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Path integrals

Rigorous approach for application to diffusion magnetic resonance imaging

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Abstract

We would like to apply the path integral formalism to diffusion MRI. There are certain path integrals which are on one hand of special interest in this context, and on the other hand insufficiently covered in the literature or treated in a mathematically non-transparent fashion. These include the Euclidean free path integral, a Lagrangian Euclidean path integral for the harmonic oscillator (quadratic potential), and a path integral representing anisotropic diffusion. This work provides a mathematically rigorous and transparent treatment of these path integrals. Moreover, physical interpretations of the rigorous path integrals are discussed where possible. The most important results are closed forms of the treated path integrals, derived in a mathematically rigorous fashion. Due to the Lagrangian formulation of the path integrals, these expressions are valid on a restricted domain of definition only, except for the free path integral. Additional results include varying physical interpretations of the free path integral, as well as a partial interpretation of the 1-dimensional Lagrangian Euclidean path integral for the harmonic oscillator. The problems of the domain of definition of the closed expressions and further interpretation of the harmonic oscillator path integral may serve as starting points for future research.

Contents

Chapter 1

Introduction

Magnetic resonance imaging (MRI) is one of the most widely used diagnostic tools in modern healthcare. One particular variant of MRI is *diffusion* MRI (often called *diffusion-weighted imaging* or DWI). This technique relies on diffusion of water molecules in the brain of the patient, which is essentially movement of water induced by the MRI scanner. The water molecules cannot move arbitrarily in any direction, since nerve fibers or *axons* act as barriers, meaning that there is more diffusion in some directions than in others, depending on where the axons are located. Based on the observed diffusion, an image of brain is generated. Such an image is called a tractogram. The tractogram depicts nerve tracts in the brain, which are bundles of axons. An example is shown in figure 1.1. In order to improve tractography, that is, the making of tractograms with diffusion MRI, it is of importance to gain a better understanding of the phenomenon of diffusion. To this end, we wish to understand and apply a different formalization of quantum mechanics instead of the usual formalism in terms of the wave function and the Schrödinger equation. This brings us to the *path integral* formalism. The present work focuses on gaining understanding of this formalism, motivated by the application to diffusion MRI.

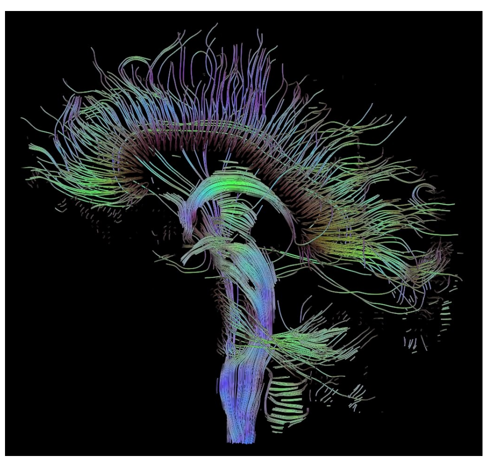

Figure 1.1: A tractogram depicting bundles of axons.
(Thomas Schultz, CC BY-SA 3.0, via Wikimedia Commons)

1.1 Feynman's idea

The concept of a path integral has fascinated physicists and mathematicians alike, ever since its introduction by Richard Feynman as a novel approach to quantum mechanics in his famous 1948 paper [1] (with preliminary work dating back to Feynman's 1942 PhD thesis [2]). Before

Feynman's work, the leading mathematical formulation of quantum mechanics was in terms of a state vector which evolves according to the Schrödinger equation. The solution of the Schrödinger equation is called the wave function, and it is a probability amplitude from which probabilities for measurements about the physical system in question can be deduced. Feynman proposed a different approach.

Inspired by Paul Dirac [3], [4], it was Feynman's idea to generalize the notion of paths and their action from classical to quantum mechanics. In classical mechanics, action is a quantity which plays a role in describing how the system changes over time. The action is different for every possible trajectory, or path, of a moving particle (see figure 1.2). For any path, which is just a continuous real function of time, the action is obtained by evaluating the *action functional* for that path.

