b-t_a)/8M\hbar}\int d^3y_b\,\delta\left(\hat{\mathbf{p}}_a\mathbf{y}_b\right)\, e^{-i\mathbf{q}\mathbf{y}_b/\hbar}\int d^3y_a \\ \times\int\mathcal{D}^3y\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}dt\,\frac{M}{2}\dot{\mathbf{y}}^2\right)\left\{\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b}dt\,V\left(\mathbf{y}+\frac{\mathbf{P}}{M}t\right)\right]-1\right\}.\end{aligned} \tag{2.739}$$

At this point it is convenient to go over to the velocity representation of the path integral (2.723). This enables us to perform trivially the integral over $\mathbf{y}_b$, and we obtain the $\mathbf{y}$ version of (2.724). The δ-function enforces a vanishing longitudinal component of $\mathbf{y}_b$. The transverse component of $\mathbf{y}_b$ will be denoted by $\mathbf{b}$:

$$\mathbf{b} \equiv \mathbf{y}_b - (\hat{\mathbf{p}}_a\mathbf{y}_b)\hat{\mathbf{p}}/a. \tag{2.740}$$

Hence we find the path integral representation

$$\begin{aligned}\langle\mathbf{p}_b|\hat{T}|\mathbf{p}_a\rangle \equiv i\frac{p}{M}\lim_{t_b-t_a\to\infty} e^{i\mathbf{q}^2 t_b/2M\hbar}\int d^2b\, e^{-i\mathbf{q}\mathbf{b}/\hbar} \\ \times\int\mathcal{D}^3v\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}dt\,\frac{M}{2}\mathbf{v}^2\right)\left[e^{i\chi_{\mathbf{b},\mathbf{p}}[\mathbf{v}]}-1\right],\end{aligned} \tag{2.741}$$

where the effect of the interaction is contained in the scattering phase

$$\chi_{\mathbf{b},\mathbf{p}}[\mathbf{v}] \equiv -\frac{1}{\hbar}\int_{t_a}^{t_b}dt\,V\left(\mathbf{b}+\frac{\mathbf{p}}{M}t-\int_t^{t_b}dt'\,\mathbf{v}(t')\right). \tag{2.742}$$

We can go back to a more conventional path integral by replacing the velocity paths $\mathbf{v}(t)$ by $\dot{\mathbf{y}}(t) = -\int_t^{t_b}\mathbf{v}(t)$. This vanishes at $t = t_b$. Equivalently, we can use paths $\mathbf{z}(t)$ with periodic boundary conditions and subtract from these $\mathbf{z}(t_b) = \mathbf{z}_b$.

From $\langle\mathbf{p}_b|\hat{T}|\mathbf{p}_a\rangle$ we obtain the scattering amplitude $f_{\mathbf{p}_b\mathbf{p}_a}$, whose square gives the differential cross section, by multiplying it with a factor $-M/2\pi\hbar$ [see Eq. (1.497)].

[37] L.D. Faddeev and V.N. Popov, Phys. Lett. B *25*, 29 (1967).

Note that in the velocity representation, the evaluation of the harmonic path integral integrated over $\mathbf{y}_a$ in (2.732) is much simpler than before where we needed the steps (2.733), (2.734). After the Fourier decomposition of $V(\mathbf{x})$ in (2.742), the relevant integral is

$$\int \mathcal{D}^3 v \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt \left[\frac{M}{2}\mathbf{v}^2 - \Theta(t_b - t')\mathbf{Q}\,\mathbf{v}\right]\right\} = e^{-\frac{i}{2M\hbar}\int_{t_a}^{t_b} dt\Theta^2(t_b - t')\mathbf{Q}^2} = e^{-\frac{i}{2M\hbar}(t_b - t')\mathbf{Q}^2}. \tag{2.743}$$

The first factor in (2.734) comes directly from the argument $\mathbf{Y}$ in the Fourier representation of the potential

$$V\left(\mathbf{y}_b + \frac{\mathbf{p}}{M}t - \int_t^{t_b} dt'\,\mathbf{v}(t')\right)$$

in the velocity representation of the S-matrix (2.729).

2.22.2 Improved Formulation

The prefactor $e^{i\mathbf{q}^2 t_b/2M\hbar}$ in Formula (2.741) is an obstacle to taking a more explicit limit $t_b - t_a \to \infty$ on the right-hand side. To overcome this, we represent this factor by an auxiliary path integral[38] over some vector field $\mathbf{w}(t)$:

$$e^{i\mathbf{q}^2 t_b/2M\hbar} = \int \mathcal{D}^3 w \,\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\frac{M}{2}\mathbf{w}^2(t)\right] e^{i\int_{t_a}^{t_b} dt\,\Theta(t)\mathbf{w}(t)\mathbf{q}/\hbar}. \tag{2.744}$$

The last factor changes the exponential $e^{-i\mathbf{q}\mathbf{b}/\hbar}$ in (2.741) into $e^{-i\mathbf{q}\left[\mathbf{b}+\int_{t_a}^{t_b} dt\,\Theta(t)\mathbf{w}(t)\right]/\hbar}$. Since $\mathbf{b}$ is a dummy variable of integration, we can equivalently replace $\mathbf{b} \to \mathbf{b}_\mathbf{w} \equiv \mathbf{b} - \int_{t_a}^{t_b} dt\,\Theta(t)\mathbf{w}(t)$ in the scattering phase $\chi_{\mathbf{b},\mathbf{p}}[\mathbf{v}]$ and remain with

$$\begin{aligned} f_{\mathbf{p}_b\mathbf{p}_a} &= \lim_{t_b - t_a \to \infty} \frac{p}{2\pi i\hbar}\int d^2 b\, e^{-i\mathbf{q}\mathbf{b}/\hbar}\int \mathcal{D}^3 w \\ &\times \int \mathcal{D}^3 v \exp\left[\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\,\frac{M}{2}\left(\mathbf{v}^2 - \mathbf{w}^2\right)\right]\left[\exp\left(i\chi_{\mathbf{b}_\mathbf{w},\mathbf{p}}\right) - 1\right]. \end{aligned} \tag{2.745}$$

The scattering phase in this expression can be calculated from formula (2.742) with the integral taken over the entire t-axis:

$$\chi_{\mathbf{b}_\mathbf{w},\mathbf{p}}[\mathbf{v},\mathbf{w}] = -\frac{1}{\hbar}\int_{-\infty}^{\infty} dt\,V\left(\mathbf{b} + \frac{\mathbf{p}}{M}t - \int_{t_a}^{t_b} dt'\,\left[\Theta(t'-t)\mathbf{v}(t') - \Theta(t')\mathbf{w}(t')\right]\right). \tag{2.746}$$

The fluctuations of $\mathbf{w}(t)$ are necessary to correct for the fact that the outgoing particle does not run, on the average, with the velocity $\mathbf{p}/M = \mathbf{p}_a/M$ but with velocity $\mathbf{p}_b/M = (\mathbf{p}+\mathbf{q})/M$.

