

CONTENTS

0 Preface	4
1 The Evolution Kernel	6
1.1 Review: The time-evolution Operator	6
1.2 Definition of the Propagator / Kernel	6
1.3 Basic Properties of the Kernel	7
1.4 Example: The Free Particle	9
1.5 Exercises	9
2 Towards the Path Integral Representation of the Kernel	10
2.1 From the Kernel to the Short-Time Kernel and Back	10
2.2 The Trotter Product Formula and the Dirac Short-Time Kernel	10
2.3 The Path Integral Representation of the Kernel	12
2.4 The Path Integral Representation of the Partition Function	15
2.5 Back from the Path Integral to the Schrödinger Equation	16
2.6 Convolution, Correlation Functions and Time-Ordered Products	18
2.7 Comments	20
2.8 Exercises	22
3 Gaussian Path Integrals and Determinants	23
3.1 Preliminary Remarks	23
3.2 The Free Particle and the Normalisation Constant \mathcal{N}	24
3.3 The Free Particle: Fluctuation Determinant and Mode Expansion	26
3.4 The Harmonic Oscillator	27
3.5 Gaussian Path Integrals and Determinants: the VVPM and GY Formulae	29
3.6 Some Comments on the Regularisation of Determinants	33
3.7 Exercises	37
4 Generating Functionals and Perturbative Expansions	38
4.1 The Generating Functional $Z[J]$	38
4.2 Green's Functions and the Generating Functional for Quadratic Theories	40

4.3	Perturbative Expansion and Generating Functionals	42
4.4	The Stationary Phase Approximation for Oscillatory Integrals	43
4.5	The Semi-Classical Approximation	46
4.6	Scattering Theory and the Path Integral	48
4.7	Exercises	49
A	Gaussian and Fresnel Integrals	50
A.1	Basic 1-dimensional Integrals	50
A.2	Related Integrals	51
A.3	Gaussian Integrals and Determinants	53
B	Infinite Product Identities	54
C	Equivalence of the VVPM and GY Formulae for the Fluctuation Determinant	55
D	Poor Man's Proof of some ζ-function Identities	56

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1 THE EVOLUTION KERNEL

1.1 REVIEW: THE TIME-EVOLUTION OPERATOR

The dynamical information about quantum mechanics is contained in the matrix elements of the time-evolution operator $U(t_f, t_i)$. For a time-independent Hamiltonian \hat{H} one has

$$U(t_f, t_i) = e^{-(i/\hbar)(t_f - t_i)\hat{H}} \quad (1.1)$$

whereas the general expression for a time-dependent Hamiltonian involves the time-ordered exponential

$$U(t_f, t_i) = \mathcal{T} \left(e^{-(i/\hbar) \int_{t_i}^{t_f} dt' \hat{H}(t')} \right) . \quad (1.2)$$

It satisfies the evolution equation

$$i\hbar \frac{\partial}{\partial t_f} U(t_f, t_i) = \hat{H}(t_f) U(t_f, t_i) , \quad (1.3)$$

with initial condition

$$U(t_f = t_i, t_i) = \mathbb{I} . \quad (1.4)$$

As a consequence,

$$\Psi(t_f) = U(t_f, t_i) \psi(t_i) \quad (1.5)$$

satisfies the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t_f} \Psi(t_f) = \hat{H}(t_f) \Psi(t_f) \quad (1.6)$$

with initial condition

$$\Psi(t_i) = \psi(t_i) . \quad (1.7)$$

Another key-property of the time-evolution operator is

$$U(t_f, t_i) = U(t_f, t) U(t, t_i) \quad t_i < t < t_f . \quad (1.8)$$

In words: evolution from time t_i to t_f is the same as evolving from t_i to t , followed by evolution from t to t_f .

1.2 DEFINITION OF THE PROPAGATOR / KERNEL

Our main interest will be in matrix elements of U in the position representation. We will denote these by (the letter K stands for “kernel”)

$$K(x_f, x_i; t_f - t_i) = \langle x_f | U(t_f, t_i) | x_i \rangle . \quad (1.9)$$

This can also be interpreted as the transition amplitude

$$K(x_f, x_i; t_f - t_i) = \langle x_f, t_f | x_i, t_i \rangle , \quad (1.10)$$

where (in the time-independent case)

$$|x_i, t_i \rangle = e^{(i/\hbar)t_i \hat{H}} |x_i \rangle \quad (1.11)$$

etc. Note that this is *not* the Schrödinger time-evolution of the state $|x_i \rangle$ - this would have the opposite sign in the exponent (this is related to the fact that $U(t_f, t_i)$ satisfies the Schrödinger equation with respect to t_f , not t_i). Rather, this state is characterised by the fact that it is the eigenstate of the Heisenberg picture operator $\hat{x}_H(t)$ at $t = t_i$,

$$\hat{x}_H(t) |x, t \rangle = e^{(i/\hbar)t \hat{H}} \hat{x} e^{-(i/\hbar)t \hat{H}} e^{(i/\hbar)t \hat{H}} |x \rangle = x |x, t \rangle . \quad (1.12)$$

Another way of saying this, or introducing the states $|x, t \rangle$, is the following: In general the operators $\hat{x}_H(t)$ and $\hat{x}_H(t')$ do not commute for $t \neq t'$. Hence they cannot be simultaneously diagonalised. For any given t , however, one can choose a basis in which $\hat{x}_H(t)$ is diagonal. This is the basis $\{|x, t \rangle\}$.

Matrix elements of the evolution operator between other states, say the transition amplitude between an initial state $|\psi_i \rangle$ and a final state $|\psi_f \rangle$, are determined by the kernel through

$$\begin{aligned} \langle \psi_f | U(t_f, t_i) | \psi_i \rangle &= \int dx_f \int dx_i \langle \psi_f | x_f \rangle \langle x_f | U(t_f, t_i) | x_i \rangle \langle x_i | \psi_i \rangle \\ &= \int dx_f \int dx_i \psi_f^*(x_f) \psi_i(x_i) K(x_f, x_i; t_f - t_i) . \end{aligned} \quad (1.13)$$

1.3 BASIC PROPERTIES OF THE KERNEL

Here are some of the basic properties of the Kernel:

1. With properly normalised position eigenstates, one has

$$\lim_{t_f \rightarrow t_i} \langle x_f, t_f | x_i, t_i \rangle = \langle x_f | x_i \rangle = \delta(x_f - x_i) . \quad (1.14)$$

2. The kernel satisfies the Schrödinger equation with respect to (t_f, x_f) , i.e.

$$[i\hbar \partial_{t_f} - \hat{H}(x_f, p_f = (\hbar/i) \partial_{x_f}, t_f)] \langle x_f, t_f | x_i, t_i \rangle = 0 . \quad (1.15)$$

More generally, for any ket $|\phi \rangle$ the wave function

$$\Psi_\phi(x, t) = \langle x, t | \phi \rangle \quad (1.16)$$

is a solution of the Schrödinger equation, with

$$\begin{aligned}\Psi_\phi(x, t) &= \int dx_i \langle x, t | x_i, t_i \rangle \langle x_i, t_i | \phi \rangle \\ &= \int dx_i K(x, x_i, t - t_i) \Psi_\phi(x_i, t_i) .\end{aligned}\quad (1.17)$$

3. Since we can restrict our attention to evolution forwards in time, one frequently also considers the *causal propagator* or *retarded propagator*

$$K_r(x_f, x_i; t_f - t_i) = \Theta(t_f - t_i) K(x_f, x_i; t_f - t_i) \quad (1.18)$$

where Θ is the Heavyside step function, $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for $x < 0$. It follows from the above two properties of the kernel, and $\Theta'(x) = \delta(x)$, that the retarded propagator satisfies

$$[i\hbar\partial_{t_f} - \hat{H}(x_f, p_f = (\hbar/i)\partial_{x_f}, t_f)]K_r(x_f, x_i; t_f - t_i) = i\hbar\delta(t_f - t_i)\delta(x_f - x_i) . \quad (1.19)$$

Thus the retarded propagator is a Green's function for the Schrödinger equation.

4. A key property of the kernel is the *convolution property*

$$K(x_f, x_i; t_f - t_i) = \int_{-\infty}^{+\infty} dx K(x_f, x; t_f - t) K(x, x_i; t - t_i) \quad (1.20)$$

(for t arbitrary subject to the condition $t_f > t > t_i$). This follows from the property (1.8) of the time-evolution operator by inserting a complete state of states in the form

$$\mathbb{I} = \int_{-\infty}^{+\infty} dx |x\rangle\langle x| . \quad (1.21)$$

One then finds

$$\begin{aligned}\langle x_f, t_f | x_i, t_i \rangle &= \langle x_f | U(t_f, t) U(t, t_i) | x_i \rangle \\ &= \int_{-\infty}^{+\infty} dx \langle x_f | U(t_f, t) | x \rangle \langle x | U(t, t_i) | x_i \rangle \\ &= \int_{-\infty}^{+\infty} dx \langle x_f, t_f | x, t \rangle \langle x, t | x_i, t_i \rangle ,\end{aligned}\quad (1.22)$$

which is the claimed result.

5. Finally, we can also expand the kernel in terms of energy eigenstates

$$\psi_n(x) = \langle x | n \rangle \quad (1.23)$$

as

$$\begin{aligned}K(x_f, x_i; t_f - t_i) &= \langle x_f | e^{-(i/\hbar)(t_f - t_i)\hat{H}} | x_i \rangle \\ &= \sum_n \langle x_f | e^{-(i/\hbar)(t_f - t_i)\hat{H}} | n \rangle \langle n | x_i \rangle \\ &= \sum_n e^{-(i/\hbar)(t_f - t_i)E_n} \psi_n(x_f) \psi_n^*(x_i) .\end{aligned}\quad (1.24)$$

1.4 EXAMPLE: THE FREE PARTICLE

For the free particle, with Hamiltonian $H = p^2/2m$, it is straightforward to determine the kernel $K = K_0$ and verify explicitly all the above properties. By inserting a complete set of momentum eigenstates $|p\rangle$,

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{(i/\hbar)px} \quad (1.25)$$

(i.e. by Fourier transform), one finds

$$\begin{aligned} K_0(x_f, x_i; t_f - t_i) &= \langle x_f | e^{-(i/\hbar)(t_f - t_i)\hat{p}^2/2m} | x_i \rangle \\ &= \int_{-\infty}^{+\infty} dp \langle x_f | p \rangle e^{-(i/\hbar)(t_f - t_i)p^2/2m} \langle p | x_i \rangle \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp e^{(i/\hbar)[p(x_f - x_i) - (t_f - t_i)p^2/2m]} . \end{aligned} \quad (1.26)$$

Using the Fresnel integral formulae from Appendix A, one thus finds

$$K_0(x_f, x_i; t_f - t_i) = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} e^{i\frac{m}{\hbar} \frac{(x_f - x_i)^2}{2(t_f - t_i)}} \quad (1.27)$$

Note that the exponent has the interpretation as the “classical action”, i.e. as the action S_0 of the free particle evaluated on the classical path $x_c(t)$ satisfying the free equations of motion and the boundary conditions $x_c(t_f) = x_f, x_c(t_i) = x_i$,

$$S_0[x_c] = \frac{m}{2} \frac{(x_f - x_i)^2}{(t_f - t_i)} . \quad (1.28)$$

This at this stage rather mysterious fact has a very natural explanation from the path integral point of view.

1.5 EXERCISES

1. Verify the results (1.27) and (1.28) for the evolution kernel of the free particle.
2. Verify that (1.27) is normalised as in (1.14), and satisfies the convolution property (1.20) and the free particle Schrödinger equation (1.15).
3. Prove the basic integral identity (A.31),

$$\int_{-\infty}^{+\infty} d^d x e^{-A_{ab}x^a x^b/2} = \left(\det \frac{A}{2\pi} \right)^{-1/2} . \quad (1.29)$$

for Gaussian integrals (A_{ab} is a real symmetric positive matrix), and calculate the integral

$$\int_{-\infty}^{+\infty} d^d x e^{-A_{ab}x^a x^b/2 + J_a x^a} \quad (1.30)$$

by completing the square (remember that A_{ab} is invertible).

2 TOWARDS THE PATH INTEGRAL REPRESENTATION OF THE KERNEL

2.1 FROM THE KERNEL TO THE SHORT-TIME KERNEL AND BACK

In general, it is a difficult (if not impossible) task to find a closed form expression for the kernel. However, the convolution property allows us to reduce the determination of the finite-time kernel to that of the short-time (or even infinitesimal time) kernel $K(x, y; \epsilon)$ and, as we will see later on, this allows us to make some progress.

First of all we note that we can write (once again in the time-independent case, but the argument works in general)

$$\langle x_f | e^{-(i/\hbar)(t_f - t_i)\hat{H}} | x_i \rangle = \langle x_f | \left(e^{-(i/\hbar)\frac{(t_f - t_i)}{N}\hat{H}} \right)^N | x_i \rangle . \quad (2.1)$$

We think of this as dividing the time-interval $[t_i, t_f]$ into N equal time-intervals $[t_k, t_{k+1}]$ of length ϵ ,

$$\epsilon = t_{k+1} - t_k = (t_f - t_i)/N . \quad (2.2)$$

Here $k = 0, \dots, N-1$ and we identify $t_f = t_N$ and $t_i = t_0$. We can now insert $N-1$ resolutions of unity at times t_k , $k = 1, \dots, N-1$ into the above expression for the kernel to find

$$K(x_f, x_i; t_f - t_i) = \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dx_k \right] \left[\prod_{k=0}^{N-1} K(x_{k+1}, x_k; \epsilon = t_{k+1} - t_k) \right] , \quad (2.3)$$

where $x_f = x_N$ and $x_i = x_0$.

Now this expression holds for any N . But for finite N , the kernel is still difficult to calculate. As we will see below, things simplify in the limit $\epsilon \rightarrow 0$, equivalently $N \rightarrow \infty$. In this limit, the kernel

$$K(x_f, x_i; t_f - t_i) = \lim_{N \rightarrow \infty} \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dx_k \right] \left[\prod_{k=0}^{N-1} K(x_{k+1}, x_k; \epsilon = (t_f - t_i)/N) \right] \quad (2.4)$$

is determined by the short-time kernel $K(x_{k+1}, x_k; \epsilon)$ as $\epsilon \rightarrow 0$.

2.2 THE TROTTER PRODUCT FORMULA AND THE DIRAC SHORT-TIME KERNEL

Formally, it is not difficult to see that in the limit $N \rightarrow \infty$ we only need to know this short-time kernel $K(x_{k+1}, x_k; \epsilon)$ to order ϵ . If everything in sight were commuting (instead of operators), the argument for this would be the following: one writes

$$e^x = \left(e^{x/N} \right)^N = \left(1 + x/N + \mathcal{O}(1/N^2) \right)^N \quad (2.5)$$

and compares with the formula

$$e^x = \lim_{N \rightarrow \infty} (1 + x/N)^N \quad (2.6)$$

to conclude that in the limit $N \rightarrow \infty$ the subleading $\mathcal{O}(N^{-2})$ terms in (2.5) can indeed be dropped.¹ Of course, to establish an analogous result for (unbounded) operators requires some functional analysis.

We will now assume that the Hamiltonian is of the standard form

$$H = T(p) + V(x) = \frac{p^2}{2m} + V(x) . \quad (2.7)$$

We are thus interested in determining the kernel

$$K(x_{k+1}, x_k; \epsilon) = \langle x_{k+1} | e^{-(i/\hbar)\epsilon(\hat{T} + \hat{V})} | x_k \rangle . \quad (2.8)$$

Provided that we can justify dropping terms of $\mathcal{O}(\epsilon^2)$, things simplify quite a bit. Indeed, even though \hat{T} and \hat{V} are non-commuting operators, $\epsilon\hat{T}$ and $\epsilon\hat{V}$ commute up to order ϵ^2 , because their commutator is $\epsilon^2[\hat{T}, \hat{V}]$. Thus, using the Baker-Campbell-Hausdorff formula one has

$$e^{-(i/\hbar)\epsilon(\hat{T} + \hat{V})} = e^{-(i/\hbar)\epsilon\hat{T}} e^{-(i/\hbar)\epsilon\hat{V}} + \mathcal{O}(\epsilon^2) . \quad (2.9)$$

To justify dropping these $\mathcal{O}(\epsilon^2)$ commutator terms, however, one needs some control over the operator $[\hat{T}, \hat{V}]$ which should not become too singular.