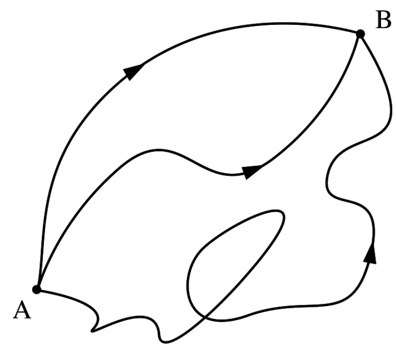

Figure 1.2: Different paths from A to B.
(Drawn by Matt McIrvin, CC BY-SA 3.0, via Wikimedia Commons)

In this way, the classical equations of motion for the system can be derived via the principle of least action, which asserts that a classical particle will traverse that path which has the least action, i.e. the path which makes the action functional stationary. Feynman introduced these concepts in the quantum world by proposing that the probability amplitude of a quantum particle should be given by a *"sum over all possible histories"* [5], each weighed by their likelihood. More precisely, according to Feynman the transition amplitude for a particle in point a at time t_a to point b at time t_b should be given by an integration over all possible paths from a to b over time $[t_a, t_b]$ that the particle can traverse, with the integrand representing in some sense the likelihood of each of those paths (that is, how likely a particle is to *actually* traverse that path). This likelihood is given by the exponential of a term proportional to the action, so that the action of a path in some sense dictates which path materializes, as in the classical setting. The resulting object, which Feynman dubbed the path integral, is in its most basic form given by

$$\int \exp\left(\frac{i}{\hbar} S[\gamma]\right) \mathcal{D}\gamma \ , \tag{1.1}$$

where S denotes the action functional, γ a path and $\mathcal{D}\gamma$ some mysterious measure on the space of paths. The integration domain is a set of paths with a certain fixed starting and end point. According to Feynman, it should then be possible to express the wave function ψ in terms of a path integral, namely

$$\psi(t, x) = \int \psi(0, \gamma(0)) \exp\left(\frac{i}{\hbar} S[\gamma]\right) \mathcal{D}\gamma \ . \tag{1.2}$$

Here, we integrate over those paths which start in a certain fixed point at time 0 and are in x at time t, that is, continuous real functions γ on $[0, \infty)$ such that $\gamma(0) = a$ for some $a \in \mathbb{R}$ and $\gamma(t) = x$ [6]. Although (1.1) and (1.2) look appealing and result from a rather intuitive and elegant idea, it is not yet clear how this path integration should work. In fact, when Feynman came up with his idea, it was mostly a heuristic tool and not a formal way of treating quantum mechanics. Although he did in his original paper [1] attempt to formalize his path integration to a certain extent, it is clear from his remarks that Feynman realized that his method was not particularly mathematically rigorous.

1.2 Mathematical difficulties

From the moment Feynman coined his path integral formalism, mathematicians and (to a lesser extent) physicists have attempted to come up with a mathematically rigorous definition of path integration, which proved no easy task. Feynman himself was already aware of the difficulties of working with his path integrals in a rigorous fashion, as becomes apparent in the following quote:

> *"(...) one feels as Cavalieri must have felt calculating the volume of a pyramid before the invention of calculus."* [1]

Although significant progress has been made, there still has been no success in formulating a general theory of path integration. Sophisticated analytic methods for broad classes of path integrals exist (see for example [7], [8], as well as the overview in [9] and the references therein), but they are still restricted to special cases. The key point is that to rigorously define path integration in general, one is essentially asking for a rigorous general treatment of infinite-dimensional integration, namely integration on a suitable infinite-dimensional function space which serves as the space of paths. If we would be able to rigorously define the as of yet heuristic measure on path space $\mathcal{D}\gamma$, we would know from measure theory how to integrate in the space of paths, and we would be done. Unfortunately, things are not that simple. A quite simple argument shows that a Lebesgue-type measure cannot be defined on infinite-dimensional Hilbert spaces, and the same holds true for Banach spaces [5]. Thus, we cannot hope to find a general, reasonable measure $\mathcal{D}\gamma$ on a complete infinite-dimensional path space equipped with at least some vector space structure. In principle this says nothing about the possibility of defining such a measure on a space with less constraints, i.e. a space which is not complete or has no vector space structure, but it seems unlikely that we end up with a useful theory if we cannot even put these requirements on the path space. Similarly, it is undesirable to look at non-Lebesgue type of measures, that is, measures which need not be rotation or translation invariant, need not assign a finite, positive value to bounded open sets of paths, or need not be σ-additive. In short, it seems impossible to define a reasonable measure $\mathcal{D}\gamma$ on a suitable space of paths, which destroys our hopes of rigorously defining Feynman's path integration in a general way through measure theory.