We may also go back to a more conventional path integral by inserting $\mathbf{y}(t) = -\int_t^{t_b}\mathbf{v}(t)$ and setting similarly $\mathbf{z}(t) = -\int_t^{t_b}\mathbf{w}(t)$. Then we obtain the alternative representation

$$\begin{aligned} f_{\mathbf{p}_b\mathbf{p}_a} &= \lim_{t_b - t_a \to \infty} \frac{p}{2\pi i\hbar}\int d^2 b\, e^{-i\mathbf{q}\mathbf{b}/\hbar}\int d^3 y_a \int d^3 z_a \\ &\times \int \mathcal{D}^3 y \int \mathcal{D}^3 z \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\frac{M}{2}\left(\dot{\mathbf{y}}^2 - \dot{\mathbf{z}}^2\right)\right]\left[e^{i\chi_{\mathbf{b}_\mathbf{z},\mathbf{p}}[\mathbf{y}]} - 1\right], \end{aligned} \tag{2.747}$$

[38] See R. Rosenfelder, notes of a lecture held at the ETH Zürich in 1979: *Pfadintegrale in der Quantenphysik*, 126 p., PSI Report 97-12, ISSN 1019-0643, and Lecture held at the 7th Int. Conf. on Path Integrals in Antwerpen, *Path Integrals from Quarks to Galaxies*, 2002; Phys. Rev. A **79**, 012701 (2009).

with

$$\chi_{\mathbf{b}_\mathbf{z},\mathbf{p}}[\mathbf{y}] \equiv -\frac{1}{\hbar}\int_{t_a}^{t_b} dt\, V\left(\mathbf{b}+\frac{\mathbf{p}}{M}t+\mathbf{y}(t)-\mathbf{z}(0)\right), \tag{2.748}$$

where the path integrals run over all paths with $\mathbf{y}_b = 0$ and $\mathbf{z}_b = 0$. In Section 3.26 this path integral will be evaluated perturbatively.

2.22.3 Eikonal Approximation to the Scattering Amplitude

To lowest approximation, we neglect the fluctuating variables $\mathbf{y}(t)$ and $\mathbf{z}(t)$ in (2.748). Since the integral

$$\int d^3y_a \int d^3z_a \int \mathcal{D}^3y \int \mathcal{D}^3z \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \frac{M}{2}\left(\dot{\mathbf{y}}^2-\dot{\mathbf{z}}^2\right)\right] \tag{2.749}$$

in (2.747) has unit normalization [recall the calculation of (2.734)], we obtain directly the eikonal approximation to the scattering amplitude

$$f^{\rm ei}_{\mathbf{p}_b\mathbf{p}_a} \equiv \frac{p}{2\pi i\hbar}\int d^2b\, e^{-i\mathbf{qb}/\hbar}\left[\exp\left(i\chi^{\rm ei}_{\mathbf{b},\mathbf{p}}\right)-1\right], \tag{2.750}$$

with

$$\chi^{\rm ei}_{\mathbf{b},\mathbf{p}} \equiv -\frac{1}{\hbar}\int_{-\infty}^{\infty} dt\, V\left(\mathbf{b}+\frac{\mathbf{p}}{M}t\right). \tag{2.751}$$

The time integration can be converted into a line integration along the direction of the incoming particles by introducing a variable $z \equiv pt/M$. Then we can write

$$\chi^{\rm ei}_{\mathbf{b},\mathbf{p}} \equiv -\frac{M}{p}\frac{1}{\hbar}\int_{-\infty}^{\infty} dz\, V\left(\mathbf{b}+\hat{\mathbf{p}}z\right). \tag{2.752}$$

If $V(\mathbf{x})$ is rotationally symmetric, it depends only on $r \equiv |\mathbf{x}|$. Then we shall write the potential as $V(r)$ and calculate (2.752) as the integral

$$\chi^{\rm ei}_{\mathbf{b},\mathbf{p}} \equiv -\frac{M}{p}\frac{1}{\hbar}\int_{-\infty}^{\infty} dz\, V\left(\sqrt{b^2+z^2}\right). \tag{2.753}$$

Inserting this into (2.750), we can perform the integral over all angles between $\mathbf{q}$ and $\mathbf{b}$ using the formula

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\, \exp\left(\frac{i}{\hbar}qb\cos\theta\right) = J_0(qb), \tag{2.754}$$

where $J_0(\xi)$ is the Bessel function, and find

$$f^{\rm ei}_{\mathbf{p}_b\mathbf{p}_a} = \frac{p}{i\hbar}\int db\, b\, J_0(qb)\left[\exp\left(i\chi^{\rm ei}_{\mathbf{b},\mathbf{p}}\right)-1\right]. \tag{2.755}$$

The variable of integration b coincides with the impact parameter b introduced in Eq. (1.500). The result (2.755) is precisely the eikonal approximation (1.500) with $\chi^{\rm ei}_{\mathbf{b},\mathbf{p}}/2$ playing the role of the scattering phases $\delta_l(p)$ of angular momentum $l = pb/\hbar$:

$$\chi^{\rm ei}_{\mathbf{b},\mathbf{p}} = 2i\delta_{pb/\hbar}(p). \tag{2.756}$$

2.23 Heisenberg Operator Approach to Time Evolution Amplitude

An interesting alternative to the path integral derivation of the time evolution amplitudes of harmonic systems is based on quantum mechanics in the Heisenberg picture. It bears a close similarity with the path integral derivation in that it requires solving the classical equations of motion with given initial and final positions to obtain the exponential of the classical action $e^{i\mathcal{A}/\hbar}$. The fluctuation factor, however, which accompanies this exponential is obtained quite differently from commutation rules of the operatorial orbits at different times as we shall now demonstrate.

2.23.1 Free Particle

We want to calculate the matrix element of the time evolution operator

$$(\mathbf{x}\, t|\mathbf{x}'\, 0) = \langle \mathbf{x}|e^{-i\hat{H}t/\hbar}|\mathbf{x}'\rangle, \tag{2.757}$$

where $\hat{H}$ is the Hamiltonian operator

$$\hat{H} = H(\hat{\mathbf{p}}) = \frac{\hat{\mathbf{p}}^2}{2M}. \tag{2.758}$$

We shall calculate the time evolution amplitude (2.757) by solving the differential equation

$$\begin{aligned} i\hbar\partial_t\langle \mathbf{x}\, t|\mathbf{x}'\, 0\rangle &\equiv \langle \mathbf{x}|\hat{H}\, e^{-i\hat{H}t/\hbar}|\mathbf{x}'\rangle = \langle \mathbf{x}|e^{-i\hat{H}t/\hbar}\left[e^{i\hat{H}t/\hbar}\hat{H}\, e^{-i\hat{H}t/\hbar}\right]|\mathbf{x}'\rangle \\ &= \langle \mathbf{x}\, t|H(\hat{\mathbf{p}}(t))|\mathbf{x}'\, 0\rangle. \end{aligned} \tag{2.759}$$

The argument contains now the time-dependent Heisenberg picture of the operator $\hat{\mathbf{p}}$. The evaluation of the right-hand side will be based on re-expressing the operator $H(\hat{\mathbf{p}}(t))$ as a function of initial and final position operators in such a way that all final position operators stand to the left of all initial ones:

$$\hat{H} = H(\hat{\mathbf{x}}(t), \hat{\mathbf{x}}(0); t). \tag{2.760}$$

Then the matrix elements on the right-hand side can immediately be evaluated using the eigenvalue equations

$$\langle \mathbf{x}\, t|\hat{\mathbf{x}}(t) = \mathbf{x}\langle \mathbf{x}\, t|, \qquad \hat{\mathbf{x}}(0)|\mathbf{x}'\, 0\rangle = \mathbf{x}'|\mathbf{x}'\, 0\rangle, \tag{2.761}$$

as being

$$\langle \mathbf{x}\, t|H(\hat{\mathbf{x}}(t), \hat{\mathbf{x}}(0); t)|\hat{\mathbf{x}}\, 0\rangle = H(\mathbf{x}, \mathbf{x}'; t)\langle \mathbf{x}\, t|\mathbf{x}'\, 0\rangle, \tag{2.762}$$

and the differential equation (2.759) becomes

$$i\hbar\partial_t\langle \mathbf{x}\, t|\mathbf{x}'\, 0\rangle \equiv H(\mathbf{x}, \mathbf{x}'; t)\langle \mathbf{x}\, t|\mathbf{x}'\, 0\rangle, \tag{2.763}$$

or

$$\langle \mathbf{x}\, t|\mathbf{x}'\, 0\rangle = C(\mathbf{x}, \mathbf{x}')E(\mathbf{x}, \mathbf{x}'; t) \equiv C(\mathbf{x}, \mathbf{x}')e^{-i\int_t dt'\, H(\mathbf{x}, \mathbf{x}'; t')/\hbar}. \tag{2.764}$$

The prefactor $C(\mathbf{x}, \mathbf{x}')$ contains a possible constant of integration resulting from the time integral in the exponent.