Concretely, what one needs is the validity of the *Trotter product formula*

$$e^{\hat{A} + \hat{B}} = \left(e^{\hat{A}/N} e^{\hat{B}/N} \right)^N \stackrel{?}{=} \lim_{N \rightarrow \infty} \left(e^{\hat{A}/N} e^{\hat{B}/N} \right)^N \quad (2.10)$$

for $\hat{A} = \hat{T}$ and $\hat{B} = \hat{V}$.

This identity is not difficult to prove for bounded operators. The case of interest, unbounded operators, is trickier. The identity holds, for instance, on the common domain of A and B , provided that both are self-adjoint operators that are bounded from below. Once again, we will gloss over these functional analysis complications and proceed with the assumption that it is legitimate to drop the commutator terms (while keeping in mind that this assumption is not valid e.g. for the Coulomb potential!).

¹The identity (2.6) can be proved directly, e.g. via a binomial expansion or by showing that

$$\frac{d}{dx} \lim_{N \rightarrow \infty} (1 + x/N)^N = \lim_{N \rightarrow \infty} (1 + x/N)^N$$

With the above assumptions, to order ϵ we can write the short-time kernel as

$$K(x_{k+1}, x_k; \epsilon) = \langle x_{k+1} | e^{-(i/\hbar)\epsilon\hat{T}} e^{-(i/\hbar)\epsilon\hat{V}} | x_k \rangle . \quad (2.11)$$

To diagonalise the operator \hat{T} we introduce a complete set of momentum eigenstates $|p_k\rangle$ with

$$\langle x | p_k \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{(i/\hbar)p_k x} \quad (2.12)$$

and calculate

$$\begin{aligned} K(x_{k+1}, x_k; \epsilon) &= \int_{-\infty}^{+\infty} dp_k \langle x_{k+1} | e^{-(i/\hbar)\epsilon\hat{T}} | p_k \rangle \langle p_k | e^{-(i/\hbar)\epsilon\hat{V}} | x_k \rangle \\ &= \int_{-\infty}^{+\infty} dp_k \langle x_{k+1} | p_k \rangle \langle p_k | x_k \rangle e^{-(i/\hbar)\epsilon(\frac{p_k^2}{2m} + V(x_k))} \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp_k e^{(i/\hbar)\epsilon[p_k \frac{(x_{k+1}-x_k)}{\epsilon} - H(p_k, x_k)]} \end{aligned} \quad (2.13)$$

This is a lovely result, first obtained by Dirac in 1933. In the exponential, where we once had operators, we now encounter the Legendre transform of the classical Hamiltonian, i.e. the Lagrangian! Indeed, if we identify

$$\frac{x_{k+1} - x_k}{\epsilon} = \frac{x_{k+1} - x_k}{t_{k+1} - t_k} \rightarrow \frac{dx_k}{dt} , \quad (2.14)$$

as a discretised time-derivative, the exponent takes the classical form $p_k \dot{x}_k - H(p_k, x_k)$. We can implement the Legendre transformation explicitly by performing the Gaussian (Fresnel) integral over p_k (see Appendix A) to find

$$\begin{aligned} K(x_{k+1}, x_k; \epsilon) &= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp_k e^{(i/\hbar)[p_k(x_{k+1} - x_k) - \epsilon(\frac{p_k^2}{2m} + V(x_k))]} \\ &= \sqrt{\frac{m}{2\pi i \hbar \epsilon}} e^{(i/\hbar)\epsilon L(x_k, \dot{x}_k)} \end{aligned} \quad (2.15)$$

where the Lagrangian L is

$$L(x_k, \dot{x}_k) = \frac{m(x_{k+1} - x_k)^2}{2\epsilon^2} - V(x_k) \rightarrow \frac{m\dot{x}_k^2}{2} - V(x_k) . \quad (2.16)$$

2.3 THE PATH INTEGRAL REPRESENTATION OF THE KERNEL

Having obtained the above explicit formula for the short-time kernel in terms of the Lagrangian, we can now go back to (2.4) to obtain an expression for the finite-time kernel. We can use either the phase space expression (2.13) or the configuration space expression (2.15). This iteration of Dirac's result is due to Feynman (1942).

In this way we arrive at

$$\begin{aligned}
K(x_f, x_i; t_f - t_i) &= \lim_{N \rightarrow \infty} \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dx_k \right] \left[\prod_{k=0}^{N-1} \int_{-\infty}^{\infty} \frac{dp_k}{2\pi\hbar} \right] e^{(i/\hbar)\epsilon \sum_{k=0}^{N-1} [p_k \frac{x_{k+1} - x_k}{\epsilon} - H(p_k, x_k)]} \\
&= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{N/2} \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dx_k \right] e^{(i/\hbar)\epsilon \sum_{k=0}^{N-1} L(x_k, \dot{x}_k)} \quad (2.17)
\end{aligned}$$

Note that in the phase space representation of the kernel there is always one more momentum than position integral. This is a consequence of the fact that each short-time propagator contains one momentum integral whereas the position integrals are inserted between the short-time propagators and the two end-points x_i and x_f are not integrated over.

In the $\epsilon \rightarrow 0$ or $N \rightarrow \infty$ limit, we interpret the points x_k as defining a continuous (but almost certainly nowhere differentiable - see below) curve, any two successive points being joined by a straight line. That is, we think of them as defining a curve $x(t)$ with endpoints

$$x(t_i) = x_i \quad x(t_f) = x_f \quad (2.18)$$

and

$$x_k = x(t_i + k\epsilon) \quad (2.19)$$

Likewise, we think of the p_k as defining a curve $p(t)$ in momentum space such that

$$p_0 = p(t_i) \quad p_k = p(t_i + k\epsilon) \quad (2.20)$$

With this interpretation the exponents in the integrand of the kernel can be written as

$$\begin{aligned}
\lim_{N \rightarrow \infty} \epsilon \sum_{k=0}^{N-1} [p_k \frac{x_{k+1} - x_k}{\epsilon} - H(p_k, x_k)] &= \int_{t_i}^{t_f} dt [p(t)\dot{x}(t) - H(p(t), x(t))] \\
\lim_{N \rightarrow \infty} \epsilon \sum_{k=0}^{N-1} L(x_k, \dot{x}_k) &= \int_{t_i}^{t_f} dt L(x(t), \dot{x}(t)) = S[x(t); t_f, t_i] \quad (2.21)
\end{aligned}$$

In the same spirit, we formally now write the integrals as integrals over paths, introducing the notation

$$\begin{aligned}
\lim_{N \rightarrow \infty} \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dx_k \right] &= \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] \\
\lim_{N \rightarrow \infty} \left[\prod_{k=0}^{N-1} \int_{-\infty}^{\infty} \frac{dp_k}{2\pi\hbar} \right] &= \int D[p(t)/2\pi\hbar] \quad (2.22)
\end{aligned}$$

With this notation, we can now write the kernel as a *path integral*,

$$\begin{aligned}
K(x_f, x_i; t_f - t_i) &= \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] \int D[p(t)/2\pi\hbar] e^{(i/\hbar) \int_{t_i}^{t_f} dt [p(t)\dot{x}(t) - H(p(t), x(t))]} \\
&= \mathcal{N} \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar) S[x(t)]} \quad (2.23)
\end{aligned}$$

This is an integral over all paths $x(t)$ with the specified boundary conditions and, in the first version, all paths $p(t)$ with $t \in [t_i, t_f]$.

Some remarks:

1. The first line, a phase space path integral, is valid for general Hamiltonians $H(p, x) = T(p) + V(x)$ (possibly time-dependent). The measure appears to be an infinite-dimensional analogue of the canonical Liouville measure. The latter is of course invariant under canonical transformations. This should however not lead one to believe that the path integral representation of the kernel also enjoys this invariance. Indeed, this cannot possibly be true since it is well known that under a canonical transformation any Hamiltonian can be mapped to zero (the Hamilton-Jacobi transformation) and hence into any other Hamiltonian, while the kernel depends non-trivially on the Hamiltonian.
2. To pass to the second line, a configuration space path integral, we used the explicit quadratic form $T = p^2/2m$ to perform the Gaussian integral over p . The derivation of the path integral for a Hamiltonian with a velocity dependent potential, such as the magnetic interaction $(p - A)^2/2m$, is more subtle (the discretised version requires a “mid-point rule” for the Hamiltonian) and will not be discussed here.
3. As mentioned above, as limits of piecewise linear continuous paths these paths are continuous but not differentiable. Indeed differentiability would require existence of a finite limit of $(x_{k+1} - x_k)/\epsilon$ as $\epsilon \rightarrow 0$. But x_{k+1} and x_k are independent variables, and hence there is no reason for the difference $x_{k+1} - x_k$ to go to zero as $\epsilon \rightarrow 0$. Hence the paths entering the above sum/integral are typically nowhere differentiable. Evidently, then, things like $\dot{x}(t)$ require some (perhaps stochastic or probabilistic) interpretation, but we will not open this Pandora’s box.
4. Finally, \mathcal{N} is formally an infinite normalisation constant,

$$\mathcal{N} = \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i \hbar (t_f - t_i)} \right)^{N/2} \quad (2.24)$$

(we have replaced ϵ by $(t_f - t_i)/N$) whose sole purpose in life is to make the combined expression \mathcal{N} times the integral well defined, finite and equal to the left hand side (provided that all our functional analysis assumptions are satisfied).

We could have absorbed much of the prefactor into the definition of the measure by writing (2.17) as

$$K(x_f, x_i; t_f - t_i) = \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{1/2} \lim_{N \rightarrow \infty} \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{1/2} dx_k \right] e^{(i/\hbar)\epsilon \sum_{k=0}^{N-1} L(x_k, \dot{x}_k)} \quad (2.25)$$

and defining

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} \tilde{D}[x(t)] = \lim_{N \rightarrow \infty} \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{1/2} dx_k \right] . \quad (2.26)$$

Then the kernel is

$$K(x_f, x_i; t_f - t_i) = \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{1/2} \int_{x(t_i)=x_i}^{x(t_f)=x_f} \tilde{D}[x(t)] e^{(i/\hbar)S[x(t)]} . \quad (2.27)$$

Another useful normalisation of the measure is, as we will see in section 3, such that

$$\mathcal{N} \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar)S[x(t)]} = \sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \int_{x(t_i)=x_i}^{x(t_f)=x_f} \hat{D}[x(t)] e^{(i/\hbar)S[x(t)]} . \quad (2.28)$$

We will obtain a more informative expression for \mathcal{N} , and hence the relation between $D[x]$ and $\hat{D}[x]$, involving the determinant of a differential operator, in the next section.

2.4 THE PATH INTEGRAL REPRESENTATION OF THE PARTITION FUNCTION

In analogy with the quantum statistical (or thermal) partition function

$$Z(\beta) = \text{Tr} e^{-\beta \hat{H}} \quad (2.29)$$

one defines the quantum mechanical partition function, or *the partition function* for short, as the trace of the time evolution operator,

$$Z(t_f, t_i) = \text{Tr} U(t_f, t_i) . \quad (2.30)$$

In the time-independent case, this becomes

$$Z(t_f, t_i) = Z(t_f - t_i) = \text{Tr} e^{-(i/\hbar)(t_f - t_i)\hat{H}} , \quad (2.31)$$

and thus the quantum mechanical and thermal partition function are formally related by continuation of the time interval $(t_f - t_i)$ to the imaginary value

$$t_f - t_i = -i\hbar\beta . \quad (2.32)$$

Evaluating the trace in a basis of energy eigenstates $|n\rangle$, one finds

$$Z(t_f - t_i) = \sum_n e^{-(i/\hbar)(t_f - t_i)E_n} . \quad (2.33)$$

On the other hand, evaluating the trace in a basis of position eigenstates $|x\rangle$, one obtains

$$Z(t_f, t_i) = \int_{-\infty}^{+\infty} dx \langle x|U(t_f, t_i)|x\rangle = \int_{-\infty}^{+\infty} dx K(x, x; t_f - t_i) . \quad (2.34)$$

This means that in the discretised expression (2.17) for the kernel there are now an equal number of momentum and position integrals. In the continuum version (2.23), setting $x_f = x_i = x$ means that one is integrating not over all paths but over all closed paths (loops) at x , and the integration over x means that one is integrating over all closed loops,

$$\begin{aligned} Z(t_f, t_i) &= \mathcal{N} \int_{-\infty}^{+\infty} dx \int_{x(t_i)=x}^{x(t_f)=x} D[x(t)] e^{(i/\hbar)S[x(t)]} \\ &= \mathcal{N} \int_{x(t_f)=x(t_i)} D[x(t)] e^{(i/\hbar)S[x(t)]} . \end{aligned} \quad (2.35)$$

Since we now have an equal number of x - and p -integrals, in terms of the measure $\tilde{D}[x]$ (2.26) the partition function reads

$$Z(t_f, t_i) = \int_{x(t_f)=x(t_i)} \tilde{D}[x(t)] e^{(i/\hbar)S[x(t)]} . \quad (2.36)$$

Comparison with (2.33) shows that, if we are able to calculate this path integral over all closed loops we should (in the time-independent case only, of course) be able to read off the energy spectrum.

The relation between statistical mechanics and quantum mechanics at imaginary time is rather deep. In particular, for quantum field theory this implies a relation between finite temperature quantum field theory in Minkowski space and quantum field theory in Euclidean space with one compact (Euclidean “time”) direction. This has far-reaching consequences (none of which will be explored here).

2.5 BACK FROM THE PATH INTEGRAL TO THE SCHRÖDINGER EQUATION

Since inside the path integral one is dealing with classical functions and functionals rather than with operators, fairly simple “classical” manipulations of the path integral can lead to non-trivial quantum mechanical identities.

As an example, consider the “trivial” statement that the path integral is invariant under an overall shift

$$x(t) \rightarrow x(t) + y(t) \quad y(t_i) = y(t_f) = 0 \quad (2.37)$$

of the integration variable,

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar)S[x(t)]} = \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar)S[x(t) + y(t)]} \quad (2.38)$$

which follows from the (presumed) translation invariance of the measure.

Infinitesimally, with $y(t) = \delta x(t)$ and

$$S[x(t) + \delta x(t)] = S[x(t)] + \delta S[x(t)] \quad , \quad (2.39)$$

this statement reduces to

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] \delta S[x(t)] e^{(i/\hbar)S[x(t)]} = 0 \quad . \quad (2.40)$$

Sometimes this statement is paraphrased as “the path integral of a total derivative is zero”,

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] \frac{\delta}{\delta x(t)} e^{(i/\hbar)S[x(t)]} = 0 \quad . \quad (2.41)$$

Consequences derived from such identities are known as “Schwinger-Dyson equations” in the quantum field theory context.

Since the variation of the action with $\delta x(t)$ vanishing at the endpoints gives the Euler-Lagrange equations,

$$\delta S[x(t)] = \int_{t_i}^{t_f} dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t) \quad , \quad (2.42)$$

and since (2.40) holds for any such $\delta x(t)$, we deduce that the classical equation of motion are valid inside the path integral (!),

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) e^{(i/\hbar)S[x(t)]} = 0 \quad . \quad (2.43)$$

This is the path integral version of Ehrenfest’s theorem.

Since this was so easy, let us generalise this a bit and consider variations of the path which fix $x(t_i)$ but change $x(t_f)$,

$$\delta x(t_i) = 0 \quad \delta x(t_f) \neq 0 \quad . \quad (2.44)$$

This means that we are calculating

$$\delta \langle x_f, t_f | x_i, t_i \rangle = \delta x(t_f) \frac{\partial}{\partial x_f} \langle x_f, t_f | x_i, t_i \rangle \quad . \quad (2.45)$$

In this case, the variation of the action is

$$\begin{aligned} \delta S[x(t)] &= \int_{t_i}^{t_f} dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t) + \frac{\partial L}{\partial \dot{x}} \delta x|^{t_f} \\ &= \int_{t_i}^{t_f} dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t) + p(t_f) \delta x(t_f) \quad , \end{aligned} \quad (2.46)$$

where $p(t_f) \equiv p_f$ is the canonical momentum at $t = t_f$. This leads to the standard Hamilton-Jacobi relation

$$p_f = \frac{\partial S[x_c]}{\partial x_f} . \quad (2.47)$$

We deduce that

$$\frac{\partial}{\partial x_f} \langle x_f, t_f | x_i, t_i \rangle = \frac{i}{\hbar} \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] p(t_f) e^{(i/\hbar)S[x(t)]} , \quad (2.48)$$

which is nothing other than the familiar statement that in the position representation one has

$$\hat{p}_f = \frac{\hbar}{i} \frac{\partial}{\partial x_f} . \quad (2.49)$$

In the same way, by considering a variation of t_f , and using

$$L(x_f, \dot{x}_f) = \frac{d}{dt_f} S[x(t)] = \frac{\partial S}{\partial t_f} + p_f \dot{x}_f \quad (2.50)$$

(modulo the Euler-Lagrange equations), and therefore

$$\frac{\partial S[x_c]}{\partial t_f} = -H(x_f, p_f) , \quad (2.51)$$

one obtains a path integral of the statement (1.15) that the kernel satisfies the Schrödinger equation (Exercise),

$$\left(i\hbar \frac{\partial}{\partial t_f} - \hat{H}(\hat{x}_f, \hat{p}_f = \frac{\hbar}{i} \frac{\partial}{\partial x_f}) \right) \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar)S[x(t)]} = 0 . \quad (2.52)$$

We had initially derived the path integral from the standard description, and now we have employed path integral manipulations to pass back from the path integral to the Schrödinger representation. This essentially completes the (formal) proof of the equivalence of the path integral description of quantum mechanics and the standard Schrödinger representation. One piece of the dictionary that is still missing is how to translate matrix elements other than the basic transition amplitude $\langle x_f, t_f | x_i, t_i \rangle$ into the path integral language. This will be the subject of the next subsection.