This, however, is not to say that it is impossible to define useful infinite-dimensional integration in any way. In fact, a theory of infinite-dimensional integration by Norbert Wiener already existed at the time Feynman wrote his thesis. It is unknown whether Feynman was actually aware of this. As it turns out, there is actually a connection between Feynman's heuristic path integral and Wiener's well-defined infinite-dimensional Wiener integral. This connection was discovered by Mark Kac, who noted the similarity between Feynman's work and his own work while attending a lecture of Feynman at Cornell University [10]. At the time, Kac was studying the distributions of certain Wiener functionals [11]. His main result was that the expectation of this type of Wiener functional, which is just a Wiener integral, is related to the fundamental solution of the heat equation. Kac remarked that this equation is, in his own words, *"quite similar"* [11] to the Schrödinger equation. Indeed, the heat equation is obtained from the Schrödinger equation by making the transformation $t \to -it$ [1], which is essentially a sort of analytic continuation to purely imaginary time. But then the assertion of Feynman (1.2) implies that the solution to the heat equation should be represented by the path integral that arises from the transformation $t \to -it$

[1] Sometimes referred to as the *Wick rotation*.

in Feynman's original path integral. This path integral is, in the simple case of a free particle (only having kinetic energy) of unit-mass and setting $\hbar = 1$,

$$\int \exp\left(-S_0[\gamma]\right)\mathcal{D}\gamma\ , \tag{1.3}$$

where S_0 is the action functional for a free particle (the definition of S_0 is at this point irrelevant). Together with Kac's result, this meant that the path integral (1.3) could be written as a rigorous Wiener integral. A generalization of this result called the Feynman-Kac formula has become one of the most fundamental and important results in the mathematical theory of path integration.

1.3 The Euclidean path integral

Consider again Feynman's path integral (1.1), for which a general definition is still unclear, and compare it to Kac's path integral (1.3), which can be written as a Wiener integral. Disregarding the fact that Kac's path integral is given in terms of the simplified action functional S_0, the essential difference is the factor in front of the action functional. In Feynman's path integral we see the complex factor $i/\hbar$, whereas in Kac's path integral we have the real factor -1. In the remainder of this work, we shall only discuss path integrals of the latter type, with a real exponent. We remark that most of the literature on path integrals focuses on the type with complex exponent, but this case is not of primary interest in the context of diffusion. Moreover, this type of path integral is even more troublesome than the type with real exponent. A thorough discussion would require, among others, functional analysis too technical to present here. We refer those interested to [7], [8].

The path integrals that we will mainly be looking at are of the form

$$K_V(a,b;t_a,t_b) := \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\dot{\gamma}^2}{2} - V(\gamma,t)dt\right)\mathcal{D}\gamma \tag{1.4}$$

with $t_a, t_b \in \mathbb{R}_+ \cup \{0\}$, $t_b > t_a$, $a, b \in \mathbb{R}$ and $\mathcal{D}\gamma$ denoting the heuristic measure on 1-dimensional path space, and its n-dimensional generalization

$$K_V(a,b;t_a,t_b) := \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\|\dot{\gamma}\|^2}{2} - V(\gamma,t)dt\right)\mathcal{D}\gamma \tag{1.5}$$

with $t_a, t_b \in \mathbb{R}_+ \cup \{0\}$, $t_b > t_a$, $a, b \in \mathbb{R}^n$ and $\mathcal{D}\gamma$ denoting the heuristic measure on n-dimensional path space. The integration bounds in the path integral indicate that we integrate over those paths γ which start in point a at time t_a and end in point b at time t_b, i.e. over continuous functions