The Hamiltonian operator is brought to the time-ordered form (2.760) by solving the Heisenberg equations of motion

$$\frac{d\hat{\mathbf{x}}(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{\mathbf{x}}(t)\right] = \frac{\hat{\mathbf{p}}(t)}{M}, \tag{2.765}$$

$$\frac{d\hat{\mathbf{p}}(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{\mathbf{p}}(t)\right] = 0. \tag{2.766}$$

The second equation shows that the momentum is time-independent:

$$\hat{\mathbf{p}}(t) = \hat{\mathbf{p}}(0), \tag{2.767}$$

so that the first equation is solved by

$$\hat{\mathbf{x}}(t) - \hat{\mathbf{x}}(0) = t\,\frac{\hat{\mathbf{p}}(t)}{M}, \tag{2.768}$$

which brings (2.758) to

$$\hat{H} = \frac{M}{2t^2}\left[\hat{\mathbf{x}}(t) - \hat{\mathbf{x}}(0)\right]^2. \tag{2.769}$$

This is not yet the desired form (2.760) since there is one factor which is not time-ordered. The proper order is achieved by rewriting $\hat{H}$ as

$$\hat{H} = \frac{M}{2t^2}\left\{\hat{\mathbf{x}}^2(t) - 2\hat{\mathbf{x}}(t)\hat{\mathbf{x}}(0) + \hat{\mathbf{x}}^2(0) + [\hat{\mathbf{x}}(t), \hat{\mathbf{x}}(0)]\right\}, \tag{2.770}$$

and calculating the commutator from Eq. (2.768) and the canonical commutation rule $[\hat{p}_i, \hat{x}_j] = -i\hbar\delta_{ij}$ as

$$[\hat{\mathbf{x}}(t), \hat{\mathbf{x}}(0)] = -\frac{i\hbar}{M}Dt, \tag{2.771}$$

so that we find the desired expression

$$\hat{H} = H(\hat{\mathbf{x}}(t), \hat{\mathbf{x}}(0); t) = \frac{M}{2t^2}\left[\hat{\mathbf{x}}^2(t) - 2\hat{\mathbf{x}}(t)\hat{\mathbf{x}}(0) + \hat{\mathbf{x}}^2(0)\right] - i\hbar\frac{D}{2t}. \tag{2.772}$$

Its matrix elements (2.762) can now immediately be written down:

$$H(\mathbf{x}, \mathbf{x}'; t) = \frac{M}{2t^2}\left(\mathbf{x} - \mathbf{x}'\right)^2 - i\hbar\frac{D}{2t}. \tag{2.773}$$

From this we find directly the exponential factor in (2.764)

$$E(\mathbf{x}, \mathbf{x}'; t) = e^{-i\int dt\, H(\mathbf{x}, \mathbf{x}'; t)/\hbar} = \exp\left[\frac{i}{\hbar}\frac{M}{2t}\left(\mathbf{x} - \mathbf{x}'\right)^2 - \frac{D}{2}\log t\right]. \tag{2.774}$$

Inserting (2.774) into Eq. (2.764), we obtain

$$\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle = C(\mathbf{x}, \mathbf{x}')\,\frac{1}{t^{D/2}}\exp\left[\frac{i}{\hbar}\frac{M}{2t}\left(\mathbf{x} - \mathbf{x}'\right)^2\right]. \tag{2.775}$$

A possible constant of integration in (2.774) depending on $\mathbf{x}, \mathbf{x}'$ is absorbed in the prefactor $C(\mathbf{x}, \mathbf{x}')$. This is fixed by differential equations involving $\mathbf{x}$:

$$\begin{aligned}
-i\hbar\boldsymbol{\nabla}\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle &= \langle \mathbf{x}|\hat{\mathbf{p}}e^{-i\hat{H}t/\hbar}|\mathbf{x}'\rangle = \langle \mathbf{x}|e^{-i\hat{H}t}\left[e^{i\hat{H}t/\hbar}\hat{\mathbf{p}}e^{-i\hat{H}t/\hbar}\right]|\mathbf{x}'\rangle = \langle \mathbf{x}\, t|\hat{\mathbf{p}}(t)|\mathbf{x}'\, 0\rangle. \\
i\hbar\boldsymbol{\nabla}'\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle &= \langle \mathbf{x}|e^{-i\hat{H}t/\hbar}\hat{\mathbf{p}}|\mathbf{x}'\rangle\langle \mathbf{x}\, t|\hat{\mathbf{p}}(0)|\mathbf{x}'\, 0\rangle.
\end{aligned} \tag{2.776}$$

Inserting (2.768) and using the momentum conservation (2.767), these become

$$\begin{aligned}
-i\hbar\boldsymbol{\nabla}\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle &= \frac{M}{t}(\mathbf{x} - \mathbf{x}')\,\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle, \\
i\hbar\boldsymbol{\nabla}'\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle &= \frac{M}{t}(\mathbf{x} - \mathbf{x}')\,\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle.
\end{aligned} \tag{2.777}$$

Inserting here the previous result (2.775), we obtain the conditions

$$-i\boldsymbol{\nabla}C(\mathbf{x}, \mathbf{x}') = 0, \quad i\boldsymbol{\nabla}'C(\mathbf{x}, \mathbf{x}') = 0, \tag{2.778}$$

which are solved only by a constant C. The constant, in turn, is fixed by the initial condition

$$\lim_{t\to 0}\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle = \delta^{(D)}(\mathbf{x} - \mathbf{x}'), \tag{2.779}$$

to be

$$C = \sqrt{\frac{M}{2\pi i\hbar}}^{D}, \tag{2.780}$$

so that we find the correct free-particle amplitude (2.74)

$$\langle \mathbf{x}\, t | \mathbf{x}'\, 0\rangle \equiv \sqrt{\frac{M}{2\pi i\hbar t}}^{D}\exp\left[\frac{i}{\hbar}\frac{M}{2t}(\mathbf{x} - \mathbf{x}')^2\right]. \tag{2.781}$$

Note that the fluctuation factor $1/t^{D/2}$ emerges in this approach as a consequence of the commutation relation (2.771).