2.6 CONVOLUTION, CORRELATION FUNCTIONS AND TIME-ORDERED PRODUCTS

As we saw in section 1 and above, a crucial property of the kernel is the convolution property (1.20). How is this encoded in the path integral representation (2.23)

$$K(x_f, x_i; t_f - t_i) = \mathcal{N} \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar)S[x(t); t_f, t_i]} \quad (2.53)$$

of the kernel? We need to consider separately the integrand and the measure. As far as the integrand is concerned, the action $S[x(t); t_f, t_i]$ obviously satisfies

$$S[x(t); t_f, t_i] = S[x(t); t_f, t_0] + S[x(t); t_0, t_i] \quad (2.54)$$

for any $t_f > t_0 > t_i$ since

$$\int_{t_i}^{t_f} (\dots) = \int_{t_0}^{t_f} (\dots) + \int_{t_i}^{t_0} (\dots) . \quad (2.55)$$

And for the path integral measure we have

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] = \int_{-\infty}^{+\infty} dx_0 \int_{x(t_0)=x_0}^{x(t_f)=x_f} D[x(t)] \int_{x(t_i)=x_i}^{x(t_0)=x_0} D[x(t)] \quad (2.56)$$

In words: we can perform the integral over all paths from x_i to x_f , by considering all paths from x_i to x_0 and x_0 to x_f for some fixed $x_0 = x(t_0)$ and then integrating over x_0 . Taken together, the statements about the action and the measure imply² the convolution property (1.20).

So far we have only discussed the transition amplitude $\langle x_f, t_f | x_i, t_i \rangle$, but it is also possible to represent matrix elements of operators as path integrals. The most natural operators to consider in the present context are products of Heisenberg operators $\hat{x}_H(t_1)\hat{x}_H(t_2)\dots$

We begin with a single operator $\hat{x}_H(t_0)$ with $t_f > t_0 > t_i$ and, to simplify the notation, we will from now on drop the subscript H on Heisenberg operators. By elementary manipulations we find

$$\begin{aligned} \langle x_f, t_f | \hat{x}(t_0) | x_i, t_i \rangle &= \int_{-\infty}^{+\infty} dx(t_0) \langle x_f, t_f | \hat{x}(t_0) | x(t_0), t_0 \rangle \langle x(t_0), t_0 | x_i, t_i \rangle \\ &= \int_{-\infty}^{+\infty} dx(t_0) \langle x_f, t_f | x(t_0), t_0 \rangle \langle x(t_0), t_0 | x_i, t_i \rangle x(t_0) . \end{aligned}$$

Turning this into a statement about path integrals, using the convolution property, we therefore conclude that

$$\langle x_f, t_f | \hat{x}(t_0) | x_i, t_i \rangle = \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] x(t_0) e^{(i/\hbar)S[x(t); t_f, t_i]} . \quad (2.57)$$

Thus the insertion of an operator in the usual prescription corresponds to the insertion of a classical function in the path integral formulation. While this is very charming, and in line with the replacement of the Hamiltonian operator by the Lagrange function and

²At least as long as one pretends that $\mathcal{N} = 1$ or that \mathcal{N} has somehow been incorporated into the definition of a suitably regularised path integral. This is the recommended attitude at the present level of rigour (better: non-rigour), and one that we will adopt henceforth.

its action, it also immediately raises a puzzle. Namely, since $x(t_1)$ and $x(t_2)$ commute, does the insertion of $x(t_1)x(t_2)$ into the path integral calculate the matrix elements of $\hat{x}(t_1)\hat{x}(t_2)$ or $\hat{x}(t_2)\hat{x}(t_1)$ or ...? To answer this question, we reverse the above calculation, but this time with the insertion of $x(t_1)x(t_2)$. In order to use the convolution property of the kernel or path integral, we need to distinguish the two cases $t_2 > t_1$ and $t_2 < t_1$. Then one finds

$$\begin{aligned}
& \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] x(t_1)x(t_2) e^{(i/\hbar)S[x(t);t_f,t_i]} \\
&= \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] x(t_2)x(t_1) e^{(i/\hbar)S[x(t);t_f,t_i]} \\
&= \begin{cases} \langle x_f, t_f | \hat{x}(t_2)\hat{x}(t_1) | x_i, t_i \rangle & t_2 > t_1 \\ \langle x_f, t_f | \hat{x}(t_1)\hat{x}(t_2) | x_i, t_i \rangle & t_2 < t_1 \end{cases} \quad (2.58)
\end{aligned}$$

Using the time-ordering operator we can summarise these results as

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] x(t_1)x(t_2) e^{(i/\hbar)S[x(t);t_f,t_i]} = \langle x_f, t_f | \mathcal{T}(\hat{x}(t_1)\hat{x}(t_2)) | x_i, t_i \rangle . \quad (2.59)$$

This immediately generalises to

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] x(t_1) \dots x(t_n) e^{(i/\hbar)S[x(t);t_f,t_i]} = \langle x_f, t_f | \mathcal{T}(\hat{x}(t_1) \dots \hat{x}(t_n)) | x_i, t_i \rangle . \quad (2.60)$$

Thus the path integral always evaluates matrix elements of time-ordered products of operators. This explains why the ordering inside the path integral is irrelevant and how the ordering ambiguity is resolved on the operator side.

As a final variation of this theme, we consider the path integral representation of transition amplitudes between states other than the position eigenstates $|x, t\rangle$. To obtain these, we simply use the formula (1.13),

$$\langle \psi_f | U(t_f, t_i) | \psi_i \rangle = \int dx_f \int dx_i \psi_f^*(x_f) \psi_i(x_i) K(x_f, x_i; t_f - t_i) , \quad (2.61)$$

and the path integral expression for the kernel $K(x_f, x_i; t_f - t_i)$.

2.7 COMMENTS

We have thus passed from a formulation of quantum mechanics based on the Hamiltonian (and operators and Hilbert spaces) to a Lagrangian description in which there are only commuting objects, no operators. In this framework, the quantum nature, which in the usual Hamiltonian approach is reflected in the non-commutativity of operators,

arises because one is instructed to consider not only *classical paths*, i.e. extrema of the action (solutions to the classical equations of motion) but all possible paths, weighted by the exponential of (i/\hbar) times the action.

This provides an extremely intuitive picture of quantum mechanics in which one is never led to ask questions like "which path did the electron take?". One also sees very explicitly how classical mechanics emerges in the limit $\hbar \rightarrow 0$. In that case, the path integral will be dominated by contributions from the extrema of the action (by the usual stationary phase approximation), i.e. precisely by those paths that are solutions to the classical equations of motion (see the discussion in section 4.6).

It is important to note that at this point the path integral notation that we have introduced is largely symbolic. It is a shorthand notation for the $N \rightarrow \infty$ limit (2.17). Provided that all our assumptions are satisfied, this is just another (albeit complicated looking) way of writing the propagator.

However, the significance of introducing this symbolic notation should not be underestimated. Indeed, if one always had to calculate path integrals as the limit of an infinite number of integrals, then path integrals might be conceptually interesting but that approach would hardly be an efficient calculational tool. One might like to draw an analogy here with Riemann integrals, defined as the limits of an infinite sum. In practice, of course, one does not calculate integrals that way. Rather, one can use that definition to establish certain basic properties of the resulting infinite sum, symbolically denoted by the continuum sum (integral) \int , and then one determines definite and indefinite integrals directly, without resorting to the discretised description. Of course, in this process one may be glossing over several mathematical subtleties (which will ultimately lead to the development of measure theory, the Lebesgue integral etc.), but this does not mean that one cannot reliably calculate simple integrals without knowing about these things.

The attitude regarding path integrals we will adopt in the following will be similar in spirit. We will deduce some properties of path integrals from their "discretised" version and then try to pass as quickly as possible to continuum integrals which will allow us to perform path integrals via one "functional integration" instead of an infinite number of ordinary integrations. Once again, this will be sweeping many important mathematical subtleties under the rug (not the least of which is "does something like what you have called $D[x]$ exist at all?"), but that does not mean that we cannot trust the results that we have obtained.³

³By the way, the answer to that questions is "no", but that is irrelevant - it is simply not the right question to ask. A more pertinent question might be "can one make sense of $\int D[x] \exp(i/\hbar)S[x]$ as something like a measure (or linear functional)?"

For some historical comments on “*efforts to give an improved mathematical meaning to Feynman’s path integral formulation of quantum mechanics*”, see e.g.

J.R. Klauder, *The Feynman Path Integral: An Historical Slice*, [quant-ph/0303034](#).

2.8 EXERCISES

1. Using the Baker-Campbell-Hausdorff formula, determine the operator \hat{X} , defined by

$$e^{-(i/\hbar)\epsilon(\hat{T} + \hat{V})} = e^{-(i/\hbar)\epsilon\hat{T}} e^{-(i/\hbar)\epsilon\hat{V}} e^{-(\epsilon/\hbar)^2\hat{X}} , \quad (2.62)$$

to order ϵ .

2. Generalise the derivation of the path integral to systems with $d > 1$ degrees of freedom. Assume that the Hamiltonian has the standard form

$$H = \frac{\vec{p}^2}{2m} + V(\vec{x}) , \quad (2.63)$$

where $\vec{x} = (x^1, \dots, x^d)$ etc.

3. Spell out the proof of (2.52) (the path integral satisfies the Schrödinger equation) in detail.

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3 GAUSSIAN PATH INTEGRALS AND DETERMINANTS

3.1 PRELIMINARY REMARKS

The path integral expression for the propagator we have obtained is

$$K(x_f, x_i; t_f - t_i) = \mathcal{N} \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar)S[x(t)]} . \quad (3.1)$$

We thus now need to make sense of, and develop rules for evaluating, such path integrals.

For a general system described by an action $S[x]$ an exact evaluation of the path integral is certainly too much to hope for. Indeed, even in the finite-dimensional case integrals of exponentials of elementary functions can typically be evaluated in closed form only in the purely quadratic (Gaussian, Fresnel) case, whereas more general integrals are then evaluated ‘perturbatively’ in terms of a generating function as in (A.26).

For path integrals, the situation is quite analogous. Typically, the path integrals that can be calculated in closed form are purely quadratic (Gaussian, Fresnel) integrals, i.e. actions of the general time-dependent harmonic oscillator type

$$S[x] = \frac{m}{2} \int_{t_i}^{t_f} (\dot{x}(t)^2 - \omega(t)^2 x(t)^2) , \quad (3.2)$$

perhaps with the addition of a ‘source’ term,

$$S[x] \rightarrow S[x] + \int j(t)x(t) . \quad (3.3)$$

Then the strategy to deal with more general path integrals, corresponding e.g. to an action of the form

$$S[x] = \int_{t_i}^{t_f} \left(\frac{m}{2} \dot{x}(t)^2 - V(x(t)) \right) , \quad (3.4)$$

is to reduce it to an expansion about a quadratic action. In practice this is achieved in one of two ways. Either the potential is of the harmonic oscillator form plus a perturbation, $V(x) = V_0(x) + \lambda W(x)$, and one defines the path integral via a power series expansion in λ , a *perturbative expansion*. Or one defines the path integral by an expansion around a classical solution $x_c(t)$ of the equations of motion $m\ddot{x} = -V'(x)$. To quadratic order in the ‘quantum fluctuations’ around the classical solution one then finds the action (3.2) with $\omega(t)^2 = \frac{1}{m}V''(x_c(t))$. This turns out to lead to an expansion of the path integral in a power series in \hbar , a *semi-classical expansion*.

In either case, the Gaussian path integral can be evaluated in reasonably closed form and the complete path integral is then defined in terms of the generating functional associated with this quadratic action. In this section 3 we will deal exclusively with Gaussian integrals. The evaluation of more general integrals in terms of generating functionals will then be one of the subjects of section 4.

3.2 THE FREE PARTICLE AND THE NORMALISATION CONSTANT \mathcal{N}

We are now ready to tackle our first path integral. For obvious reasons we will consider the simplest dynamical system, namely the free particle, with Lagrangian

$$L_0(x(t), \dot{x}(t)) = \frac{m}{2} \dot{x}(t)^2 . \quad (3.5)$$

We thus need to calculate

$$K_0(x_f, x_i; t_f - t_i) = \mathcal{N} \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar) S_0[x(t)]} , \quad (3.6)$$

and we know that we should find the result (1.27),

$$K_0(x_f, x_i; t_f - t_i) = \sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} e^{(i/\hbar) \frac{m}{2} \frac{(x_f - x_i)^2}{(t_f - t_i)}} \quad (3.7)$$

Since in this case we already know the result, we can use this calculation to determine the overall normalisation of the path integral from the continuum point of view (since \mathcal{N} is universal: it depends only on m and $(t_f - t_i)$ and not on the potential $V(x)$).

As described above, the general strategy is to expand the paths around a solution to the classical equations of motion. Here the starting action is already quadratic, but this expansion will have the added benefit of eliminating the boundary conditions $x(t_{i,f}) = x_{i,f}$ from the path integral. We thus split any path satisfying these boundary conditions into the sum of the classical path $x_c(t)$,

$$x_c(t) = x_i + \frac{x_f - x_i}{t_f - t_i} (t - t_i) , \quad (3.8)$$

and a *quantum fluctuation* $y(t)$,

$$x(t) = x_c(t) + y(t) , \quad (3.9)$$

with $y(t)$ satisfying the homogeneous boundary conditions

$$y(t_i) = y(t_f) = 0 . \quad (3.10)$$

Plugging this into the action, one finds

$$S_0[x_c + y] = S_0[x_c] + \frac{m}{2} \int_{t_i}^{t_f} \dot{y}(t)^2 \quad (3.11)$$

where $S_0[x_c]$ is the classical action, already given in (1.28),

$$S_0[x_c] = \frac{m}{2} \frac{(x_f - x_i)^2}{(t_f - t_i)} . \quad (3.12)$$

There is no linear term in $y(t)$ because we are expanding around a critical point of the action $S_0[x(t)]$, and there are no higher than quadratic terms because the free particle action itself is quadratic.

In the path integral, instead of integrating over all paths $x(t)$ with the specified boundary conditions we now integrate over all paths $y(t)$ with the boundary conditions (3.10). We thus find that the path integral expression for the kernel becomes

$$K_0(x_f, x_i; t_f - t_i) = e^{(i/\hbar)S_0[x_c]} \mathcal{N} \int_{y(t_i)=y(t_f)=0} D[y(t)] e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_i}^{t_f} \dot{y}(t)^2} \quad (3.13)$$

We thus automatically produce the classical action in the exponent, as in (3.7).