$$\gamma : [t_a, \infty) \to \mathbb{R} \tag{1.6}$$

such that $\gamma(t_a) = a$ and $\gamma(t_b) = b$ (so the paths do not actually "end" and there is no such thing as the end point, but we will only be considering the segments of the paths over closed time intervals $[t_a, t_b]$ which justifies the terminology used here). The exponent contains the action functional

$$S(t_a,t_b)[\gamma] := \int\limits_{t_a}^{t_b} \mathcal{L}(\gamma,\dot{\gamma},t)dt \tag{1.7}$$

with the *Lagrangian*

$$\mathcal{L}(\gamma, \dot{\gamma}, t) := \frac{\|\dot{\gamma}\|^2}{2} - V(\gamma, t) \ , \tag{1.8}$$

viz.

$$K_V(a, b; t_a, t_b) = \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-S(t_a, t_b)[\gamma]\right) \mathcal{D}\gamma = \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \mathcal{L}(\gamma, \dot{\gamma}, t) dt\right) \mathcal{D}\gamma \ . \tag{1.9}$$

The term $\|\dot{\gamma}\|^2/2$ in the Lagrangian denotes kinetic energy, whereas the function V represents the potential energy. We see that (1.5) is a generalization of (1.3) to the general action functional S instead of S_0, the latter corresponding to $V = 0$ in the Lagrangian. Observe that we implicitly assume that the particle can traverse *any* path from a to b, even though this is not quite true: in reality, the particle's speed is bounded by the speed of light. This is in general not taken into account in the theory of path integrals, to maintain at least some simplicity in an already difficult topic, but some interesting ideas are sketched in [12].

At this point, we must note that there is a difference between the type of path integral with real exponent that is usually treated in the literature, and our path integral K_V. Indeed, observe that the transformation $t \to -it$ in Feynman's original path integral (1.1) actually gives the path integral

$$\int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\|\dot{\gamma}\|^2}{2} + V(\gamma, t) dt\right) \mathcal{D}\gamma \ . \tag{1.10}$$

This is almost the same as our path integral K_V, except that the sign in front of the potential function V is flipped. Whereas we recognize the action functional with the Lagrangian in K_V, the path integral that arises from Feynman's path integral by substituting $t \to -it$ contains the *Hamiltonian* instead, viz.

$$\int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\|\dot{\gamma}\|^2}{2} + V(\gamma, t) dt\right) \mathcal{D}\gamma = \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} H(\dot{\gamma}, \gamma, t) dt\right) \mathcal{D}\gamma \ , \tag{1.11}$$

with the Hamiltonian H being defined as

$$H(\gamma, \dot{\gamma}, t) := \frac{\|\dot{\gamma}\|^2}{2} + V(\gamma, t) \ . \tag{1.12}$$

Although the difference is only a sign, there is a fundamental difference between Lagrangian and Hamiltonian formalism from the physical viewpoint [13]. Hence, there is a clear conceptual difference between these types of path integrals. It will turn out that this has quite severe implications for the mathematics behind the path integrals as well, which we will discuss in detail from chapter 3 onward. Path integrals of the type (1.11) are often called *Euclidean* path integrals, and this is the type of path integral with real exponent that one usually encounters in the literature. The path integral K_V which we will be studying is for $V \neq 0$ hardly ever discussed in the literature. This is unfortunate, since it is precisely this formulation that we are interested in in the context of diffusion MRI. We will henceforth also refer to path integrals of the type (1.5) as Euclidean path integrals. Whenever necessary, we shall distinguish between the type (1.5) and (1.11) with the terms *Lagrangian* and *Hamiltonian*, respectively.

The main goal of this work is to present a mathematically rigorous treatment of certain path integrals which are of particular interest for application to diffusion MRI. This consists of special cases of this Lagrangian Euclidean path integral, as well as a slightly different, more general type of path integral with real exponent, all of which are insufficiently covered in the literature. We will also be looking at the Euclidean path integral with $V = 0$, for which there is no difference between the Lagrangian and Hamiltonian formulation. This case *is* discussed in a multitude of literature sources, but often from a physical point of view which is mathematically non-transparent. As such, we will treat this case from a more mathematical point of view, which yields a transparent treatment and at the same time serves as a basis to build on for the other, more complicated path integrals. The secondary goal is to offer physical interpretations of the path integrals that we will treat, where possible, once we have made them mathematically rigorous.