2.23.2 Harmonic Oscillator

Here we are dealing with the Hamiltonian operator

$$\hat{H} = H(\hat{\mathbf{p}}, \hat{\mathbf{x}}) = \frac{\hat{\mathbf{p}}^2}{2M} + \frac{M\omega^2}{2}\mathbf{x}^2, \tag{2.782}$$

which has to be brought again to the time-ordered form (2.760). We must now solve the Heisenberg equations of motion

$$\frac{d\hat{\mathbf{x}}(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{\mathbf{x}}(t)\right] = \frac{\hat{\mathbf{p}}(t)}{M}, \tag{2.783}$$

$$\frac{d\hat{\mathbf{p}}(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{\mathbf{p}}(t)\right] = -M\omega^2\hat{\mathbf{x}}(t). \tag{2.784}$$

By solving these equations we obtain [compare (2.158)]

$$\hat{\mathbf{p}}(t) = M\frac{\omega}{\sin\omega t}\left[\hat{\mathbf{x}}(t)\cos\omega t - \hat{\mathbf{x}}(0)\right]. \tag{2.785}$$

Inserting this into (2.782), we obtain

$$\hat{H} = \frac{M\omega^2}{2\sin^2\omega t}\left\{\left[\hat{\mathbf{x}}(t)\cos\omega t - \hat{\mathbf{x}}(0)\right]^2 + \sin^2\omega t\,\hat{\mathbf{x}}^2(t)\right\}, \tag{2.786}$$

which is equal to

$$\hat{H} = \frac{M\omega^2}{2\sin^2\omega t}\left\{\hat{\mathbf{x}}^2(t) + \hat{\mathbf{x}}^2(0) - 2\cos\omega t\,\hat{\mathbf{x}}(t)\hat{\mathbf{x}}(0) + \cos\omega t\,\left[\hat{\mathbf{x}}(t), \hat{\mathbf{x}}(0)\right]\right\}. \tag{2.787}$$

By commuting Eq. (2.785) with $\hat{\mathbf{x}}(t)$, we find the commutator [compare (2.771)]

$$\left[\hat{\mathbf{x}}(t), \hat{\mathbf{x}}(0)\right] = -\frac{i\hbar}{M}D\frac{\sin\omega t}{\omega}, \tag{2.788}$$

so that we find the matrix elements of the Hamiltonian operator in the form (2.762) [compare (2.773)]

$$H(\mathbf{x}, \mathbf{x}'; t) = \frac{M\omega^2}{2\sin^2\omega t}\left(\mathbf{x}^2 + \mathbf{x}'^2 - 2\cos\omega t\,\mathbf{x}\mathbf{x}'\right) - i\hbar\frac{D}{2}\omega\cot\omega t. \tag{2.789}$$

This has the integral [compare (2.774)]

$$\int dt\,H(\mathbf{x}, \mathbf{x}'; t) = -\frac{M\omega}{2\sin\omega t}\left[\left(\mathbf{x}^2 + \mathbf{x}'^2\right)\cos\omega t - 2\,\mathbf{x}\,\mathbf{x}'\right] - i\hbar\,\frac{D}{2}\log\frac{\sin\omega t}{\omega}. \tag{2.790}$$

Inserting this into Eq. (2.764), we find precisely the harmonic oscillator amplitude (2.177), apart from the factor $C(\mathbf{x}, \mathbf{x}')$. This is again determined by the differential equations (2.776), leaving only a simple normalization factor fixed by the initial condition (2.779) with the result (2.780).

Again, the fluctuation factor has its origin in the commutator (2.788).

2.23.3 Charged Particle in Magnetic Field

We now turn to a charged particle in three dimensions in a magnetic field treated in Section 2.18, where the Hamiltonian operator is most conveniently expressed in terms of the operator of the covariant momentum (2.644),

$$\hat{\mathbf{P}} \equiv \hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}(\hat{\mathbf{x}}), \tag{2.791}$$

as [compare (2.643)]

$$\hat{H} = H(\hat{\mathbf{p}}, \hat{\mathbf{x}}) = \frac{\hat{\mathbf{P}}^2}{2M}. \tag{2.792}$$

In the presence of a magnetic field, its components do not commute but satisfy the commutation rules:

$$[\hat{P}_i, \hat{P}_j] = -\frac{e}{c}\,[\hat{p}_i, \hat{A}_j] - \frac{e}{c}\,[\hat{A}_i, \hat{p}_j] = i\,\frac{e\hbar}{c}\,(\nabla_i A_j - \nabla_j A_i) = i\,\frac{e\hbar}{c} B_{ij}, \tag{2.793}$$

where $B_{ij} = \epsilon_{ijk} B_K$ is the usual antisymmetric tensor representation of the magnetic field.

We now have to solve the Heisenberg equations of motion

$$\frac{d\hat{\mathbf{x}}(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{\mathbf{x}}\,(t)\right] = \frac{\hat{\mathbf{P}}(t)}{M} \tag{2.794}$$

$$\frac{d\hat{\mathbf{P}}(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{\mathbf{P}}(t)\right] = \frac{e}{Mc} B(\hat{\mathbf{x}}(t))\hat{\mathbf{P}}(t) + i\frac{e\hbar}{Mc}\nabla_j B_{ji}(\hat{\mathbf{x}}(t)), \tag{2.795}$$

where $B(\hat{\mathbf{x}}(t))\hat{\mathbf{P}}(t)$ is understood as the product of the matrix $B_{ij}(\hat{\mathbf{x}}(t))$ with the vector $\hat{\mathbf{P}}$. In a *constant* field, where $B_{ij}(\hat{\mathbf{x}}(t))$ is a constant matrix B_{ij}, the last term in the second equation is absent and we find directly the solution

$$\hat{\mathbf{P}}(t) = e^{\Omega_L t}\hat{\mathbf{P}}(0), \tag{2.796}$$

where Ω_L is a matrix version of the Landau frequency (2.648)

$$\Omega_{L\,ij} \equiv \frac{e}{Mc} B_{ij}, \tag{2.797}$$

which can also be rewritten with the help of the Landau frequency vector

$$\boldsymbol{\omega}_L \equiv \frac{e}{Mc}\mathbf{B} \tag{2.798}$$

and the 3×3-generators of the rotation group

$$(L_k)_{ij} \equiv -i\epsilon_{kij} \tag{2.799}$$

as

$$\Omega_L = i\,\mathbf{L}\cdot\boldsymbol{\omega}_L. \tag{2.800}$$

Inserting this into Eq. (2.794), we find

$$\hat{\mathbf{x}}(t) = \hat{\mathbf{x}}(0) + \frac{e^{\Omega_L t} - 1}{\Omega_L}\frac{\hat{\mathbf{P}}(0)}{M}, \tag{2.801}$$

where the matrix on the right-hand side is again defined by a power series expansion

$$\frac{e^{\Omega_L t} - 1}{\Omega_L} = t + \Omega_L\,\frac{t^2}{2} + \Omega_L^2\,\frac{t^3}{3!} + \dots\ . \tag{2.802}$$

We can invert (2.801) to find

$$\frac{\hat{\mathbf{P}}(0)}{M} = \frac{\Omega_L/2}{\sinh \Omega_L t/2} e^{-\Omega_L t/2}\left[\hat{\mathbf{x}}(t) - \hat{\mathbf{x}}(0)\right]. \tag{2.803}$$

Using (2.796), this implies

$$\hat{\mathbf{P}}(t) = MN(\Omega_L t)\left[\hat{\mathbf{x}}(t) - \hat{\mathbf{x}}(0)\right], \tag{2.804}$$

with the matrix

$$N(\Omega_L t) \equiv \frac{\Omega_L/2}{\sinh \Omega_L t/2} e^{\Omega_L t/2}. \tag{2.805}$$

By squaring (2.804) we obtain

$$\frac{\hat{\mathbf{P}}^2(t)}{2M} = \frac{M}{2} \left[\hat{\mathbf{x}}(t) - \hat{\mathbf{x}}(0)\right]^T K(\Omega_L t) \left[\hat{\mathbf{x}}(t) - \hat{\mathbf{x}}(0)\right], \tag{2.806}$$

where

$$K(\Omega_L t) = N^T(\Omega_L t) N(\Omega_L t). \tag{2.807}$$

Using the antisymmetry of the matrix Ω_L, we can rewrite this as

$$K(\Omega_L t) = N(-\Omega_L t) N(\Omega_L t) = \frac{\Omega_L^2/4}{\sinh^2 \Omega_L t/2}. \tag{2.808}$$