To get a handle on the path integral over $y(t)$, we integrate by parts in the action to obtain

$$\int_{y(t_i)=y(t_f)=0} D[y(t)] e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_i}^{t_f} \dot{y}(t)^2} = \int_{y(t_i)=y(t_f)=0} D[y(t)] e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_i}^{t_f} y(t) (-\partial_t^2) y(t)} \quad (3.14)$$

Comparing with the fundamental Fresnel integral formula (A.32),

$$\int_{-\infty}^{+\infty} d^d x e^{iA_{ab}x^a x^b/2} = \left(\det \frac{A}{2\pi i} \right)^{-1/2}, \quad (3.15)$$

we deduce that what this path integral formally calculates is the determinant of the differential operator $(-\partial_t^2)$,

$$\int_{y(t_i)=y(t_f)=0} D[y(t)] e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_i}^{t_f} y(t) (-\partial_t^2) y(t)} = \left(\text{Det} \frac{m}{2\pi i \hbar} [-\partial_t^2] \right)^{-1/2}. \quad (3.16)$$

I denote the (functional) determinant of an operator by Det to distinguish it from a standard finite-dimensional determinant. We will discuss this determinant in more detail momentarily. First of all, we note that comparison of (3.7) and (3.13) shows that the infinite normalisation constant \mathcal{N} is related to this determinant by

$$\mathcal{N} = \sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \left(\text{Det} \frac{m}{2\pi i \hbar} [-\partial_t^2] \right)^{+1/2}. \quad (3.17)$$

We also see that the normalised path integral measure $\hat{D}[y(t)]$ introduced in (2.28) is such that it normalises the free particle Gaussian fluctuation integral to unity,

$$\int_{y(t_i)=y(t_f)=0} \hat{D}[y(t)] e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_i}^{t_f} y(t) (-\partial_t^2) y(t)} = 1. \quad (3.18)$$

3.3 THE FREE PARTICLE: FLUCTUATION DETERMINANT AND MODE EXPANSION

Now let us return to the definition of the determinant of a differential operator. As in the finite-dimensional case, this determinant is formally defined as the product of the eigenvalues. That this is indeed what the path integral gives rise to can be seen more explicitly by expanding $y(t)$ in normalised eigenmodes $y_n(t)$ of the operator $(-\partial_t^2)$,

$$y(t) = \sum_n c_n y_n(t) \quad , \quad (3.19)$$

with

$$\begin{aligned} (-\partial_t^2) y_n(t) &= \lambda_n y_n(t) \\ \int_{t_i}^{t_f} y_n(t) y_m(t) &= \delta_{m,n} \\ y_n(t_i) = y_n(t_f) &= 0 \quad . \end{aligned} \quad (3.20)$$

In terms of this decomposition, the action becomes

$$\frac{m}{2} \int_{t_i}^{t_f} y(t) (-\partial_t^2) y(t) = \frac{m}{2} \sum_n \lambda_n c_n^2 \quad . \quad (3.21)$$

Thus the expansion of $y(t)$ in terms of eigenmodes is tantamount to diagonalising the operator (this statement is obviously true more generally). Then the path integral over all $y(t)$ becomes an integral over the c_n ,

$$\int_{y(t_i)=y(t_f)=0} D[y(t)] = \prod_n \left(\int_{-\infty}^{+\infty} dc_n \right) \quad , \quad (3.22)$$

and thus the path integral reduces to an infinite product of finite-dimensional Gaussian integrals, with the result

$$\begin{aligned} \int_{y(t_i)=y(t_f)=0} D[y(t)] e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_i}^{t_f} y(t) (-\partial_t^2) y(t)} &= \prod_n \left(\int_{-\infty}^{+\infty} dc_n \right) e^{\frac{i}{\hbar} \frac{m}{2} \sum_n \lambda_n c_n^2} \\ &= \left(\prod_n \frac{m}{2\pi i \hbar} \lambda_n \right)^{-1/2} \quad . \end{aligned} \quad (3.23)$$

It is this infinite product which we have defined as the determinant.

It will be useful for later to know explicitly the eigenvalues λ_n . The properly normalised eigenfunctions are

$$y_n(t) = \sqrt{\frac{2}{t_f - t_i}} \sin n\pi \frac{t - t_i}{t_f - t_i} \quad . \quad (3.24)$$

Since $y_{-n}(t) = -y_n(t)$, the linearly independent solutions are $y_n(t)$ with $n \in \mathbb{N}$ and the corresponding eigenvalues are

$$\lambda_n = \frac{n^2 \pi^2}{(t_f - t_i)^2} \quad . \quad (3.25)$$

We thus have

$$\text{Det}[-\partial_t^2] = \prod_{n=1}^{\infty} \frac{n^2 \pi^2}{(t_f - t_i)^2} \quad (3.26)$$

This is clearly infinite, and thus $\text{Det}^{-1/2}[-\partial_t^2]$ is zero, but this is compensated by the infinite normalisation constant in precisely such a way that one obtains the finite result (3.17).

$$\mathcal{N} \left(\text{Det} \frac{m}{2\pi i \hbar} [-\partial_t^2] \right)^{-1/2} = \sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \quad (3.27)$$

For more comments on determinants and regularised determinants see sections 3.5 and 3.6.

3.4 THE HARMONIC OSCILLATOR

We have now accumulated all the techniques we need to tackle a more interesting example, namely the time-independent harmonic oscillator, with action

$$S[x] = \frac{m}{2} \int_{t_i}^{t_f} (\dot{x}(t)^2 - \omega_0^2 x(t)^2) dt. \quad (3.28)$$

Following the same strategy as for the free particle, we decompose the path into a classical path $x_c(t)$ and the fluctuation $y(t)$, determine the classical action and the (still quadratic) action for $y(t)$, and then perform the Gaussian integral over $y(t)$.

The classical path and action are (see Exercise 1)

$$\begin{aligned} x_c(t) &= x_i \frac{\sin \omega_0(t_f - t)}{\sin \omega_0(t_f - t_i)} + x_f \frac{\sin \omega_0(t - t_i)}{\sin \omega_0(t_f - t_i)} \\ S[x_c] &= \frac{m \omega_0}{2 \sin \omega_0(t_f - t_i)} \left[(x_i^2 + x_f^2) \cos \omega_0(t_f - t_i) - 2x_i x_f \right]. \end{aligned} \quad (3.29)$$

Expanding the action around $x_c(t)$, one finds

$$S[x_c + y] = S[x_c] + \frac{m}{2} \int_{t_i}^{t_f} y(t) (-\partial_t^2 - \omega_0^2) y(t) dt \quad (3.30)$$

Thus the path integral we need to calculate is

$$K(x_f, x_i; t_f - t_i) = e^{(i/\hbar)S[x_c]} \mathcal{N} \int_{y(t_i)=y(t_f)=0} D[y(t)] e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_i}^{t_f} y(t) (-\partial_t^2 - \omega_0^2) y(t) dt} \quad (3.31)$$

This is once again a straightforward Gaussian (Fresnel) integral, and thus one finds, using the result (3.17),

$$\begin{aligned} K(x_f, x_i; t_f - t_i) &= \sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \sqrt{\frac{\text{Det} \frac{m}{2\pi i \hbar} [-\partial_t^2]}{\text{Det} \frac{m}{2\pi i \hbar} [-\partial_t^2 - \omega_0^2]}} e^{(i/\hbar)S[x_c]} \\ &= \sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \sqrt{\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega_0^2]}} e^{(i/\hbar)S[x_c]} \end{aligned} \quad (3.32)$$

Since in writing the above we have taken into account the normalisation factor, the result should be well defined and finite. This is indeed the case. To calculate this ratio of determinants, we observe first of all that if the eigenvalues of the operator $(-\partial_t^2)$ are λ_n , the eigenvalues μ_n of the operator $(-\partial_t^2 - \omega_0^2)$ are $\mu_n = \lambda_n - \omega_0^2$. Thus the ratio of determinants is

$$\begin{aligned} \sqrt{\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega_0^2]}} &= \left(\prod_n \frac{\lambda_n}{\lambda_n - \omega_0^2} \right)^{1/2} \\ &= \left(\prod_n \left(1 - \frac{\omega_0^2}{\lambda_n}\right) \right)^{-1/2}. \end{aligned} \quad (3.33)$$

Even though this may not be obvious from this expression, the result is actually an elementary function. First of all, using the explicit expression for the λ_n , one has

$$\prod_{n=1}^{\infty} \left(1 - \frac{\omega_0^2}{\lambda_n}\right) = \prod_{n=1}^{\infty} \left(1 - \frac{\omega_0^2(t_f - t_i)^2}{n^2\pi^2}\right). \quad (3.34)$$

The function

$$f(x) = \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2\pi^2}\right) \quad (3.35)$$

is an even function of x with $f(0) = 1$ and simple zeros at $x = \pm n\pi$. This shows (see also Appendix B) that this is an infinite product representation of

$$f(x) = \frac{\sin x}{x}. \quad (3.36)$$

Therefore, the final result for the ratio of determinants is

$$\sqrt{\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega_0^2]}} = \sqrt{\frac{\omega_0(t_f - t_i)}{\sin \omega_0(t_f - t_i)}}, \quad (3.37)$$

and our final compact result for the propagator of the harmonic oscillator is

$$\begin{aligned} K(x_f, x_i; t_f - t_i) &= \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} \sqrt{\frac{\omega_0(t_f - t_i)}{\sin \omega_0(t_f - t_i)}} e^{(i/\hbar)S[x_c]} \\ &= \sqrt{\frac{m\omega_0}{2\pi i\hbar \sin \omega_0(t_f - t_i)}} e^{(i/\hbar)S[x_c]} \end{aligned} \quad (3.38)$$

with

$$S[x_c] = \frac{m}{2} \frac{\omega_0}{\sin \omega_0(t_f - t_i)} \left[(x_i^2 + x_f^2) \cos \omega_0(t_f - t_i) - 2x_i x_f \right]. \quad (3.39)$$

It is easy to see that this result reduces to that for the free particle in the limit $\omega_0 \rightarrow 0$.

Given the above result for the kernel, we also immediately obtain an expression for the partition function by setting $x_i = x_f = x$ and integrating over x . This is a Fresnel integral, and the result is

$$Z(t_f - t_i) = \frac{1}{2i \sin \frac{\omega_0(t_f - t_i)}{2}} . \quad (3.40)$$

This can be expanded as

$$Z(t_f - t_i) = \sum_{n=0}^{\infty} e^{-(i/\hbar)(t_f - t_i)E_n} , \quad (3.41)$$

where (cf. (2.33))

$$E_n = \hbar\omega_0(n + \frac{1}{2}) \quad (3.42)$$

are the harmonic oscillator energy levels. (Exercise)

3.5 GAUSSIAN PATH INTEGRALS AND DETERMINANTS: THE VVPM AND GY FORMULAE

Frequently one encounters time-dependent harmonic oscillators with Hamiltonian

$$H(t) = \frac{1}{2m}p^2 + \frac{m\omega(t)^2}{2}x^2 \quad (3.43)$$

and the quadratic action

$$S[x] = \frac{m}{2} \int_{t_i}^{t_f} (\dot{x}(t)^2 - \omega(t)^2 x(t)^2) . \quad (3.44)$$

For instance, expanding the general action

$$S[x] = \frac{m}{2} \int_{t_i}^{t_f} (\dot{x}(t)^2 - \frac{2}{m}V(x(t))) \quad (3.45)$$

to second order around a classical solution $x_c(t)$ of the equations of motion $m\ddot{x} = -V'(x)$, one finds the action (3.44) with

$$\omega(t)^2 = \frac{1}{m}V''(x_c(t)) . \quad (3.46)$$

The resulting path integral is still Gaussian, and exactly the same strategy as above can be used to show that the path integral result for the kernel of the evolution operator is (cf. (3.32))

$$\langle x_f | \hat{T} e^{-(i/\hbar) \int_{t_i}^{t_f} dt \hat{H}(t)} | x_i \rangle = \sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \sqrt{\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega(t)^2]}} e^{(i/\hbar)S[x_c]} . \quad (3.47)$$

Here $x_c(t)$ now denotes the classical harmonic oscillator solution with the given boundary condition, $x_c(t_i) = x_i$ and $x_c(t_f) = x_f$, $S[x_c]$ is the classical action, and the fluctuation determinants are to be calculated for zero (Dirichlet) boundary conditions.

In order to evaluate the result for the propagator (3.47), one needs to determine the classical action and the ratio of fluctuation determinants. The former is rather straightforward provided that one can find the classical solution. An integration by parts shows that the classical action can be calculated in terms of the boundary values of $x_c(t)$ and $\dot{x}_c(t)$ at $t = t_i, t_f$,

$$S[x_c] = \frac{m}{2} \int_{t_i}^{t_f} (\dot{x}_c(t)^2 - \omega(t)^2 x_c(t)^2) = \frac{m}{2} [x_f \dot{x}_c(t_f) - x_i \dot{x}_c(t_i)] . \quad (3.48)$$

The calculation of the ratio of determinants would be complicated if one tried to calculate these determinants directly, as we did in the time-independent case. Fortunately there are two elegant shortcuts to calculating this ratio of determinants which are finite-dimensional in nature and do not require the calculation of a functional determinant. I will briefly describe these below.

One can for instance use the useful and remarkable result that the ratio of determinants can be calculated *from the classical action* via the Van Vleck - Pauli - Morette (VVPM) formula

$$\sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \sqrt{\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega(t)^2]}} = \frac{1}{\sqrt{2\pi i \hbar}} \sqrt{-\frac{\partial^2 S[x_c]}{\partial x_i \partial x_f}} \quad (3.49)$$

More generally, for a d -dimensional quantum system, the 2nd derivative of the classical action would be replaced by the d -dimensional VVPM determinant

$$\frac{\partial^2 S[x_c]}{\partial x_i \partial x_f} \rightarrow \det \left[\frac{\partial^2 S[x_c]}{\partial x_i^\mu \partial x_f^\nu} \right] .$$

This is a non-trivial but standard and well-known result. Notice that, to evaluate the ratio of *quantum* fluctuations in this manner, one only needs to know the *classical* action.

In the case of the harmonic oscillator with constant frequency, agreement between the VVPM formula and the result we obtained in (3.38) can be immediately verified from the classical action (3.39) which gives

$$-\frac{\partial^2 S[x_c]}{\partial x_i \partial x_f} = \frac{m\omega_0}{\sin \omega_0(t_f - t_i)} . \quad (3.50)$$

Alternatively, instead of the VVPM result one can use the equally remarkable, but apparently much less well known, Gelfand-Yaglom (GY) formula that states that

$$\frac{\text{Det}[-\partial_t^2 - \omega(t)^2]}{\text{Det}[-\partial_t^2]} = \frac{F_\omega(t_f)}{t_f - t_i} \quad (3.51)$$

where $F_\omega(t)$ is the solution of the classical harmonic oscillator equation

$$(\partial_t^2 + \omega(t)^2)F_\omega(t) = 0 \quad (3.52)$$

with the initial conditions

$$F_\omega(t_i) = 0 \quad \dot{F}_\omega(t_i) = 1 \quad . \quad (3.53)$$

Thus one has the simple result

$$\sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \sqrt{\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega(t)^2]}} = \sqrt{\frac{m}{2\pi i \hbar F_\omega(t_f)}} \quad (3.54)$$

It is quite remarkable that the ratio of fluctuation determinants, which involves the product over all eigenvalues of the operator $-(\partial_t^2 + \omega(t)^2)$ (with zero boundary conditions), can be expressed in terms of the zero mode (solution with zero eigenvalue) of the same operator with the GY boundary conditions (3.53).

Once again, as an example we consider the constant frequency harmonic oscillator. The solution of the classical equations of motion satisfying the GY boundary conditions is evidently

$$F_{\omega_0}(t) = \frac{1}{\omega_0} \sin \omega_0(t - t_i) \quad . \quad (3.55)$$

Thus

$$F_{\omega_0}(t_f) = \frac{1}{\omega_0} \sin \omega_0(t_f - t_i) \quad (3.56)$$

and the GY formula predicts

$$\frac{\text{Det}[-\partial_t^2 - \omega_0^2]}{\text{Det}[-\partial_t^2]} = \frac{\sin \omega_0(t_f - t_i)}{\omega_0(t_f - t_i)} \quad , \quad (3.57)$$

in perfect agreement with the result (3.37).

Some comments:

1. If $f(t)$ is a solution of the harmonic oscillator equation with $f(t_i) = 0$, the GY solution is evidently $F_\omega(t) = f(t)/\dot{f}(t_i)$ with

$$F_\omega(t_f) = \frac{f(t_f)}{\dot{f}(t_i)} \quad . \quad (3.58)$$

If, on the other hand, $f(t)$ is any solution of the harmonic oscillator equation with $f(t_i) \neq 0$, the GY solution can be constructed from it as

$$F_\omega(t) = f(t_i)f(t) \int_{t_i}^t dt' \frac{1}{f(t')^2} \quad (3.59)$$

In particular, one has

$$F_\omega(t_f) = f(t_i)f(t_f) \int_{t_i}^{t_f} dt \frac{1}{f(t)^2} \quad . \quad (3.60)$$

2. The denominator $t_f - t_i$ in the GY formula (3.51) can be interpreted as $F_0(t_f)$, where

$$F_0(t) = t - t_i \quad (3.61)$$

solves the free-particle ($\omega = 0$) equations of motion with the GY boundary conditions, so that one can write (3.51) in the more suggestive form

$$\frac{\text{Det}[-\partial_t^2 - \omega(t)^2]}{\text{Det}[-\partial_t^2]} = \frac{F_\omega(t_f)}{F_0(t_f)} . \quad (3.62)$$

3. Comparison with the VVPM formula gives the relation

$$\frac{\partial^2 S[x_c]}{\partial x_i \partial x_f} = -\frac{m}{F_\omega(t_f)} . \quad (3.63)$$

With a bit of effort this purely classical (in the sense of classical mechanics) formula can be proved directly via Hamilton-Jacobi theory (see Appendix C), but this by itself provides no insight into the reason for the validity of either the VVPM or the GY formula.