This work is written in such a way that only a minimal amount of preliminary knowledge is required. Elementary knowledge of calculus, linear algebra, real analysis, and probability theory should suffice for most parts. Knowledge of measure theory and mathematical physics is beneficial, but these parts have been made as self-contained as possible so that it is not an absolute necessity. We will begin by analyzing the 1-dimensional Euclidean path integral for the simple case $V = 0$ in chapter 2. In chapter 3, we will look at a quadratic potential function V in the Lagrangian Euclidean path integral, first in the 1-dimensional case and then in the general n-dimensional case. The latter case will also yield an n-dimensional generalization of the case $V = 0$. In chapter 4, we will discuss a path integral slightly different from but closely related to the Euclidean type. The last section of chapter 4 (section 4.3) will, as a special case, yield a result for the Lagrangian Euclidean path integral for another class of potential functions. We will end with a summary of the main results and an outline of possible future research in chapter 5.

Chapter 2

The free path integral

In this section, we shall begin by analyzing the simplest form of the 1-dimensional Euclidean path integral (1.4), namely the case where we set the potential $V = 0$, given by

$$K_0(a,b;t_a,t_b) := \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}(t)^2}{2} dt \right) \mathcal{D}\gamma \ . \tag{2.1}$$

The path integral given by (2.1) shall henceforth be referred to as the *free path integral*, because it corresponds to a particle moving in a region of uniform (non-varying) potential, which can be set to 0 arbitrarily. Thus, the particle moves freely in that its movement is not restricted by any potential field. This is not a good representation of the water molecules in diffusion MRI, since their movement *is* restricted due to the structure of the brain, as explained in chapter 1. Nonetheless, it is crucial to understand the free path integral before moving on to more complicated versions. Treating the free path integral first will give a good idea of how the path integral works from a mathematical point of view and what it represents on a deeper physical level, while avoiding mathematical problems which arise for nonzero potentials. We consider the 1-dimensional case here for simplicity. A generalization to the n-dimensional analogue of (2.1) will follow in chapter 3, as a corollary of the main result in that chapter.

2.1 Defining the free path integral

Let us start by discussing the most obvious issue: how to give meaning to the right-hand side of (2.1)? The problem is two-fold. On one hand, we would like to rigorously define this integration with respect to the heuristic measure on path space, and on the other hand, we want to do this in such a way that the intuitive properties of the original idea are preserved. A natural way to proceed is to infer a rigorous definition from certain properties that one would like the path integral to have. One desired property is, for a general n-dimensional Euclidean path integral K_V, the following:

$$K_V(a,b;t_a,t_b) = \int_{\mathbb{R}^n} K_V(a,c;t_a,t_c) K_V(c,b;t_c,t_b) dc \tag{2.2}$$

for all $t_c \in (t_a, t_b)$. In particular, the one-dimensional free path integral should satisfy

$$K_0(a,b;t_a,t_b) = \int_{\mathbb{R}} K_0(a,c;t_a,t_c) K_0(c,b;t_c,t_b) dc \tag{2.3}$$

for all $t_c \in (t_a, t_b)$. Equation (2.2) essentially says that we can introduce an arbitrary intermediate point c on any path between a and b at a fixed time t_c, allowing us to split the paths and consequently the path integral itself in two parts, and in order to consider all admissible paths from a to b we integrate over all possible intermediate points c. This requirement will form the basis of a rigorous definition of the Euclidean path integral. Inspired by (2.3), we now consider N intermediate points. By repeatedly applying (2.3), we then find

$$K_0(a,b;t_a,t_b) = \int\limits_{\mathbb{R}^N} \prod_{j=0}^{N} K_0(x_j,x_{j+1};t_j,t_{j+1})dx \ , \tag{2.4}$$

with $x_0 := a,\ t_0 := t_a,\ x_{N+1} := b,\ t_{N+1} := t_b$ and $dx := dx_1 \dots dx_N$. We can simplify this by considering equidistant time points, that is, we set $t_{j+1} - t_j = \varepsilon := \frac{t_b - t_a}{N+1}$ for $j = 0, \dots, N$. If we denote the corresponding path integrals by $K_0(x_j, x_{j+1}; \varepsilon)$, this gives

$$K_0(a,b;t_a,t_b) = \int\limits_{\mathbb{R}^N} \prod_{j=0}^{N} K_0(x_j,x_{j+1};\varepsilon)dx \ . \tag{2.5}$$