The commutator between two operators $\hat{\mathbf{x}}(t)$ at different times is, due to Eq. (2.801),

$$[\hat{\mathbf{x}}_i(t), \hat{\mathbf{x}}_j(0)] = -\frac{i}{M} \left(\frac{e^{\Omega_L t} - 1}{\Omega_L}\right)_{ij}, \tag{2.809}$$

and

$$\begin{aligned} \left[\hat{\mathbf{x}}_i(t), \hat{\mathbf{x}}_j(0)\right] + [\hat{\mathbf{x}}_j(t), \hat{\mathbf{x}}_i(0)] &= -\frac{i}{M} \left(\frac{e^{\Omega_L t} - 1}{\Omega_L} + \frac{e^{\Omega_L^T t} - 1}{\Omega_L^T}\right)_{ij} \\ = \quad -\frac{i}{M} \left(\frac{e^{\Omega_L t} - e^{-\Omega_L t}}{\Omega_L}\right)_{ij} &= -2\frac{i}{M} \left[\frac{\sinh \Omega_L t}{\Omega_L}\right]_{ij}. \end{aligned} \tag{2.810}$$

Respecting this, we can expand (2.806) in powers of operators $\hat{\mathbf{x}}(t)$ and $\hat{\mathbf{x}}(0)$, thereby time-ordering the later operators to the left of the earlier ones as follows:

$$\begin{aligned} H(\hat{\mathbf{x}}(t), \hat{\mathbf{x}}(0)) &= \frac{M}{2} \left[\hat{\mathbf{x}}^T(t) K(\Omega_L t) \hat{\mathbf{x}}(t) - 2\hat{\mathbf{x}}^T K(\Omega_L t) \hat{\mathbf{x}}(0) + \hat{\mathbf{x}}^T K(\Omega_L t) \hat{\mathbf{x}}(0)\right] \\ &- \frac{i\hbar}{2} \mathrm{tr} \left[\frac{\Omega_L}{2} \coth \frac{\Omega_L t}{2}\right]. \end{aligned} \tag{2.811}$$

This has to be integrated in t, for which we use the formulas

$$\int dt\, K(\Omega_L t) = \int dt\, \frac{\Omega_L^2/2}{\sinh^2 \Omega_L t/2} = -\frac{\Omega_L}{2} \coth \frac{\Omega_L t}{2}, \tag{2.812}$$

and

$$\int dt\, \frac{1}{2}\, \mathrm{tr} \left[\frac{\Omega_L}{2} \coth \frac{\Omega_L t}{2}\right] = \mathrm{tr} \log \frac{\sinh \Omega_L t/2}{\Omega_L/2} = \mathrm{tr} \log \frac{\sinh \Omega_L t/2}{\Omega_L t/2} + 3 \log t, \tag{2.813}$$

these results following again from a Taylor expansion of both sides. The factor 3 in the last term is due to the three-dimensional trace. We can then immediately write down the exponential factor $E(\mathbf{x}, \mathbf{x}'; t)$ in (2.764):

$$E(\mathbf{x}, \mathbf{x}'; t) = \frac{1}{t^{3/2}} \exp \left\{\frac{i}{\hbar} \frac{M}{2} (\mathbf{x} - \mathbf{x}')^T \left(\frac{\Omega_L}{2} \coth \frac{\Omega_L t}{2}\right) (\mathbf{x} - \mathbf{x}') - \frac{1}{2} \mathrm{tr} \log \frac{\sinh \Omega_L t/2}{\Omega_L t/2}\right\}. \tag{2.814}$$

The last term gives rise to a prefactor

$$\left[\det \frac{\sinh \Omega_L t/2}{\Omega_L t/2}\right]^{-1/2}. \tag{2.815}$$

As before, the time-independent integration factor $C(\mathbf{x},\mathbf{x}')$ in (2.764) is fixed by differential equations in $\mathbf{x}$ and $\mathbf{x}'$, which involve here the covariant derivatives:

$$\begin{aligned}\left[-i\hbar\boldsymbol{\nabla}-\frac{e}{c}\mathbf{A}(\mathbf{x})\right]\langle\mathbf{x}\,t|\mathbf{x}'\,0\rangle &= \langle\mathbf{x}|\hat{\mathbf{P}}e^{-i\hat{H}t/\hbar}|\mathbf{x}'\rangle=\langle\mathbf{x}|e^{-i\hat{H}t/\hbar}\left[e^{i\hat{H}t/\hbar}\hat{\mathbf{P}}e^{-i\hat{H}t/\hbar}\right]|\mathbf{x}'\rangle\\ &= \langle\mathbf{x}\,t|\hat{\mathbf{P}}(t)|\mathbf{x}'\,0\rangle=L(\Omega_Lt)(\mathbf{x}-\mathbf{x}')\langle\mathbf{x}\,t|\mathbf{x}'\,0\rangle, \qquad (2.816)\\ \left[\;i\hbar\boldsymbol{\nabla}'-\frac{e}{c}\mathbf{A}(\mathbf{x})\right]\langle\mathbf{x}\,t|\mathbf{x}'\,0\rangle &= \langle\mathbf{x}|e^{-i\hat{H}t/\hbar}\hat{\mathbf{P}}|\mathbf{x}'\rangle\\ &= \langle\mathbf{x}\,t|\hat{\mathbf{P}}(0)|\mathbf{x}'\,0\rangle=L(\Omega_Lt)(\mathbf{x}-\mathbf{x}')\langle\mathbf{x}\,t|\mathbf{x}'\,0\rangle. \qquad (2.817)\end{aligned}$$

Calculating the partial derivative we find

$$\begin{aligned}-i\hbar\boldsymbol{\nabla}\langle\mathbf{x}\,t|\mathbf{x}'\,0\rangle &=[-i\hbar\boldsymbol{\nabla}C(\mathbf{x},\mathbf{x}')]E(\mathbf{x},\mathbf{x}';t)+C(\mathbf{x},\mathbf{x}')[-i\hbar\boldsymbol{\nabla}E(\mathbf{x},\mathbf{x}';t)]\\ &=[-i\hbar\boldsymbol{\nabla}C(\mathbf{x},\mathbf{x}')]E(\mathbf{x},\mathbf{x}';t)+C(\mathbf{x},\mathbf{x}')M\left(\frac{\Omega_L}{2}\coth\frac{\Omega_Lt}{2}\right)(\mathbf{x}-\mathbf{x}')E(\mathbf{x},\mathbf{x}';t).\end{aligned}$$

Subtracting the right-hand side of (2.816) leads to

$$M\left(\frac{\Omega_L}{2}\coth\frac{\Omega_Lt}{2}\right)(\mathbf{x}-\mathbf{x}')-ML(\Omega_Lt)(\mathbf{x}-\mathbf{x}')=-\frac{M}{2}\Omega_L(\mathbf{x}-\mathbf{x}'), \qquad (2.818)$$

so that $C(\mathbf{x},\mathbf{x}')$ satisfies the time-independent differential equation

$$\left[-i\hbar\boldsymbol{\nabla}-\frac{e}{c}A(\mathbf{x})-\frac{M}{2}\Omega_L(\mathbf{x}-\mathbf{x}')\right]C(\mathbf{x},\mathbf{x}')=0. \qquad (2.819)$$

A similar equation is found from the second equation (2.817):

$$\left[\quad i\hbar\boldsymbol{\nabla}'-\frac{e}{c}A(\mathbf{x})-\frac{M}{2}\Omega_L(\mathbf{x}-\mathbf{x}')\right]C(\mathbf{x},\mathbf{x}')=0. \qquad (2.820)$$