A slick proof of the GY formula, in the form (3.62) has been given by S. Coleman in his Erice lectures on *The uses of instantons* (Appendix A), reprinted in

S. Coleman, *Aspects of Symmetry, Selected Erice Lectures*, Cambridge University Press (1985).

This proof is also reproduced in

L.S. Schulman, *Techniques and Applications of Path Integration*, Dover (2005).

It works roughly as follows (to make this argument more precise one should insert words like “Fredholm operators” etc. in appropriate places):

Let $F_{\omega,\lambda}(t)$ be the solution of the equation

$$(-\partial_t^2 - \omega(t)^2)F_{\omega,\lambda}(t) = \lambda F_{\omega,\lambda}(t) \quad (3.64)$$

with the GY boundary conditions

$$F_{\omega,\lambda}(t_i) = 0 \quad , \quad \dot{F}_{\omega,\lambda}(t_i) = 1 . \quad (3.65)$$

Thus $F_{\omega,0}(t)$ is what we called $F_\omega(t)$ above, and $F_{\omega,\lambda}(t)$ has the property that $F_{\omega,\lambda}(t_f) = 0$ iff λ is an eigenvalue of the operator $(-\partial_t^2 - \omega(t)^2)$ with zero Dirichlet boundary conditions (because then $F_{\omega,\lambda}(t)$ is the corresponding eigenfunction).

The claim is now that

$$\frac{\text{Det}[-\partial_t^2 - \omega(t)^2 - \lambda]}{\text{Det}[-\partial_t^2 - \lambda]} = \frac{F_{\omega,\lambda}(t_f)}{F_{0,\lambda}(t_f)} \quad (3.66)$$

for all $\lambda \in \mathbb{C}$. Here, Det is again defined to be the product of all eigenvalues. In particular, this implies the GY result (3.62) for $\lambda = 0$.

To establish this claim, one considers the left and right hand sides as functions of the complex variable λ . The left hand side is a meromorphic function of λ with a simple zero at each eigenvalue λ_n of $(-\partial_t^2 - \omega(t)^2)$ (an eigenvalue λ_n of $(-\partial_t^2 - \omega(t)^2)$ is a zero eigenvalue of $(-\partial_t^2 - \omega(t)^2) - \lambda_n$), and a simple pole at each eigenvalue $\lambda_{0,n}$ of $(-\partial_t^2)$ (for the same reason). By the remark above (3.66), exactly the same is true of the right hand side. In particular, the ratio of the left and the right hand sides has no poles and is therefore an *analytic* function of λ .

Moreover, provided that $\omega(t)$ is a bounded function of t , for λ sufficiently large, $|\lambda| \rightarrow \infty$, one can ignore $\omega(t)$, and hence both the left and the right hand side go to 1 in that limit (everywhere except on the real positive line where one can find large real eigenvalues).

Putting these two observations together, one concludes that the ratio of the two sides is an analytic function of λ that goes to 1 in any direction except perhaps along the positive real axis, and this implies that the ratio is equal to 1 identically, which concludes the proof of the identity (3.66).

Another elegant continuum (i.e. non-discretised) proof of the GY formula (3.51) can be found in

H. Kleinert, A. Chervyakov, *Simple Explicit Formulas for Gaussian Path Integrals with Time-Dependent Frequencies*, Phys. Lett. A245 (1998) 345-357; [quant-ph/9803016](#).

Yet another proof can be assembled from sections 3.3, 3.5 and 34.2 of

J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Oxford Science Publications, 1989).

A proof along these lines is also outlined in Appendix A of

R. Rajaraman, *Solitons and Instantons* (North Holland 1982, 1987)

3.6 SOME COMMENTS ON THE REGULARISATION OF DETERMINANTS

In the above we have repeatedly encountered determinants of infinite-dimensional operators, and we have treated them in quite a formal and cavalier way. In the following, I want to (very) briefly indicate some ways to define these objects in a more satisfactory manner.

There are certain infinite-dimensional operators for which the definition of a determinant poses no real problem. For example, for most intents and purposes, trace class operators K (i.e. operators for which the trace exists), and operators of the form $\mathbb{I} + K$, where \mathbb{I} is

the identity operator and K a trace class operator, behave like finite-dimensional linear operators (matrices). For invertible $(n \times n)$ -matrices M one can write the determinant (with $K = \mathbb{I} - M$) as

$$\det M = \det(\mathbb{I} + K) = 1 + \text{tr } K + \text{tr}(\wedge^2 K) + \dots + \text{tr}(\wedge^n K) . \quad (3.67)$$

Here $\wedge^p K$ (the p 'th anti-symmetric power of K) denotes the operator implementing the induced action of K on anti-symmetric p -vectors. Analogously, one can define the (Fredholm) determinant of an invertible operator $\mathbb{I} + K$ with K trace class by

$$\text{Det}_F(\mathbb{I} + K) = 1 + \text{Tr } K + \text{Tr}(\wedge^2 K) + \dots , \quad (3.68)$$

since this series is absolutely convergent. However, most operators appearing in physics are not of this form, and hence one needs to be more creative.

In section 3.4 we had seen that, even though $\text{Det}(-\partial_t^2 - \omega_0^2)$ (the product of the eigenvalues) diverges, the ratio of this determinant and the (equally divergent) free particle determinant gave us a finite result. More generally, the ratio of determinants that appears in (3.47) can be interpreted as defining a *regularised* functional determinant of the operator $(-\partial_t^2 - \omega(t)^2)$, in the sense of

$$\text{Det}_{reg}[-\partial_t^2 - \omega(t)^2] := \frac{\text{Det}[-\partial_t^2 - \omega(t)^2]}{\text{Det}[-\partial_t^2]} \quad (3.69)$$

It is this regularised determinant that the normalised path integral with measure $\hat{D}[x]$ computes (cf. (2.28,3.18)),

$$\int_{y(t_i)=y(t_f)=0} \hat{D}[y(t)] e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_i}^{t_f} y(t) (-\partial_t^2 - \omega(t)^2) y(t)} = \left(\text{Det}_{reg}[-\partial_t^2 - \omega(t)^2] \right)^{-1/2} . \quad (3.70)$$

However, usually in the physics literature one adopts a slightly different attitude. Instead of regularising explicitly by means of the free particle determinant (which is nevertheless natural from the path integral point of view) one attempts to define meaningful individual (instead of ratios of) regularised functional determinants in other ways, e.g. via the so-called ζ -function or heat kernel regularisation.

For a sufficiently reasonable (elliptic, self-adjoint, ...) operator A with eigenvalues λ_n , define the *spectral ζ -function* of A to be the function

$$\zeta_A(s) = \sum_n \lambda_n^{-s} . \quad (3.71)$$

This generalises the definition of the ordinary Riemann ζ -function $\zeta(s)$,

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s} . \quad (3.72)$$

To see the relation between the spectral ζ -function and the determinant, one differentiates once,

$$\zeta'_A(s) = - \sum_n n^{-s} \log \lambda_n , \quad (3.73)$$

to conclude that

$$\zeta'_A(0) = - \sum_n \log \lambda_n = - \log \prod_n \lambda_n . \quad (3.74)$$

Formally, therefore, one has

$$\prod_n \lambda_n = e^{-\zeta'_A(0)} , \quad (3.75)$$

but, at this point, the left hand side is as ill-defined as the right hand side because $\zeta_A(s)$, as it stands, will be convergent only for $\text{Re}(s)$ sufficiently large and positive (and not at $s = 0$).

Likewise, the ordinary Riemann ζ -function, as it stands, converges only for $\text{Re}(s) > 1$. However, in that case it is well known that $\zeta(s)$ can be analytically continued to a meromorphic function of s in the entire complex s -plane, with a pole only at $s = 1$. In particular, one then has cute results like

$$\begin{aligned} \zeta(0) &= -\frac{1}{2} & \left(\sum_{n=1}^{\infty} 1 \right) \\ \zeta(-1) &= -\frac{1}{12} & \left(\sum_{n=1}^{\infty} n \right) \\ \zeta(-2) &= 0 & \left(\sum_{n=1}^{\infty} n^2 \right) \end{aligned} \quad (3.76)$$

(for a poor man's (handwaving) proof of these identities, see Appendix D) as well as (we will need this below)

$$\zeta'(0) = -\frac{1}{2} \log 2\pi . \quad (3.77)$$

Note that, with

$$\zeta'(0) = - \sum_{n=1}^{\infty} \log n , \quad (3.78)$$

this result can be written as the equally cute and astounding identity

$$\prod_{n=1}^{\infty} n^2 = 2\pi . \quad (3.79)$$

Analogously, under favourable circumstances the spectral ζ -function $\zeta_A(s)$ can be extended to a meromorphic function of s which is holomorphic at $s = 0$, and then (3.75) can be used to define the ζ -function regularised determinant of A via

$$\text{Det}_{\zeta} A = e^{-\zeta'_A(0)} . \quad (3.80)$$

To illustrate this method, let us go back to the calculation of the free particle determinant in section 3.3. There we had seen that the eigenvalues of the operator $A = -\partial_t^2$

(with Dirichlet boundary conditions) are

$$\lambda_n = \frac{n^2 \pi^2}{T^2} \quad n = 1, 2, \dots \quad (3.81)$$

where $T = t_f - t_i$. To define the determinant, we construct the spectral ζ -function

$$\zeta_A(s) = \sum_{n=1}^{\infty} \left(\frac{n\pi}{T} \right)^{-2s} = \left(\frac{T}{\pi} \right)^{2s} \zeta(2s) = e^{2s \log(T/\pi)} \zeta(2s) \quad (3.82)$$

and calculate

$$\zeta'_A(0) = 2\zeta(0) \log(T/\pi) + 2\zeta'(0) = -\log(T/\pi) - \log(2\pi) = -\log(2T) \quad (3.83)$$

Thus we conclude that, with ζ -function regularisation,

$$\text{Det}_\zeta[-\partial_t^2] = 2T \quad (3.84)$$

Likewise, for the harmonic oscillator determinant of section 3.4 with

$$\lambda_n = \frac{n^2 \pi^2}{T^2} - \omega_0^2 \quad n = 1, 2, \dots \quad (3.85)$$

one finds

$$\text{Det}_\zeta[-\partial_t^2 - \omega_0^2] = 2T \frac{\sin T\omega_0}{T\omega_0} \quad (3.86)$$

In particular, we have

$$\frac{\text{Det}_\zeta[-\partial_t^2 - \omega_0^2] \frac{\sin T\omega_0}{T\omega_0}}{\text{Det}_\zeta[-\partial_t^2]} = \frac{\sin T\omega_0}{T\omega_0} \quad (3.87)$$

in perfect agreement with the previously obtained result (3.37),

$$\sqrt{\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega_0^2]}} = \sqrt{\frac{\omega_0(t_f - t_i)}{\sin \omega_0(t_f - t_i)}} \quad (3.88)$$

While this ζ -function regularised definition of the determinant captures most of the essential properties of the standard determinant, some care is required in manipulating these objects. For example, one important property of the standard determinant in the finite-dimensional case is its multiplicativity $\det(MN) = \det(M) \det(N)$. To what extent an analogous identity

$$\text{Det}_\zeta(AB) \stackrel{?}{=} \text{Det}_\zeta A \text{Det}_\zeta B \quad (3.89)$$

holds in the infinite-dimensional case is discussed e.g. in elementary terms in

hep-th/9804118; E. Elizalde, *On the concept of determinant for the differential operators of Quantum Physics*, hep-th/9906229,

and, from a more mathematical point of view, in (warning: not for the faint of heart)

M. Kontsevich, S. Vishik, *Determinants of elliptic pseudo-differential operators* (155 p., hep-th/9404046).

3.7 EXERCISES

1. Verify (3.29). Instead of calculating the classical action by integration, try to determine it in an intelligent way by proving first that only boundary terms contribute to the classical action,

$$S[x_c] = \frac{m}{2} [x_f \dot{x}_c(t_f) - x_i \dot{x}_c(t_i)] . \quad (3.90)$$

2. Verify that the harmonic oscillator kernel (3.38)
 - satisfies the harmonic oscillator Schrödinger equation (1.15)
 - and the initial condition (1.14),
 - and reduces to the free particle propagator for $\omega_0 \rightarrow 0$.
3. Verify the result (3.40) for the partition function of the harmonic oscillator, and the expansion (3.41).
4. Fill in the missing steps in the proof of the identity (3.63) given in Appendix C. In particular, verify (C.10).
5. Find an elementary proof of the VVPM formula

$$\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega(t)^2]} = -\frac{(t_f - t_i)}{m} \frac{\partial^2 S[x_c]}{\partial x_i \partial x_f} \quad (3.91)$$

or the GY formula

$$\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega(t)^2]} = \frac{F_0(t_f)}{F_\omega(t_f)} \quad (3.92)$$

and publish it and/or tell me about it.

4 GENERATING FUNCTIONALS AND PERTURBATIVE EXPANSIONS

In this section we will study some other important properties of the path integral, in particular the perturbative and semi-classical expansion of non-Gaussian path integrals. The treatment in this section is somewhat more cursory than in the previous sections - the main intention is to give a flavour of things to come (in a course on quantum field theory, say).

4.1 THE GENERATING FUNCTIONAL $Z[J]$

The main objects of interest in quantum field theory are vacuum expectation values of time-ordered products of field operators. These matrix elements can be obtained from a generating functional which, in turn, can be expressed as a path integral. This motivates the following discussion of these concepts in the quantum mechanical context.

Before turning to the path integral, we introduce the generating functionals for the correlation functions (n -point functions)

$$\begin{aligned} G_{fi}(x(t_1), \dots, x(t_n)) &= \langle x_f, t_f | \mathcal{T}(\hat{x}(t_1) \dots \hat{x}(t_n)) | x_i, t_i \rangle \\ G(x(t_1), \dots, x(t_n)) &= \langle 0 | \mathcal{T}(\hat{x}(t_1) \dots \hat{x}(t_n)) | 0 \rangle . \end{aligned} \quad (4.1)$$

They are defined as

$$\begin{aligned} Z_{fi}[j] &= \sum_{n=0}^{\infty} \frac{(i/\hbar)^n}{n!} \int_{t_i}^{t_f} dt_1 \dots dt_n j(t_1) \dots j(t_n) G_{fi}(x(t_1), \dots, x(t_n)) \\ &= \langle x_f, t_f | \mathcal{T} e^{(i/\hbar) \int_{t_i}^{t_f} dt j(t) \hat{x}(t)} | x_i, t_i \rangle \end{aligned} \quad (4.2)$$

$$\begin{aligned} Z[j] &= \sum_{n=0}^{\infty} \frac{(i/\hbar)^n}{n!} \int_{-\infty}^{+\infty} dt_1 \dots dt_n j(t_1) \dots j(t_n) G(x(t_1), \dots, x(t_n)) \\ &= \langle 0 | \mathcal{T} e^{(i/\hbar) \int_{-\infty}^{+\infty} dt j(t) \hat{x}(t)} | 0 \rangle . \end{aligned} \quad (4.3)$$

From these generating functionals, the individual correlation functions can evidently be reconstructed by differentiation,

$$\begin{aligned} G_{fi}(x(t_1), \dots, x(t_n)) &= \left(\frac{\hbar}{i} \right)^n \frac{\delta^n Z_{fi}[j]}{\delta j(t_1) \dots \delta j(t_n)} \Big|_{j(t)=0} \\ G(x(t_1), \dots, x(t_n)) &= \left(\frac{\hbar}{i} \right)^n \frac{\delta^n Z[j]}{\delta j(t_1) \dots \delta j(t_n)} \Big|_{j(t)=0} . \end{aligned} \quad (4.4)$$

For $Z_{fi}[j]$ we can easily deduce a path integral representation. Using (2.60) and the definition (4.2), one finds

$$Z_{fi}[j] = \mathcal{N} \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar) S[x(t); j(t); t_f, t_i]} , \quad (4.5)$$

where

$$S[x(t); j(t); t_f, t_i] = S[x(t); t_f, t_i] + \int_{t_i}^{t_f} dt j(t)x(t) \quad (4.6)$$

is the action with a source term (or the action with a coupling of $x(t)$ to the current $j(t)$). Thus the generating functional $Z_{fi}[j]$ is the path integral for the action with a source term.