Equation (2.5) does not seem very insightful, since the to-be-defined path integral appears on both sides. The crucial trick is to consider the limit $N \to \infty$. In this case, we partition the time interval $[t_a, t_b]$ in infinitesimally small parts, viz. $\varepsilon = \frac{t_b - t_a}{N+1} \downarrow 0$. We obtain

$$K_0(a,b;t_a,t_b) = \lim_{N\to\infty} \int\limits_{\mathbb{R}^N} \prod_{j=0}^{N} K_0(x_j,x_{j+1};\varepsilon)dx \ . \tag{2.6}$$

In the integrand, we then have the path integrals

$$K_0(x_j,x_{j+1};\varepsilon) = \int\limits_{\gamma(t_j)=x_j}^{\gamma(t_{j+1})=x_{j+1}} \exp\left(-\int\limits_{t_j}^{t_{j+1}} \frac{\dot\gamma(t)^2}{2} dt\right) \mathcal{D}\gamma \ , \tag{2.7}$$

but since the partition of $[t_a, t_b]$ gets infinitesimally fine as $N \to \infty$, we restrict the path at arbitrarily many points in time, so that the freedom within the path integration effectively vanishes and the path integrations together resemble integration over *just the intermediate points* $x_1, \dots, x_N$. Consequently, using the approximation

$$\exp\left(-\int\limits_{t_j}^{t_{j+1}} \frac{\dot\gamma(t)^2}{2} dt\right) \approx \exp\left(-\frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right) \ , \tag{2.8}$$

we define the free path integral through (2.6) as follows.

Definition 2.1 (**Free path integral**)**.** The free path integral (2.1) is defined as

$$\begin{aligned} K_0(a,b;t_a,t_b) &:= \lim_{N\to\infty} \frac{1}{Z_N} \int\limits_{\mathbb{R}^N} \prod_{j=0}^{N} \exp\left(-\frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right) dx \\ &= \lim_{N\to\infty} \frac{1}{Z_N} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N} \frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right) dx \ , \end{aligned}$$

where $\varepsilon = \varepsilon(N) := \frac{t_b - t_a}{N+1} > 0$, $x_0 := a$, $x_{N+1} := b$, $dx := dx_1 \dots dx_N$ and $\frac{1}{Z_N}$ denotes a suitable normalization constant to ensure convergence in the limit.

Although definition 2.1 may seem cumbersome, it actually provides a very natural interpretation of the path integral. Namely, we can apparently view integration in the space of paths as "ordinary" integration over infinitely many intermediate points which lie on the path, via a limiting procedure of Riemann integrals over $\mathbb{R}^N$. Of course, we can never control the path at every single point in time by simply introducing enough intermediate points, for any path consists of uncountably many points, but an arbitrarily small neighborhood of any point in time $t \in (t_a, t_b)$ will eventually contain such an intermediate time epoch t_j when N gets sufficiently large. Thus, when N grows large, integration over the N "control points" $x_1, \ldots, x_N$ closely resembles heuristic integration in path space. For these reasons, and others which will become apparent later on, definition 2.1 and analogues thereof are the standard in literature on path integrals, see for example [14], [15]. In fact, Feynman himself proposed a more general version of this definition for his path integral (1.1) [1], but only in the Euclidean case this definition is relatively straightforward. In the most general case, convergence of the limit is not at all guaranteed, and a rigorous treatment involves complicated machinery which is well beyond the scope of this work. For those interested, we refer to [7], [8].