These equations are solved by

$$C(\mathbf{x},\mathbf{x}')=C\,\exp\left\{\frac{i}{\hbar}\int_{\mathbf{x}'}^{\mathbf{x}}d\boldsymbol{\xi}\left[\frac{e}{c}\mathbf{A}(\boldsymbol{\xi})+\frac{M}{2}\Omega_L(\boldsymbol{\xi}-\mathbf{x}')\right]\right\}. \qquad (2.821)$$

The contour of integration is arbitrary since the vector field in brackets,

$$\frac{e}{c}\mathbf{A}'(\boldsymbol{\xi})\equiv\frac{e}{c}\mathbf{A}(\boldsymbol{\xi})+\frac{\Omega_L}{2}(\boldsymbol{\xi}-\mathbf{x}')=\frac{e}{c}\left[\mathbf{A}(\boldsymbol{\xi})-\frac{1}{2}\mathbf{B}\times(\boldsymbol{\xi}-\mathbf{x}')\right] \qquad (2.822)$$

has a vanishing curl, $\boldsymbol{\nabla}\times\mathbf{A}'(\mathbf{x})=0$. We can therefore choose the contour to be a straight line connecting $\mathbf{x}'$ and $\mathbf{x}$, in which case $d\boldsymbol{\xi}$ points in the same direction of $\mathbf{x}-\mathbf{x}'$ as $\boldsymbol{\xi}-\mathbf{x}'$ so that the cross product vanishes. Hence we may write for a straight-line connection the Ω_L-term

$$C(\mathbf{x},\mathbf{x}')=C\,\exp\left\{i\,\frac{e}{c}\int_{\mathbf{x}'}^{\mathbf{x}}d\boldsymbol{\xi}\,\mathbf{A}(\boldsymbol{\xi})\right\}. \qquad (2.823)$$

Finally, the normalization constant C is fixed by the initial condition (2.779) to have the value (2.780).

Collecting all terms, the amplitude is

$$\begin{aligned}\langle\mathbf{x}\,t|\mathbf{x}'\,0\rangle &= \frac{1}{\sqrt{2\pi i\hbar^2t/M}^{\,3}}\left[\det\frac{\sinh\Omega_Lt/2}{\Omega_Lt/2}\right]^{-1/2}\exp\left\{i\,\frac{e}{c}\int_{\mathbf{x}'}^{\mathbf{x}}d\boldsymbol{\xi}\,\mathbf{A}(\boldsymbol{\xi})\right\}\\ &\times\;\exp\left\{\frac{i}{\hbar}\frac{M}{2}(\mathbf{x}-\mathbf{x}')^T\left(\frac{\Omega_L}{2}\coth\frac{\Omega_Lt}{2}\right)(\mathbf{x}-\mathbf{x}')\right\}. \qquad (2.824)\end{aligned}$$

All expressions simplify if we assume the magnetic field to point in the z-direction, in which case the frequency matrix becomes

$$\Omega_L = \begin{pmatrix} 0 & \omega_L & 0 \\ -\omega_L & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{2.825}$$

so that

$$\cos\frac{\Omega_L t}{2} = \begin{pmatrix} \cos\omega_L t/2 & 0 & 0 \\ 0 & \cos\omega_L t/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2.826}$$

and

$$\frac{\sinh\Omega_L t/2}{\Omega_L t/2} = \begin{pmatrix} 0 & \sin\omega_L t/2 & 0 \\ -\sin\omega_L t/2 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2.827}$$

whose determinant is

$$\det\frac{\sinh\Omega_L t/2}{\Omega_L t/2} = \left(\frac{\sinh\omega_L t/2}{\omega_L t/2}\right)^2. \tag{2.828}$$

Let us calculate the exponential involving the vector potential in (2.824) explicitly. We choose the gauge in which the vector potential points in the y-direction [recall (2.636)], and parametrize the straight line between $\mathbf{x}'$ and $\mathbf{x}$ as

$$\boldsymbol{\xi} = \mathbf{x}' + s(\mathbf{x} - \mathbf{x}'), \qquad s \in [0,1]. \tag{2.829}$$

Then we find

$$\begin{aligned} \int_{\mathbf{x}'}^{\mathbf{x}} d\boldsymbol{\xi}\, \mathbf{A}(\boldsymbol{\xi}) &= B(y-y')\int_0^1 ds\,[x' + s(x-x')] = B(y-y')(x+x') \\ &= B(xy - x'y') + B(x'y - xy'). \end{aligned} \tag{2.830}$$

Inserting this and (2.828) into (2.764), we recover the earlier result (2.668).

Appendix 2A Baker-Campbell-Hausdorff Formula and Magnus Expansion

The standard Baker-Campbell-Hausdorff formula, from which our formula (2.9) can be derived, reads

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{C}}, \tag{2A.1}$$

where

$$\hat{C} = \hat{B} + \int_0^1 dt g(e^{\mathrm{ad}\,A\,t}e^{\mathrm{ad}\,B})[\hat{A}], \tag{2A.2}$$

and $g(z)$ is the function

$$g(z) \equiv \frac{\log z}{z-1} = \sum_{n=0}^{\infty}\frac{(1-z)^n}{n+1}, \tag{2A.3}$$

and $\mathrm{ad}\,B$ is the operator associated with $\hat{B}$ in the so-called *adjoint representation*, which is defined by

$$\mathrm{ad}\,B[\hat{A}] \equiv [\hat{B},\hat{A}]. \tag{2A.4}$$

One also defines the trivial adjoint operator $(\mathrm{ad}\,B)^0[\hat{A}] = 1[\hat{A}] \equiv \hat{A}$. By expanding the exponentials in Eq. (2A.2) and using the power series (2A.3), one finds the explicit formula

$$\hat{C} = \hat{B} + \hat{A} + \sum_{n=1}^{\infty} \frac{(-1)^n}{n+1} \sum_{p_i,q_i;p_i+q_i\ge 1} \frac{1}{1+\sum_{i=1}^{n} p_i} \times \frac{(\mathrm{ad}\,A)^{p_1}}{p_1!}\frac{(\mathrm{ad}\,B)^{q_1}}{q_1!}\cdots\frac{(\mathrm{ad}\,A)^{p_n}}{p_n!}\frac{(\mathrm{ad}\,B)^{q_n}}{q_n!}[\hat{A}]. \tag{2A.5}$$

The lowest expansion terms are

$$\begin{aligned} \hat{C} &= \hat{B} + \hat{A} - \frac{1}{2}\left[\tfrac{1}{2}\mathrm{ad}\,A + \mathrm{ad}\,B + \tfrac{1}{6}(\mathrm{ad}\,A)^2 + \tfrac{1}{2}\mathrm{ad}\,A\,\mathrm{ad}\,B + \tfrac{1}{2}(\mathrm{ad}\,B)^2 + \ldots\right][\hat{A}] \\ &\quad + \frac{1}{3}\left[\tfrac{1}{3}(\mathrm{ad}\,A)^2 + \tfrac{1}{2}\mathrm{ad}\,A\,\mathrm{ad}\,B + \tfrac{1}{2}\mathrm{ad}\,B\,\mathrm{ad}\,A + (\mathrm{ad}\,B)^2 + \ldots\right][\hat{A}] \\ &= \hat{A} + \hat{B} + \frac{1}{2}[\hat{A},\hat{B}] + \frac{1}{12}([\hat{A},[\hat{A},\hat{B}]] + [\hat{B},[\hat{B},\hat{A}]]) + \frac{1}{24}[\hat{A},[[\hat{A},\hat{B}],\hat{B}]] \ldots . \end{aligned} \tag{2A.6}$$