Our aim is now to find a similar path integral representation for $Z[j]$. For that we need to project from the states $|x, t\rangle$ to the ground state $|0\rangle$. To that end we first expand the state $|x, t\rangle$ in a basis of eigenstates $|n\rangle$ of the Hamiltonian,

$$|x, t\rangle = e^{(i/\hbar)t\hat{H}}|x\rangle = \sum_n e^{(i/\hbar)t\hat{H}}|n\rangle \langle n|x\rangle = \sum_n e^{(i/\hbar)tE_n} \psi_n^*(x)|n\rangle \quad (4.7)$$

Thus for the correlation functions (2.60) of time-ordered products of operators one finds

$$G_{fi}(x(t_1), \dots, x(t_n)) = \sum_{m,n} e^{-(i/\hbar)t_f E_n + (i/\hbar)t_i E_m} \times \psi_n(x_f) \psi_m^*(x_i) \langle n|\mathcal{T}(\hat{x}(t_1) \dots \hat{x}(t_n))|m\rangle \quad (4.8)$$

To accomplish the projection onto the vacuum expectation value, we now take the limit $t_{f,i} \rightarrow \pm\infty$. This can be understood in a number of related ways. They all amount to the statement that, in the sense of distributions, $\exp(-itE) \rightarrow 0$ for $t \rightarrow \infty$, the dominant contribution in that limit coming from the smallest possible value of E , i.e. from the ground state. Explicitly, one can for instance replace $E_n \rightarrow (1 - i\epsilon)E_n$ for a small positive ϵ and then take the limit $\epsilon \rightarrow 0$ at the end. Alternatively, one can “analytically continue” to imaginary time, take the limit there, and then continue back to real time. In whichever way one proceeds, one can conclude that

$$G(x(t_1), \dots, x(t_n)) = \langle 0|\mathcal{T}(\hat{x}(t_1) \dots \hat{x}(t_n))|0\rangle \quad (4.9)$$

$$= \lim_{t_{f,i} \rightarrow \pm\infty} \frac{e^{(i/\hbar)(t_f - t_i)E_0}}{\psi_0(x_f)\psi_0^*(x_i)} \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] x(t_1) \dots x(t_n) e^{(i/\hbar)S[x(t); t_f, t_i]} \quad .$$

As the left hand side is independent of the boundary conditions $x_{f,i}$ imposed at $t \rightarrow \pm\infty$, so is the right hand side. Passing now to the generating functional $Z[j]$ (4.3), we can once again rewrite the infinite sum as an exponential in the path integral to deduce (suppressing the dependence on the boundary conditions) that

$$Z[j] \sim \int D[x(t)] e^{(i/\hbar)S[x(t); j(t); t_{f,i} = \pm\infty]} \quad , \quad (4.10)$$

where

$$S[x(t); j(t), t_{f,i} = \pm\infty] = \int_{-\infty}^{+\infty} dt [L(x(t), \dot{x}(t)) + j(t)x(t)] \quad . \quad (4.11)$$

The proportionality factor (normalisation constant) is fixed by

$$Z[j = 0] = \langle 0|0 \rangle = 1 . \quad (4.12)$$

We therefore obtain the final result

$$Z[j] = \frac{\int D[x(t)] e^{(i/\hbar)S[x(t); j(t); t_{f,i} = \pm\infty]}}{\int D[x(t)] e^{(i/\hbar)S[x(t); t_{f,i} = \pm\infty]}} . \quad (4.13)$$

The right hand side is independent of the boundary conditions imposed at $t = \pm\infty$ provided that one chooses the same boundary conditions in the numerator and the denominator.

4.2 GREEN'S FUNCTIONS AND THE GENERATING FUNCTIONAL FOR QUADRATIC THEORIES

As we will reduce the calculation of a general path integral and its generating functional to that of a quadratic theory, in this section we will determine explicitly the generating functional for the latter.

For finite-dimensional Fresnel integrals one has (see e.g. Exercise 1.5.3 and equation (A.13))

$$\int d^d x e^{iA_{ab}x^a x^b/2 + i j_a x^a} = \left(\det \frac{A}{2\pi i} \right)^{-1/2} e^{-iG^{ab} j_a j_b/2} , \quad (4.14)$$

where G^{ab} is the inverse matrix ("Green's function") to A_{ab} , $G^{ab} A_{bc} = \delta_c^a$. Thus the "generating function" is

$$\begin{aligned} z_0[j] &:= \frac{\int d^d x e^{iA_{ab}x^a x^b/2 + i j_a x^a}}{\int d^d x e^{iA_{ab}x^a x^b/2}} \\ &= e^{-iG^{ab} j_a j_b/2} . \end{aligned} \quad (4.15)$$

It follows from this that the "2-point function"

$$\langle x_c x_d \rangle := \frac{\int d^d x x_c x_d e^{iA_{ab}x^a x^b/2}}{\int d^d x e^{iA_{ab}x^a x^b/2}} \quad (4.16)$$

is

$$\begin{aligned} \langle x_c x_d \rangle &= \left[\frac{1}{i} \frac{\partial}{\partial j_c} \frac{1}{i} \frac{\partial}{\partial j_d} z_0[j] \right]_{j=0} \\ &= \left[\frac{1}{i} \frac{\partial}{\partial j_c} \left(-G^{ad} j_a z_0[j] \right) \right]_{j=0} \\ &= iG^{cd} . \end{aligned} \quad (4.17)$$

Thus the “2-point function” is the “Green’s function” of the Fresnel integral.

Higher moments (n -point functions) can be calculated in a similar way. For n odd they are manifestly zero. For the 4-point function one finds (Exercise)

$$\langle x_a x_b x_c x_d \rangle = \langle x_a x_b \rangle \langle x_c x_d \rangle + \langle x_a x_c \rangle \langle x_b x_d \rangle + \langle x_a x_d \rangle \langle x_b x_c \rangle \quad (4.18)$$

etc. The general result, expressing the $2n$ -point functions as a sum over all possible pairings $P(x_1, \dots, x_{2n})$,

$$\langle x_1 \dots x_{2n} \rangle = \sum_{P(x_1, \dots, x_{2n})} \langle x_{i_1} x_{i_2} \rangle \dots \langle x_{i_{2n-1}} x_{i_{2n}} \rangle \quad (4.19)$$

(there are $(2n - 1)!!$ terms) is also easily deduced from the generating function $z_0[j]$. In the quantum field theory context, this result is known as *Wick’s Theorem* and, even though a simple result, is of enormous practical significance in perturbative calculations.

We now consider the analogous question for harmonic oscillator path integrals. In this case, one finds, in precise analogy with the finite-dimensional case,

$$Z_0[j] = e^{-\frac{i}{m\hbar} \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' j(t) G(t, t') j(t') / 2} \quad (4.20)$$

where $G(t, t')$ is a Green’s function (the inverse) of the operator $-\partial_t^2 - \omega(t)^2$,

$$(-\partial_t^2 - \omega(t)^2) G_0(t, t') = \delta(t - t') \quad (4.21)$$

For the finite-time path integral, the Green’s function that appears here would have been determined by the Dirichlet (zero) boundary conditions at $t_{i,f}$ to be the Green’s function with

$$G_0(t, t_i) = G_0(t, t_f) = 0 \quad (4.22)$$

In the present case (infinite time interval), the relevant Green’s function is implicitly determined by an $i\epsilon$ prescription. In particular, for the time-independent harmonic oscillator with constant frequency ω_0 one finds

$$G_0(t, t') = \frac{1}{2i\omega_0} e^{-i\omega_0 |t - t'|} \quad (4.23)$$

Once we know the generating functional, we can use it to calculate n -point functions. In particular, for the two-point function one has

$$\begin{aligned} \langle 0 | \mathcal{T}(\hat{x}(t) \hat{x}(t')) | 0 \rangle &= \left[\frac{\hbar}{i} \frac{\delta}{\delta j(t)} \frac{\hbar}{i} \frac{\delta}{\delta j(t')} Z_0[j] \right]_{j=0} \\ &= \frac{i\hbar}{m} G_0(t, t') \quad (4.24) \end{aligned}$$

That the time-ordered product $\langle 0 | \mathcal{T}(\hat{x}(t) \hat{x}(t')) | 0 \rangle$ is a Green’s function can of course also be verified directly in the standard operator formulation of quantum mechanics (Exercise). Likewise, higher n -point functions can be expressed in terms of products of 2-point functions (Wick’s theorem again).

4.3 PERTURBATIVE EXPANSION AND GENERATING FUNCTIONALS

As we have seen, the generating functional $Z[j]$ encodes all the information about the n -point functions $G(x_1, \dots, x_n)$. However, this is only useful if supplemented by a prescription for how to calculate $Z[j]$. Since in practice the only path integrals that we can do explicitly are Gaussian path integrals and their close relatives, the question arises how to reduce the evaluation of $Z[j]$ to an evaluation of Gaussian integrals. This is achieved via a perturbative expansion of the path integral around a quadratic (Gaussian) action. The (assumed) small perturbation expansion parameter can be a coupling constant λ , as in

$$\hat{H} = \hat{H}_0 + \lambda \hat{W} \ , \quad (4.25)$$

with \hat{H}_0 a harmonic oscillator Hamiltonian. In this case one is studying a path integral counterpart of standard quantum mechanical perturbation theory.

Alternatively, the small parameter could be Planck's constant \hbar itself. In this case one is interested in evaluating the path integral

$$\int D[x] e^{(i/\hbar)S[x]} \quad (4.26)$$

for $\hbar \rightarrow 0$ as a power series in \hbar by expanding the action around a classical solution $x_c(t)$. This is a semi-classical expansion of the path integral, a counterpart of the standard WKB approximation of quantum mechanics.

Both physically and technically (in one case one has a small parameter in front of a part of the action, the perturbation, in the other a large parameter $1/\hbar$ in front of the entire action) these two expansions appear to be quite distinct. Calculationally, however, they are rather similar, since in both cases the path integral can be reduced to a series expansion in derivatives of the generating functional of the quadratic theory. This is immediate for the perturbative λ -expansion (which we will consider in this section) but requires a minor bit of trickery for the \hbar -expansion (hence the excursion into the stationary phase approximation for finite-dimensional integrals in section 4.5).

For definiteness, we will assume that the perturbation \hat{W} arises from a velocity-independent perturbation of the potential

$$V(x) = V_0(x) + \lambda W(x) \ , \quad (4.27)$$

with $V_0(x)$ a harmonic oscillator potential. For more complicated perturbations one would have to go back to the phase space path integral, introduce sources for both $\hat{x}(t)$ and $\hat{p}(t)$, etc. Then the action takes the form

$$S[x] = S_0[x] + \lambda S_I[x] = S_0[x] - \lambda \int dt W(x(t)) \ , \quad (4.28)$$

where $S_0[x]$ is the free action, and $S_I[x]$ the perturbation or interaction term.

To calculate the path integral, one introduces a source-term for the free action $S_0[x]$,

$$S_0[x, j] = S_0[x] + \int dt j(t)x(t); \quad (4.29)$$

and determines $Z_{f_{i,0}}[j]$ or $Z_0[j]$. Focussing on the latter, the vacuum generating functional $Z[j]$ for the perturbed action can then be written in terms of that for the free action as

$$Z[j] = \mathcal{N} e^{(i\lambda/\hbar)S_I[\frac{\hbar}{i}\frac{\delta}{\delta j(t)}]} Z_0[j] . \quad (4.30)$$

The normalisation constant, determined by the condition $Z[j = 0] = 1$, is

$$\mathcal{N}^{-1} = \left[e^{(i\lambda/\hbar)S_I[\frac{\hbar}{i}\frac{\delta}{\delta j(t)}]} Z_0[j] \right]_{j=0} \quad (4.31)$$

This result for $Z[j]$ is manifestly a power series expansion in λ - and the fact that this perturbative expansion is so straightforward to obtain in the path integral formalism is one of the reasons that makes the path integral approach to quantum field theory so powerful.

Moreover, using the explicit expression (4.20) for the generating functional $Z_0[j]$ in terms of the Green's functions of the free theory, one sees that the generating functional $Z[j]$, and thus all the n -point functions of the perturbed theory, are expressed as a series expansion in terms of the Green's functions of the unperturbed theory. A graphical representation of this expansion leads to the Feynman diagram expansion of quantum mechanics (and quantum field theory).

4.4 THE STATIONARY PHASE APPROXIMATION FOR OSCILLATORY INTEGRALS

The integrals of interest in this section are oscillatory integrals of the kind

$$\int_{-\infty}^{+\infty} dx e^{(i/\hbar)f(x)} . \quad (4.32)$$

The basic tenet of the stationary phase approximation of such integrals is that for small \hbar , $\hbar \rightarrow 0$, the integrand oscillates so rapidly that the integral over any small x -interval will give zero unless one is close to a critical point x_c of $f(x)$, $f'(x_c) = 0$, for which to first order around x_c there are no oscillations. This suggests that for $\hbar \rightarrow 0$ the integral is dominated by the contribution from the neighbourhood of some critical point(s) x_c of $f(x)$, and that therefore in this limit the dominant contribution to the integral can be obtained by a Taylor expansion of $f(x)$ around $x = x_c$.

To set the stage for this discussion, we will first reconsider the Gaussian and Fresnel integrals of Appendix A from this point of view. There we had obtained the formula (A.13),

$$\int_{-\infty}^{+\infty} dx e^{iax^2/2 + ijx} = \sqrt{\frac{2\pi i}{a}} e^{-ij^2/2a} \quad (4.33)$$

by analytic continuation from the corresponding Gaussian integral and/or completing the square. A (for the following) more instructive way of obtaining this result is to consider the integral

$$\int_{-\infty}^{+\infty} dx e^{(i/\hbar)q(x)} \quad (4.34)$$

for some quadratic function of x ($q(x) = ax^2/2 + jx + c$, say). Such a function has a unique critical point x_c ($x_c = -j/a$), and since $q(x)$ is quadratic and $q'(x_c) = 0$ one can write $q(x)$ as

$$q(x) = q(x_c) + \frac{1}{2}(x - x_c)^2 q''(x_c) \quad (4.35)$$

Thus the integral is

$$\begin{aligned} \int_{-\infty}^{+\infty} dx e^{(i/\hbar)q(x)} &= e^{(i/\hbar)q(x_c)} \int_{-\infty}^{+\infty} dy e^{(i/\hbar)q''(x_c)y^2/2} \\ &= e^{(i/\hbar)q(x_c)} \sqrt{\frac{2\pi i\hbar}{q''(x_c)}} \end{aligned} \quad (4.36)$$

This reproduces and generalises (4.33).

It will be more convenient to move the factor $\sqrt{2\pi i\hbar}$ to the left, so that the result is

$$\frac{1}{\sqrt{2\pi i\hbar}} \int_{-\infty}^{+\infty} dx e^{(i/\hbar)q(x)} = \frac{1}{\sqrt{q''(x_c)}} e^{(i/\hbar)q(x_c)} \quad (4.37)$$

We see that a Fresnel integral is determined exactly by the contribution from the critical point and the quadratic fluctuations around it. Another way of saying this is that, as we will see, for a Gaussian Fresnel integral the stationary phase approximation is exact.

Now let us consider the oscillatory integral

$$I[f] = \frac{1}{\sqrt{2\pi i\hbar}} \int_{-\infty}^{+\infty} dx e^{(i/\hbar)f(x)} \quad (4.38)$$

for a general function $f(x)$. Let x_c denote the critical point of $f(x)$ with the smallest absolute value, and assume that x_c is isolated. Then we can expand $f(x)$ around x_c as

$$f(x) = f(x_c) + \frac{1}{2}(x - x_c)^2 f''(x_c) + R(x - x_c) \quad , \quad (4.39)$$

where the rest $R(x - x_c)$ is at least cubic in $(x - x_c)$. Thus the integral is

$$I[f] = \frac{1}{\sqrt{2\pi i\hbar}} e^{(i/\hbar)f(x_c)} \int_{-\infty}^{+\infty} dx e^{(i/\hbar)[f''(x_c)(x - x_c)^2/2 + R(x - x_c)]} \quad (4.40)$$

The *stationary phase approximation* (also known as the *saddle point approximation*) to the integral amounts to ignoring the higher than quadratic terms encoded in $R(x - x_c)$ and leads to the approximate result

$$\frac{1}{\sqrt{2\pi i\hbar}} \int_{-\infty}^{+\infty} dx e^{(i/\hbar)f(x)} \approx \frac{1}{\sqrt{f''(x_c)}} e^{(i/\hbar)f(x_c)} . \quad (4.41)$$

To justify this approximation, one needs to show that the contributions due to the remainder $R(x - x_c)$ are indeed subleading in \hbar as $\hbar \rightarrow 0$. We will establish this below.