The result can be rearranged to the closely related *Zassenhaus formula*

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}\, e^{\hat{Z}_2}e^{\hat{Z}_3}e^{\hat{Z}_4}\cdots , \tag{2A.7}$$

where

$$\hat{Z}_2 = \frac{1}{2}[\hat{B},\hat{A}] \tag{2A.8}$$

$$\hat{Z}_3 = -\frac{1}{3}[\hat{B},[\hat{B},\hat{A}]] - \frac{1}{6}[\hat{A},[\hat{B},\hat{A}]]) \tag{2A.9}$$

$$\hat{Z}_4 = \frac{1}{8}\Big([[[\hat{B},\hat{A}],\hat{B}],\hat{B}] + [[[\hat{B},\hat{A}],\hat{A}],\hat{B}]\Big) + \frac{1}{24}[[[\hat{B},\hat{A}],\hat{A}],\hat{A}] \tag{2A.10}$$

$$\vdots \quad .$$

To prove formula (2A.2) and thus the expansion (2A.6), we proceed similar to the derivation of the interaction formula (1.295) by deriving and solving a differential equation for the operator function

$$\hat{C}(t) = \log(e^{\hat{A}t}e^{\hat{B}}). \tag{2A.11}$$

Its value at $t = 1$ will supply us with the desired result $\hat{C}$ in (2A.5). The starting point is the observation that for any operator $\hat{M}$,

$$e^{\hat{C}(t)}\hat{M}e^{-\hat{C}(t)} = e^{\mathrm{ad}\,C(t)}[\hat{M}], \tag{2A.12}$$

by definition of $\mathrm{ad}\,C$. Inserting (2A.11), the left-hand side can also be rewritten as $e^{\hat{A}t}e^{\hat{B}}\hat{M}e^{-\hat{B}}e^{-\hat{A}t}$, which in turn is equal to $e^{\mathrm{ad}\,A\,t}e^{\mathrm{ad}\,B}[\hat{M}]$, by definition (2A.4). Hence we have

$$e^{\mathrm{ad}\,C(t)} = e^{\mathrm{ad}\,A\,t}e^{\mathrm{ad}\,B}. \tag{2A.13}$$

Differentiation of (2A.11) yields

$$e^{\hat{C}(t)}\frac{d}{dt}e^{-\hat{C}(t)} = -\hat{A}. \tag{2A.14}$$

The left-hand side, on the other hand, can be rewritten in general as

$$e^{\hat{C}(t)}\frac{d}{dt}e^{-\hat{C}(t)} = -f(\mathrm{ad}\,C(t))[\dot{\hat{C}}(t)], \tag{2A.15}$$

where

$$f(z) \equiv \frac{e^z - 1}{z}. \tag{2A.16}$$

This will be verified below. It implies that

$$f(\text{ad}\,C(t))[\dot{\hat{C}}(t)] = \hat{A}. \tag{2A.17}$$

We now define the function $g(z)$ as in (2A.3) and see that it satisfies

$$g(e^z)f(z) \equiv 1. \tag{2A.18}$$

We therefore have the trivial identity

$$\dot{\hat{C}}(t) = g(e^{\text{ad}\,C(t)})f(\text{ad}\,C(t))[\dot{\hat{C}}(t)]. \tag{2A.19}$$

Using (2A.17) and (2A.13), this turns into the differential equation

$$\dot{\hat{C}}(t) = g(e^{\text{ad}\,C(t)})[\hat{A}] = e^{\text{ad}\,A\,t}e^{\text{ad}\,B}[\hat{A}], \tag{2A.20}$$

from which we find directly the result (2A.2).

To complete the proof we must verify (2A.15). The expression is not simply equal to $-e^{\hat{C}(t)}\dot{\hat{C}}(t)Me^{-\hat{C}(t)}$ since $\dot{\hat{C}}(t)$ does not, in general, commute with $\hat{C}(t)$. To account for this consider the operator

$$\hat{O}(s,t) \equiv e^{\hat{C}(t)s}\frac{d}{dt}e^{-\hat{C}(t)s}. \tag{2A.21}$$

Differentiating this with respect to s gives

$$\begin{aligned}\partial_s\hat{O}(s,t) &= e^{\hat{C}(t)s}\hat{C}(t)\frac{d}{dt}\left(e^{-\hat{C}(t)s}\right) - e^{\hat{C}(t)s}\frac{d}{dt}\left(\hat{C}(t)e^{-\hat{C}(t)s}\right)\\ &= -e^{\hat{C}(t)s}\dot{\hat{C}}(t)e^{-\hat{C}(t)s}\\ &= -e^{\text{ad}\,C(t)s}[\dot{\hat{C}}(t)].\end{aligned} \tag{2A.22}$$

Hence

$$\begin{aligned}\hat{O}(s,t) - \hat{O}(0,t) &= \int_0^s ds'\partial_{s'}\hat{O}(s',t)\\ &= -\sum_{n=0}^{\infty}\frac{s^{n+1}}{(n+1)!}\left(\text{ad}\,C(t)\right)^n[\dot{\hat{C}}(t)],\end{aligned} \tag{2A.23}$$

from which we obtain

$$\hat{O}(1,t) = e^{\hat{C}(t)}\frac{d}{dt}e^{-\hat{C}(t)} = -f(\text{ad}\,C(t))[\dot{\hat{C}}(t)], \tag{2A.24}$$

which is what we wanted to prove.

Note that the final form of the series for $\hat{C}$ in (2A.6) can be rearranged in many different ways, using the Jacobi identity for the commutators. It is a nontrivial task to find a form involving the smallest number of terms.[39]

The same mathematical technique can be used to derive a useful modification of the Neumann-Liouville expansion or Dyson series (1.239) and (1.251). This is the so-called *Magnus expansion*[40], in which one writes $\hat{U}(t_b,t_a) = e^{\hat{E}}$, and expands the exponent $\hat{E}$ as

$$\hat{E} \;=\; -\frac{i}{\hbar}\int_{t_a}^{t_b}dt_1\,\hat{H}(t_1) + \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2\int_{t_a}^{t_b}dt_2\int_{t_a}^{t_2}dt_1\,\left[\hat{H}(t_2),\hat{H}(t_1)\right]$$

[39] For a discussion see J.A. Oteo, J. Math. Phys. *32*, 419 (1991).

[40] See A. Iserles, A. Marthinsen, and S.P. Norsett, *On the implementation of the method of Magnus series for linear differential equations*, BIT **39**, 281 (1999) (http://www.damtp.cam.ac.uk/user/ai/Publications).

$$
+ \frac{1}{4}\left(\frac{-i}{\hbar}\right)^3 \left\{ \int_{t_a}^{t_b} dt_3 \int_{t_a}^{t_3} dt_2 \int_{t_a}^{t_2} dt_1 \left[\hat{H}(t_3), \left[\hat{H}(t_2), \hat{H}(t_1)\right]\right] \right.
$$

$$
\left. + \frac{1}{3} \int_{t_a}^{t_b} dt_3 \int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_b} dt_1 \left[\left[\hat{H}(t_3), \hat{H}(t_2)\right], \hat{H}(t_1)\right] \right\} + \ldots, \tag{2A.25}
$$

which converges faster than the Neumann-Liouville expansion.

Appendix 2B Direct Calculation of the Time-Sliced Oscillator Amplitude

After time-slicing, the amplitude (2.145) becomes a multiple integral over short-time amplitudes [using the action (2.192)]

$$
(x_n\epsilon|x_{n-1}0) = \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}} \exp\left\{\frac{i}{\hbar}\frac{M}{2}\left[\frac{(x_n - x_{n-1})^2}{\epsilon} - \epsilon\omega^2 \frac{1}{2}(x_n^2 + x_{n-1}^2)\right]\right\}. \tag{2B.26}
$$

We shall write this as

$$
(x_n\epsilon|x_{n-1}0) = \mathcal{N}_1 \exp\left\{\frac{i}{\hbar}\left[a_1(x_n^2 + x_{n-1}^2) - 2b_1 x_n x_{n-1}\right]\right\}, \tag{2B.27}
$$

with

$$
\begin{aligned}
a_1 &= \frac{M}{2\epsilon}\left[1 - 2\left(\frac{\omega\epsilon}{2}\right)^2\right], \quad b_1 = \frac{M}{2\epsilon}, \\
\mathcal{N}_1 &= \frac{1}{\sqrt{2\pi\hbar i\epsilon/M}}.
\end{aligned} \tag{2B.28}
$$

When performing the intermediate integrations in a product of N such amplitudes, the result must have the same general form

$$
(x_N\epsilon|x_{N-1}0) = \mathcal{N}_N \exp\left\{\frac{i}{\hbar}\left[a_N(x_N^2 + x_0^2) - 2b_N x_N x_0\right]\right\}. \tag{2B.29}
$$

Multiplying this by a further short-time amplitude and integrating over the intermediate position gives the recursion relations

$$
\mathcal{N}_{N+1} = \mathcal{N}_1\mathcal{N}_N\sqrt{\frac{i\pi\hbar}{a_N + a_1}}, \tag{2B.30}
$$

$$
a_{N+1} = \frac{a_N^2 - b_N^2 + a_1 a_N}{a_1 + a_N} = \frac{a_1^2 - b_1^2 + a_1 a_N}{a_1 + a_N}, \tag{2B.31}
$$

$$
b_{N+1} = \frac{b_1 b_N}{a_1 + a_N}. \tag{2B.32}
$$

From (2B.31) we find

$$
a_N^2 = b_N^2 + a_1^2 - b_1^2, \tag{2B.33}
$$

and the only nontrivial recursion relation to be solved is that for b_N. With (2B.32) it becomes

$$
b_{N+1} = \frac{b_1 b_N}{a_1 + \sqrt{b_N^2 - (b_1^2 - a_1^2)}}, \tag{2B.34}
$$

or

$$
\frac{1}{b_{N+1}} = \frac{1}{b_1}\left(\frac{a_1}{b_N} + \sqrt{1 - \frac{b_1^2 - a_1^2}{b_N^2}}\right). \tag{2B.35}
$$

We now introduce the auxiliary frequency $\tilde{\omega}$ of Eq. (2.163). Then

$$a_1 = \frac{M}{2\epsilon}\cos\tilde{\omega}, \tag{2B.36}$$

and the recursion for b_{N+1} reads

$$\frac{1}{b_{N+1}} = \frac{\cos\tilde{\omega}\epsilon}{b_N} + \frac{2\epsilon}{M}\sqrt{1 - \frac{M^2}{4\epsilon^2}\frac{\sin^2\tilde{\omega}\epsilon}{b_N^2}}. \tag{2B.37}$$

By introducing the reduced quantities

$$\beta_N \equiv \frac{2\epsilon}{M} b_N, \tag{2B.38}$$

with

$$\beta_1 = 1, \tag{2B.39}$$

the recursion becomes

$$\frac{1}{\beta_{N+1}} = \frac{\cos\tilde{\omega}\epsilon}{\beta_N} + \sqrt{1 - \frac{\sin^2\tilde{\omega}\epsilon}{\beta_N^2}}. \tag{2B.40}$$

For $N = 1, 2$, this determines

$$\begin{aligned}\frac{1}{\beta_2} &= \cos\tilde{\omega}\epsilon + \sqrt{1 - \sin^2\tilde{\omega}\epsilon} = \frac{\sin 2\tilde{\omega}\epsilon}{\sin\tilde{\omega}\epsilon},\\ \frac{1}{\beta_3} &= \cos\tilde{\omega}\epsilon\frac{\sin 2\tilde{\omega}\epsilon}{\sin\tilde{\omega}\epsilon} + \sqrt{1 - \sin^2\tilde{\omega}\epsilon\frac{\sin^2 2\tilde{\omega}\epsilon}{\sin^2\tilde{\omega}\epsilon}} = \frac{\sin 3\tilde{\omega}\epsilon}{\sin\tilde{\omega}\epsilon}.\end{aligned} \tag{2B.41}$$

We therefore expect the general result

$$\frac{1}{\beta_{N+1}} = \frac{\sin\tilde{\omega}(N+1)\epsilon}{\sin\tilde{\omega}\epsilon}. \tag{2B.42}$$

It is easy to verify that this solves the recursion relation (2B.40). From (2B.38) we thus obtain

$$b_{N+1} = \frac{M}{2\epsilon}\frac{\sin\tilde{\omega}\epsilon}{\sin\tilde{\omega}(N+1)\epsilon}. \tag{2B.43}$$

Inserting this into (2B.30) and (2B.33) yields

$$a_{N+1} = \frac{M}{2\epsilon}\sin\tilde{\omega}\epsilon\frac{\cos\tilde{\omega}(N+1)\epsilon}{\sin\tilde{\omega}(N+1)\epsilon}, \tag{2B.44}$$

$$\mathcal{N}_{N+1} = \mathcal{N}_1\sqrt{\frac{\sin\tilde{\omega}\epsilon}{\sin\tilde{\omega}(N+1)\epsilon}}, \tag{2B.45}$$

such that (2B.29) becomes the time-sliced amplitude (2.199).

Appendix 2C Derivation of Mehler Formula

Here we briefly sketch the derivation of Mehler's formula.[41] It is based on the observation that the left-hand side of Eq. (2.297), let us call it $F(x, x')$, is the Fourier transform of the function

$$\tilde{F}(k, k') = \pi\, e^{-(k^2+k'^2+akk')/2}, \tag{2C.46}$$

[41]See P.M. Morse and H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill, New York, Vol. I, p. 781 (1953).

as can easily be verified by performing the two Gaussian integrals in the Fourier representation

$$F(x;x') = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dk}{2\pi}\frac{dk'}{2\pi} e^{ikx+ik'x}\tilde{F}(k,k'). \tag{2C.47}$$

We now consider the right-hand side of (2.297) and form the Fourier transform by recognizing the exponential $e^{k^2/2-ikx}$ as the generating function of the Hermite polynomials[42]

$$e^{k^2/2-ikx} = \sum_{n=0}^{\infty} \frac{(-ik/2)^n}{n!} H_n(x). \tag{2C.48}$$

This leads to

$$\tilde{F}(k,k') = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, dx' F(x,x') e^{-ikx-ik'x} = e^{-(k^2+k'^2)/2}$$
$$\times \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, dx' F(x,x') \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty} \frac{(-ik/2)^n}{n!}\frac{(-ik'/2)^{n'}}{n'!} H_n(x)H_{n'}(x). \tag{2C.49}$$

Inserting here the expansion on the right-hand side of (2.297) and using the orthogonality relation of Hermite polynomials (2.306), we obtain once more (2C.47).

Notes and References

The basic observation underlying path integrals for time evolution amplitudes goes back to the historic article
P.A.M. Dirac, Physikalische Zeitschrift der Sowjetunion **3**, 64 (1933).
He observed that the short-time propagator is the exponential of $i/\hbar$ times the classical action. See also
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M. Kac, Bull. Am. Math. Soc. **72**, Part II, 52 (1966).
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