Another cause for concern may be that, while we have (hand-wavily) argued that the dominant contribution to the oscillatory integral should arise from a small neighbourhood of the critical point(s), in order to arrive at (4.41) we have taken the integral not over a small neighbourhood of x_c but, quite on the contrary, over $(-\infty, +\infty)$.

To justify this, consider the contribution to the integral from an interval $[a, b]$ without critical points. In that interval, one can change the integration variable from x to $f(x)$ (this would not be allowed if $f(x)$ had a critical point in the interval). Then it is easy to see (e.g. by an integration by parts) that the integral

$$\int_a^b dx e^{(i/\hbar)f(x)} = \mathcal{O}(\hbar) . \quad (4.42)$$

Thus regions without critical points contribute $\mathcal{O}(\hbar)$ terms to the integral. On the other hand, (4.41) shows that, regardless of what the neglected terms do, there are some contributions to the total integral which are of order $\mathcal{O}(\hbar^{1/2})$. Thus these must be due to the contributions from (integrals over arbitrarily small neighbourhoods of) the critical points. As these are dominant relative to the $\mathcal{O}(\hbar)$ contributions as $\hbar \rightarrow 0$, the difference between integrating over such a neighbourhood of the critical point and integrating over all x is negligible in this limit.

To analyse the contributions due to $R(x - x_c)$ and to make the dependence of the various terms on \hbar more transparent, it is convenient to define the fluctuation variable y not as $(x - x_c)$, as was implicitly done in (4.36), but via

$$x = x_c + \sqrt{\hbar}y . \quad (4.43)$$

This has the effect of making the Gaussian part of the integral independent of \hbar ,

$$(x - x_c)^2/2\hbar = y^2/2 . \quad (4.44)$$

Moreover, since $R(x - x_c)$ is at least cubic, $(1/\hbar)R(\sqrt{\hbar}y)$ is now a power series in strictly positive powers of $\sqrt{\hbar}$,

$$r(y) \equiv (1/\hbar)R(\sqrt{\hbar}y) = \hbar^{1/2}f^{(3)}(x_c)y^3/3! + \hbar f^{(4)}(x_c)y^4/4! + \dots \quad (4.45)$$

even (odd) powers of y appearing with integral (half-integral) powers of \hbar . All in all, we thus have

$$\frac{1}{\sqrt{2\pi i\hbar}} \int_{-\infty}^{+\infty} dx e^{(i/\hbar)f(x)} = \frac{1}{\sqrt{2\pi i}} e^{(i/\hbar)f(x_c)} \int_{-\infty}^{+\infty} dy e^{i[f''(x_c)y^2/2 + r(y)]} . \quad (4.46)$$

To obtain the higher order corrections to the stationary phase approximation, one can expand $\exp ir(y)$. Remembering that only even powers of y in that expansion give a non-zero contribution to the y -integral, one concludes that this expresses the integral as a power series in (integral) powers of \hbar ,

$$\frac{1}{\sqrt{2\pi i\hbar}} \int_{-\infty}^{+\infty} dx e^{(i/\hbar)f(x)} = \frac{1}{\sqrt{f''(x_c)}} e^{(i/\hbar)f(x_c)} (1 + \hbar(\dots) + \hbar^2(\dots) + \dots) \quad (4.47)$$

Alternatively, this series can be expressed in terms of generating functions as

$$1 + \hbar(\dots) + \hbar^2(\dots) + \dots = e^{ir(-i\partial/\partial j)} e^{-ij^2/2f''(x_c)}|_{j=0} . \quad (4.48)$$

The stationary phase approximation can be used to calculate the integral with reasonable accuracy for very small \hbar , $\hbar \rightarrow 0$. However, the series expansion should not be expected to converge in general, and the series is only an *asymptotic series*. If contributions from all critical points are included, it is under certain conditions possible to obtain error estimates, but in practice applications of the stationary phase approximation are usually restricted to (4.41).

4.5 THE SEMI-CLASSICAL APPROXIMATION

It is now straightforward to formally apply this stationary phase approximation to path integrals. The crucial point is that in the path integral formulation of quantum mechanics the classical limit and the emergence of classical mechanics from quantum mechanics are extremely transparent: in the limit $\hbar \rightarrow 0$, the path integral is dominated by paths that are critical points of the action, i.e. the classical solutions to the equations of motion. This should be contrasted with the much more cumbersome eikonal or WKB semi-classical approximation to the Schrödinger equation.

Essentially all the work has already been done in sections 3.5 and 4.6 and we can be brief about this here. Instead of the function $f(x)$ we have an action $S[x]$, and the semi-classical approximation amounts to expanding $S[x]$ around a critical point, i.e. a classical solution $x_c(t)$ of the corresponding Euler-Lagrange equations. This is precisely the procedure we had already advocated for how to deal with general non-Gaussian path integrals. We now see that this will lead to an expansion of the path integral in

powers of \hbar , the stationary phase approximation to the path integral agreeing with the harmonic oscillator path integral of section 3.5.

First of all, with

$$x(t) = x_c(t) + \delta x(t) \quad , \quad (4.49)$$

we expand the action as

$$\begin{aligned} S[x] &= S[x_c] + \int_{t_i}^{t_f} dt \frac{\delta S}{\delta x(t)} \Big|_{x(t)=x_c(t)} \delta x(t) \\ &\quad + \frac{1}{2} \int_{t_i}^{t_f} dt \int_{t_i}^{t_f} dt' \frac{\delta^2 S}{\delta x(t) \delta x(t')} \Big|_{x(t)=x_c(t)} \delta x(t) \delta x(t') + \dots \\ &= S[x_c] + \frac{1}{2} \int_{t_i}^{t_f} dt \int_{t_i}^{t_f} dt' \frac{\delta^2 S}{\delta x(t) \delta x(t')} \Big|_{x(t)=x_c(t)} \delta x(t) \delta x(t') + \dots \end{aligned} \quad (4.50)$$

For an action of the standard form

$$S[x] = \frac{m}{2} \int_{t_i}^{t_f} (\dot{x}(t))^2 - \frac{1}{m} V(x(t)) \quad (4.51)$$

the quadratic term is

$$\frac{1}{2} \int_{t_i}^{t_f} dt \int_{t_i}^{t_f} dt' \frac{\delta^2 S}{\delta x(t) \delta x(t')} \Big|_{x(t)=x_c(t)} \delta x(t) \delta x(t') = \frac{m}{2} \int_{t_i}^{t_f} (\delta \dot{x}(t))^2 - \frac{1}{m} V''(x_c(t)) \delta x(t)^2 \quad (4.52)$$

As already noted in section 3.5, this is the action of a harmonic oscillator with time-dependent frequency

$$\omega(t) = \frac{1}{m} V''(x_c(t)) \quad . \quad (4.53)$$

Thus the stationary phase or semi-classical approximation to the path integral is (cf. (3.47))

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] e^{(i/\hbar)S[x(t); t_f, t_i]} \approx \sqrt{\frac{m}{2\pi i \hbar (t_f - t_i)}} \sqrt{\frac{\text{Det}[-\partial_t^2]}{\text{Det}[-\partial_t^2 - \omega(t)^2]}} e^{(i/\hbar)S[x_c]} \quad . \quad (4.54)$$

This can be evaluated using either the VVPM or the GY method.

The difference between (3.47) and (4.54) is that in the former case one was dealing with a quadratic action and the result was exact (i.e. the semi-classical approximation is exact for the harmonic oscillator), whereas here this is really just the semi-classical approximation. Note also that x_c in (4.54) refers to a classical solution of the full equations of motion $m\ddot{x} = -V'(x)$ whereas x_c in (3.47) is of course a solution of the harmonic oscillator equation.

If desired, higher order corrections in \hbar to the semi-classical result can be calculated, as in (4.48), by using the generating functional of the quadratic theory.

4.6 SCATTERING THEORY AND THE PATH INTEGRAL

Formal scattering theory can be succinctly described by the evolution operator $U_I(t_f, t_i)$ in the interaction representation. Thus let the Hamiltonian be (in the simplest case of two-body potential scattering)

$$H = H_0 + V \quad (4.55)$$

where H_0 is the free-particle Hamiltonian $H_0 = \vec{p}^2/2m$. Then $U_I(t_f, t_i)$ is given by

$$U_I(t_f, t_i) = e^{(i/\hbar)t_f H_0} e^{-(i/\hbar)(t_f - t_i)H} e^{-(i/\hbar)t_i H_0} \quad (4.56)$$

The Møller operators

$$\Omega_{\pm} = \lim_{t \rightarrow \mp\infty} U_I(0, t) \quad (4.57)$$

act on free particle states $|\vec{k}_a\rangle$ (plane wave eigenstates of the free Hamiltonian H_0)

$$\langle \vec{x} | \vec{k}_a \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}_a \cdot \vec{x}} \quad (4.58)$$

$\vec{p}_a = \hbar\vec{k}_a$, $H_0|\vec{k}_a\rangle = E_a|\vec{k}_a\rangle$, to produce the stationary scattering states $\psi_a^{\pm}(\vec{x})$,

$$\Omega_{\pm}|\vec{k}_a\rangle = |\psi_a^{\pm}\rangle \quad (4.59)$$

The S-matrix elements S_{ab} are the transition amplitudes among the asymptotic in and out scattering states $|\psi_a^{\pm}\rangle$,

$$S_{ab} = \langle \psi_a^- | \psi_b^+ \rangle \quad (4.60)$$

and therefore they are the matrix elements

$$S_{ab} = \langle \vec{k}_a | S | \vec{k}_b \rangle \quad (4.61)$$

of the scattering operator

$$S = \Omega_-^\dagger \Omega_+ = \lim_{t_f, i \rightarrow \pm\infty} U_I(t_f, t_i) \quad (4.62)$$

between free particle states.

Such matrix elements can readily be expressed in terms of the path integral. First of all, we have

$$\begin{aligned} S_{ab} &= \lim_{t_f, i \rightarrow \pm\infty} \langle \vec{k}_a | e^{(i/\hbar)t_f H_0} e^{-(i/\hbar)(t_f - t_i)H} e^{-(i/\hbar)t_i H_0} | \vec{k}_b \rangle \\ &= \lim_{t_f, i \rightarrow \pm\infty} e^{(i/\hbar)(t_f E_a - t_i E_b)} \langle \vec{k}_a | e^{-(i/\hbar)(t_f - t_i)H} | \vec{k}_b \rangle \quad (4.63) \end{aligned}$$

To pass from the momentum space matrix elements of the evolution operator for H to the kernel (the position space matrix elements), we perform a double Fourier transform (this is a special case of (2.61)),

$$\langle \vec{k}_a | e^{-(i/\hbar)(t_f - t_i)H} | \vec{k}_b \rangle = \frac{1}{(2\pi)^3} \int d\vec{x}_a \int d\vec{x}_b e^{i(\vec{k}_b \cdot \vec{x}_b - \vec{k}_a \cdot \vec{x}_a)} K(\vec{x}_a, \vec{x}_b, t_f - t_i) . \quad (4.64)$$

Representing, in the usual way, the kernel by the path integral, we conclude that the S-matrix elements S_{ab} are given by a Fourier transform of the path integral. Either perturbative or semi-classical expansion techniques, as described earlier on in this section, can now be employed to obtain series expansions for these S-matrix elements.

4.7 EXERCISES

- Using the Heisenberg picture operator equations of motion or Ehrenfest's theorem, show that for a (possibly time-dependent) harmonic oscillator the time-ordered 2-point function is a Green's function,

$$(-\partial_t^2 - \omega(t)^2) \langle 0 | \mathcal{T}(\hat{x}(t)\hat{x}(t')) | 0 \rangle = \frac{i\hbar}{m} \delta(t - t') . \quad (4.65)$$

- Using the generating functional $Z_0[j]$ (4.20), express the 4-point function

$$\langle 0 | \mathcal{T}(\hat{x}(t_1)\hat{x}(t_2))\hat{x}(t_3)\hat{x}(t_4) | 0 \rangle \quad (4.66)$$

in terms of sums of products of Green's functions (2-point functions).

- Calculate the order \hbar correction to the stationary phase approximation of the integral

$$\frac{1}{\sqrt{2\pi i\hbar}} \int_{-\infty}^{+\infty} dx e^{(i/\hbar)f(x)} = \frac{1}{\sqrt{f''(x_c)}} e^{(i/\hbar)f(x_c)} (1 + \hbar(\dots) + \dots) \quad (4.67)$$

Note that *two* different terms contribute to the integral at this order.

A GAUSSIAN AND FRESNEL INTEGRALS

A.1 BASIC 1-DIMENSIONAL INTEGRALS

The basic Gaussian integral is

$$I_0[\alpha] = \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} = \sqrt{\frac{2\pi}{\alpha}} \quad \alpha \in \mathbb{R}, \alpha > 0 . \quad (\text{A.1})$$

This result can for instance be established by the standard trick of squaring the integral and passing to polar coordinates. The first generalisation we will consider is the integral

$$I_1[\alpha, j] = \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2 + jx} \quad j \in \mathbb{R} . \quad (\text{A.2})$$

By completing the square and shifting the integration variable (using translation invariance of the measure) one finds

$$I_1[\alpha, j] = \int_{-\infty}^{+\infty} dx e^{-\alpha(x - j/\alpha)^2/2 + j^2/2\alpha} = \sqrt{\frac{2\pi}{\alpha}} e^{j^2/2\alpha} . \quad (\text{A.3})$$

Another proof of this identity is based on the trivial identity

$$\int_{-\infty}^{+\infty} dx \frac{d}{dx} e^{-\alpha x^2/2 + jx} = 0 . \quad (\text{A.4})$$

Expanding this out, one finds

$$\begin{aligned} 0 &= \int_{-\infty}^{+\infty} dx (-\alpha x + j) e^{-\alpha x^2/2 + jx} \\ &= -\alpha \frac{\partial}{\partial j} I_1[\alpha, j] + j I_1[\alpha, j] . \end{aligned} \quad (\text{A.5})$$

This differential equation for $I_1[\alpha, j]$,

$$\frac{\partial}{\partial j} I_1[\alpha, j] = (j/\alpha) I_1[\alpha, j] , \quad (\text{A.6})$$

called a *Schwinger-Dyson Equation* in the quantum field theory context, is evidently solved by

$$I_1[\alpha, j] = c e^{j^2/2\alpha} , \quad (\text{A.7})$$

and the normalisation (initial) condition $I_1[\alpha, 0] = I_0[\alpha]$ then leads to

$$I_1[\alpha, j] = I_0[\alpha] e^{j^2/2\alpha} , \quad (\text{A.8})$$

which agrees with the result (A.3).

The other generalisation that will interest us is the oscillatory Fresnel integral

$$J_0[a] = I_0[-ia] = \int_{-\infty}^{+\infty} dx e^{iax^2/2} . \quad (\text{A.9})$$

It can be obtained by noting that the basic Gaussian integral is well defined for $\alpha \in \mathbb{C}$ with $\text{Re}(\alpha) > 0$, and that it continues to be well defined for $\text{Re}(\alpha) \rightarrow 0$ provided that $\text{Im}(\alpha) \neq 0$. It follows that

$$J_0[a] = \sqrt{\frac{2\pi i}{a}} = \sqrt{\frac{2\pi}{a}} e^{i\pi/4} . \quad (\text{A.10})$$

A useful way to remember this result is to relate it to the integral I_0 with a phase depending on the sign of a ,

$$J_0[a] = I_0[|a|] e^{i\text{sign}(a)\pi/4} . \quad (\text{A.11})$$

By the same reasoning, for the integral

$$J_1[a, j] = I_1[-ia, ij] = \int_{-\infty}^{+\infty} dx e^{iax^2/2 + ijx} \quad (\text{A.12})$$

one finds

$$J_1[a, j] = \sqrt{\frac{2\pi i}{a}} e^{-ij^2/2a} . \quad (\text{A.13})$$

For an alternative proof of this identity see section 4.5.

As an application, we consider an integral of the kind we encountered in sections 1 and 2, namely

$$K = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp e^{(i/\hbar)[py - \epsilon p^2/2m]} . \quad (\text{A.14})$$

By completing the square, shifting the integration variable and using the Fresnel integral formula, or directly upon using the above result for $J_1[a, j]$, one finds

$$\begin{aligned} K &= \frac{1}{2\pi\hbar} \sqrt{\frac{2\pi\hbar m}{i\epsilon}} e^{(i/\hbar)\epsilon(m/2)(y/\epsilon)^2} \\ &= \sqrt{\frac{m}{2\pi i\hbar\epsilon}} e^{\frac{i}{\hbar} \frac{m}{2} \frac{y^2}{\epsilon}} . \end{aligned} \quad (\text{A.15})$$

A.2 RELATED INTEGRALS

By symmetry considerations, one has

$$\int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} x^{2m+1} = 0 . \quad (\text{A.16})$$

The integrals of even powers x^{2m} can be calculated by relating them to the integrals I_0 or I_1 . For example, one has

$$\begin{aligned} \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} x^{2m} &= (-2)^m \frac{\partial^m}{\partial \alpha^m} \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} \\ &= (-2)^m \frac{\partial^m}{\partial \alpha^m} I_0[\alpha] . \end{aligned} \quad (\text{A.17})$$

This can be evaluated to give

$$\begin{aligned} \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} x^{2m} &= (-2)^m \sqrt{2\pi} \frac{\partial^m}{\partial \alpha^m} \alpha^{-1/2} \\ &= \sqrt{2\pi} (2m-1)!! \alpha^{-(2m+1)/2} . \end{aligned} \quad (\text{A.18})$$

However, this formula does not generalise in any useful way to path integrals. An alternative (and very slick) way to obtain the result (A.18) is to introduce, for the integrals

$$Z_\ell = \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} x^\ell , \quad (\text{A.19})$$

the *generating function*

$$Z(j) = \sum_{\ell=0}^{\infty} j^\ell Z_\ell . \quad (\text{A.20})$$

By evaluating the sum, we see that

$$Z(j) = \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2 + jx} = I_1[\alpha, j] = \sqrt{\frac{2\pi}{\alpha}} e^{j^2/2\alpha} . \quad (\text{A.21})$$

Hence, comparing powers of j , one deduces $Z_{2m+1} = 0$ and

$$Z_{2m} = \sqrt{\frac{2\pi}{\alpha}} (2\alpha)^{-m} \frac{(2m)!}{m!} . \quad (\text{A.22})$$

In view of

$$(2m)! = 2^m m! (2m-1)!! , \quad (\text{A.23})$$

this agrees precisely with (A.18).

Alternatively, instead of comparing powers, one can differentiate with respect to j , so that the result can be written as

$$\begin{aligned} \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} x^\ell &= \left[\frac{\partial^\ell}{\partial j^\ell} \int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2 + jx} \right]_{j=0} \\ &= \left[\frac{\partial^\ell}{\partial j^\ell} I_1[\alpha, j] \right]_{j=0} . \end{aligned} \quad (\text{A.24})$$

More generally, one has

$$\int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} F(x) = \left[F \left(\frac{\partial}{\partial j} \right) I_1[\alpha, j] \right]_{j=0} \quad (\text{A.25})$$

and

$$\int_{-\infty}^{+\infty} dx e^{-\alpha x^2/2} + F(x) = \left[e^{F\left(\frac{\partial}{\partial j}\right)} I_1[\alpha, j] \right]_{j=0} \quad (\text{A.26})$$

for any function $F(x)$. This justifies the name generating function and explains why the central object of interest for integrals with Gaussian weight is the integral $Z(j) = I_1[\alpha, j]$.

A.3 GAUSSIAN INTEGRALS AND DETERMINANTS

The simplest 2-dimensional Gaussian integral is

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy e^{-\alpha x^2/2 - \beta y^2/2} = \frac{2\pi}{\sqrt{\alpha\beta}}. \quad (\text{A.27})$$

This generalises to

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy e^{-(\alpha x^2 + \beta y^2 + 2\gamma xy)/2} = \frac{2\pi}{\sqrt{\alpha\beta - \gamma^2}}, \quad (\text{A.28})$$

as can be seen by completing the square.

In terms of the matrix

$$A = \begin{pmatrix} \alpha & \gamma \\ \gamma & \beta \end{pmatrix} \quad (\text{A.29})$$

the exponent of the integrand can be written as $A_{ab}x^a x^b/2$ with $x^a = (x, y)$ and the above identity reads

$$\int_{-\infty}^{+\infty} d^2x e^{-A_{ab}x^a x^b/2} = \frac{(\sqrt{2\pi})^2}{\sqrt{\det A}} = \left(\det \frac{A}{2\pi} \right)^{-1/2}. \quad (\text{A.30})$$

This way of writing this result generalises to d -dimensional integrals, $d \geq 2$. Let A be a symmetric, positive real $(d \times d)$ -matrix. Then one has

$$\int_{-\infty}^{+\infty} d^d x e^{-A_{ab}x^a x^b/2} = \left(\det \frac{A}{2\pi} \right)^{-1/2}. \quad (\text{A.31})$$

Likewise, for the oscillatory version of this integral one has

$$\int_{-\infty}^{+\infty} d^d x e^{iA_{ab}x^a x^b/2} = \left(\det \frac{A}{2\pi i} \right)^{-1/2}. \quad (\text{A.32})$$

Thus the task of calculating Gaussian integrals and their various relatives and descendants has been reduced to the purely algebraic task of calculating determinants of matrices.

The proof of the fundamental identities (A.31,A.32) is remarkably simple and will be left as an exercise. The strategy is to first prove them for A diagonal (this is trivial) and to then use the fact that any real symmetric A can be diagonalised by an orthogonal transformation, combined with the rotation invariance of the measure $d^d x$.

B INFINITE PRODUCT IDENTITIES

A useful identity, ubiquitous in determinant and index calculations, is the following infinite product representation for $(\sin x)/x$,

$$\frac{\sin x}{x} = \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2\pi^2}\right) \quad (\text{B.1})$$

The validity of this formula is plausible as the right hand side has exactly the same zeros and identical behaviour as $x \rightarrow 0$ as the left hand side. It can be proved rigorously in a variety of ways. The easiest (and closest in spirit to the rough argument in the previous sentence) is to extend $(\sin x)/x$ to a holomorphic function $(\sin z)/z$ in the complex plane and factorise using the Mittag-Leffler pole expansion - see e.g. section 7 of

G. Arfken and H. Weber, *Mathematical Methods for Physicists* Elsevier (2005).

The single identity above can be used to generate an infinite number of other identities, in the spirit of Euler. The first non-trivial one of these results from comparing the quadratic term in the expansion of the left hand side

$$\frac{\sin x}{x} = \frac{x - x^3/6 + \dots}{x} = 1 - \frac{x^2}{6} + \dots \quad (\text{B.2})$$

with the quadratic term arising from the right hand side,

$$\prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2\pi^2}\right) = 1 - \sum_{n=1}^{\infty} \frac{x^2}{n^2\pi^2} + \dots \quad (\text{B.3})$$

which provides a cute proof of the famous identity

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \quad (\text{B.4})$$

There are a host of other occasionally useful infinite product identities (none of which, however, will be used in these notes). For example, closely related infinite product representations of other trigonometric and hyperbolic functions are

$$\frac{\sinh x}{x} = \prod_{n=1}^{\infty} \left(1 + \frac{x^2}{n^2\pi^2}\right) \quad (\text{B.5})$$

$$\cos x = \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{(n - 1/2)^2\pi^2}\right) \quad (\text{B.6})$$

$$\cosh x = \prod_{n=1}^{\infty} \left(1 + \frac{x^2}{(n - 1/2)^2\pi^2}\right) \quad (\text{B.7})$$

There is also the more mysterious identity

$$\frac{\sin x}{x} = \prod_{n=1}^{\infty} \cos\left(\frac{x}{2^n}\right) . \quad (\text{B.8})$$

As another example, Euler's identity for the Riemann ζ -function

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \quad (\text{B.9})$$

is

$$\zeta(s) = \prod_{n=1}^{\infty} \frac{1}{1 - p_n^{-s}} , \quad (\text{B.10})$$

where $p_n = 2, 3, 7, 11, \dots$ is the sequence of prime numbers. This identity provides the cornerstone of the relation between number theory and complex analysis.

C EQUIVALENCE OF THE VVPM AND GY FORMULAE FOR THE FLUCTUATION DETERMINANT

The article of Kleinert and Chervyakov cited in section 3.5 contains a nice proof of the classical identity (3.63) expressing the equivalence of the VVPM (3.49) and Gelfand-Yaglom (3.51) results for the ratio of fluctuation determinants.

Consider the classical solution $x_c(t)$ with $x_c(t_{f,i}) = x_{f,i}$. This solution can equally well be regarded as a function of the initial position x_i and velocity \dot{x}_i ,

$$x_c = x_c(t, x_i, \dot{x}_i) . \quad (\text{C.1})$$

Writing this as a linear combination of two linearly independent solutions $f_1(t)$ and $f_2(t)$ of the oscillator equation,

$$x_c(t, x_i, \dot{x}_i) = x_i f_1(t) + \dot{x}_i f_2(t) \quad (\text{C.2})$$

and imposing the conditions $x_c(t_i) = x_i$ and $\dot{x}_c(t_i) = \dot{x}_i$, one finds

$$\begin{aligned} x_c(t_i) = x_i &\Rightarrow f_1(t_i) = 1 & f_2(t_i) = 0 \\ \dot{x}_c(t_i) = \dot{x}_i &\Rightarrow \dot{f}_1(t_i) = 0 & \dot{f}_2(t_i) = 1 . \end{aligned} \quad (\text{C.3})$$

This shows that $f_2(t) = F_\omega(t)$ is the GY solution,

$$F_\omega(t) = \frac{\partial x_c(t, x_i, \dot{x}_i)}{\partial \dot{x}_i} . \quad (\text{C.4})$$

At this point, one can either use directly the Hamilton-Jacobi relation

$$\frac{\partial S[x_c]}{\partial x_i} = -p_i = -m\dot{x}_i , \quad (\text{C.5})$$

to deduce (3.63). Or one can evaluate explicitly the classical action in terms of $F_\omega(t)$ and $f_1(t) \equiv G_\omega(t)$ (the “dual” GY solution, which plays a role analogous to the GY solution when one considers periodic or anti-periodic boundary conditions instead of zero boundary conditions). Thus one has

$$x_c(t) = x_i G_\omega(t) + \dot{x}_i F_\omega(t) . \quad (\text{C.6})$$

and therefore, in particular,

$$\begin{aligned} x_f &= x_i G_\omega(t_f) + \dot{x}_i F_\omega(t_f) \\ \dot{x}_f &= x_i \dot{G}_\omega(t_f) + \dot{x}_i \dot{F}_\omega(t_f) . \end{aligned} \quad (\text{C.7})$$

Since only boundary terms contribute to the classical action, it is simply given by (3.48)

$$S[x_c] = \frac{m}{2} [x_f \dot{x}_c(t_f) - x_i \dot{x}_c(t_i)] . \quad (\text{C.8})$$

Using (C.7) to eliminate $\dot{x}_{i,f}$ in favour of $x_{i,f}$, and using the fact that the Wronskian of $F_\omega(t)$ and $G_\omega(t)$ is t -independent,

$$(F_\omega \dot{G}_\omega - \dot{F}_\omega G_\omega)(t_i) = -1 = (F_\omega \dot{G}_\omega - \dot{F}_\omega G_\omega)(t_f) , \quad (\text{C.9})$$

one finds that the classical action, as a function of x_i and x_f , is

$$S[x_c] = \frac{m}{2F_\omega(t_f)} [\dot{F}_\omega(t_f) x_i^2 + G_\omega(t_f) x_i^2 - 2x_i x_f] . \quad (\text{C.10})$$

It follows that

$$\frac{\partial^2 S[x_c]}{\partial x_i \partial x_f} = -\frac{m}{F_\omega(t_f)} , \quad (\text{C.11})$$

as we set out to show.

D POOR MAN’S PROOF OF SOME ζ -FUNCTION IDENTITIES

The purpose of this appendix is to give a heuristic proof of the ζ -function identities

$$\begin{aligned} \zeta(0) &= -\frac{1}{2} & (\sum_{n=1}^{\infty} 1) \\ \zeta(-1) &= -\frac{1}{12} & (\sum_{n=1}^{\infty} n) \\ \zeta(-2) &= 0 & (\sum_{n=1}^{\infty} n^2) \end{aligned} \quad (\text{D.1})$$

where

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s} . \quad (\text{D.2})$$

Let us, for reasons that will become apparent below, start with the sum

$$Z(\epsilon) = \sum_{n=1}^{\infty} e^{-\epsilon n} \quad (\text{D.3})$$

which we consider as the regularisation of $\sum_{n=1}^{\infty} 1$ (to which it reduces as $\epsilon \rightarrow 0$). This sum is elementary,

$$Z(\epsilon) = \frac{1}{e^\epsilon - 1} \quad (\text{D.4})$$

The derivatives of $Z(\epsilon)$ are

$$\begin{aligned} Z'(\epsilon) &= -\sum_{n=1}^{\infty} n e^{-\epsilon n} \\ Z''(\epsilon) &= \sum_{n=1}^{\infty} n^2 e^{-\epsilon n} , \end{aligned} \quad (\text{D.5})$$

etc. Therefore, just as we formally have $Z(0) = \sum_n 1$, we have

$$\begin{aligned} \sum_{n=1}^{\infty} n &= -Z'(0) \\ \sum_{n=1}^{\infty} n^2 &= Z''(0) , \end{aligned} \quad (\text{D.6})$$

etc. Now let us expand $Z(\epsilon)$ for small ϵ ,

$$Z(\epsilon) = \frac{1}{\epsilon} - \frac{1}{2} + \frac{\epsilon}{12} + \mathcal{O}(\epsilon^3) \quad (\text{D.7})$$

(in particular, there is no ϵ^2 term). Therefore we also have

$$\begin{aligned} Z'(\epsilon) &= -\frac{1}{\epsilon^2} + \frac{1}{12} + \mathcal{O}(\epsilon^2) \\ Z''(\epsilon) &= \frac{2}{\epsilon^3} + \mathcal{O}(\epsilon) . \end{aligned} \quad (\text{D.8})$$

Evidently, in each case the first term is singular as $\epsilon \rightarrow 0$. Now comes the trickery. Assume that, for present purposes, the regularisation (analytic continuation) of the Riemann ζ -function amounts to nothing more and nothing less than that this term is absent. Then we find

$$\begin{aligned} \left(\sum_{n=1}^{\infty} 1\right)_{reg} &= Z(0)_{reg} = -\frac{1}{2} \\ \left(\sum_{n=1}^{\infty} n\right)_{reg} &= -Z'(0)_{reg} = -\frac{1}{12} \\ \left(\sum_{n=1}^{\infty} n^2\right)_{reg} &= Z''(0)_{reg} = 0 , \end{aligned} \quad (\text{D.9})$$

which agrees precisely with the values of $\zeta(s)$ for $s = 0, -1, -2$ respectively.

As an aside: an elegant way to obtain the analytic continuation of the Riemann ζ -function is via the (assumed known) analytic continuation of the Euler Gamma-function

$$\Gamma(s) = \int_0^\infty dt e^{-t} t^{s-1} , \quad (\text{D.10})$$

which generalises the factorial,

$$\Gamma(n+1) = n! \quad n \in \mathbb{N} . \quad (\text{D.11})$$

The first step is to establish the identity

$$\Gamma(s)\zeta(s) = \int_0^\infty dt \frac{t^{s-1}}{e^t - 1} , \quad (\text{D.12})$$

which follows from changing variables $t \rightarrow nt$ in (D.10),

$$\Gamma(s) = n^s \int_0^\infty dt e^{-nt} t^{s-1} , \quad (\text{D.13})$$

and

$$\Gamma(s)\zeta(s) = \sum_{n=1}^\infty \int_0^\infty dt e^{-nt} t^{s-1} = \int_0^\infty dt \frac{t^{s-1}}{e^t - 1} . \quad (\text{D.14})$$

From this, the expansion of $(e^t - 1)^{-1}$ (as above) and the analytic continuation of the Gamma-function, one can then obtain the analytic continuation of the ζ -function.

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