Now that we have established definition 2.1, let us briefly discuss the normalization factor $1/Z_N$. Of course, this factor should be chosen such that the right-hand side in the definition of the free path integral converges, but in principle there are many valid choices for Z_N. However, there is one particular choice which is preferred, as we shall now explain. We observe that the integral

$$\frac{1}{Z_N} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N} \frac{(x_{j+1} - x_j)^2}{2\varepsilon} \right) dx \tag{2.9}$$

is, after a change of variables $y_{i+1} = x_{i+1} - x_i$ (which has unit Jacobian determinant), the product of N Gaussian integrals. It is well known that for the standard Gaussian integral, we have

$$\int\limits_{\mathbb{R}} \exp\left(-\alpha(x+\beta)^2 \right) dx = \sqrt{\frac{\pi}{\alpha}} \ , \tag{2.10}$$

for $\alpha > 0$ and $\beta \in \mathbb{R}$, or equivalently

$$\sqrt{\frac{\alpha}{\pi}} \int\limits_{\mathbb{R}} \exp\left(-\alpha(x+\beta)^2 \right) dx = 1 \ . \tag{2.11}$$

With $\alpha = \frac{1}{2\varepsilon}$, this becomes

$$\frac{1}{\sqrt{2\pi\varepsilon}} \int\limits_{\mathbb{R}} \exp\left(-\frac{(x+\beta)^2}{2\varepsilon} \right) dx = 1 \ . \tag{2.12}$$

Note that the fact that the above integral over $\mathbb{R}$ equals 1 suggests that we can interpret the integrand as a probability density (indeed, the integrand is the probability density function of a Gaussian distribution). Inspired by this, we wish to interpret (2.9) as a probability density in b (so the entire $\mathbb{R}^N$-integral should be the probability density function in b). Therefore, we require that

$$\frac{1}{Z_N} \int\limits_{\mathbb{R}} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N} \frac{(x_{j+1} - x_j)^2}{2\varepsilon} \right) dx db = 1 \ , \tag{2.13}$$

meaning that the probability of finding the particle in an arbitrary point $b \in \mathbb{R}$ at time t_b must be equal to 1. In other words, what this requirement says is that, starting in a at time t_a, the particle has to be in *some* point $b \in \mathbb{R}$ at time t_b. Again performing the change of variables $y_{i+1} = x_{i+1} - x_i$, we see that the $\mathbb{R}^{N+1}$-integral in (2.13) is the product of $N+1$ Gaussian integrals. But then we immediately see from (2.12) that we can interpret (2.9) as a probability density in b when setting

$$\frac{1}{Z_N} = \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} , \tag{2.14}$$

which is the result of adding a factor $1/\sqrt{2\pi\varepsilon}$ in front for each of the $N+1$ Gaussian integrals. The possibility of interpreting the N-dimensional Riemann integrals within the limit as probability density functions in turn allows for a clear probabilistic interpretation of the path integral itself, as will become apparent in section 2.4. Referring back to the original idea of Feynman, namely that the path integral should represent the wave function (see equation (1.2)) which has a probabilistic physical meaning, we would indeed also like to interpret the Euclidean path integral in some probabilistic sense (even though it does not represent the wave function anymore after the transformation to imaginary time). Thus, (2.14) is a natural choice for the normalization constant, and we shall henceforth fix this choice for Z_N.

2.2 Relating the free path integral to the Wiener measure

In the preceding section, we established a definition of the free path integral in terms of a limit of Riemann $\mathbb{R}^N$-integrals. In this section, we will concisely introduce Wiener measure, and subsequently relate this measure to our definition of the free path integral. We will only consider the 1-dimensional case of the Wiener measure, but the general n-dimensional case is analogous. Some knowledge of elementary measure theory is useful, as it is beyond the scope of this work to introduce measure theory in all generality, but it is not strictly necessary. For the uninitiated reader, in particular those who are not familiar with the concept of a measure space and integration w.r.t. a measure, we refer to [16]. We also point out that a particularly interesting and elementary sketch of the main topics of this section combined with some of the results of sections 2.4.1 and 2.4.2 (as well as some results which we will see later in chapter 3) is given in chapter 9 of [17].

2.2.1 Construction of the Wiener measure

Wiener measure was first introduced by Norbert Wiener in 1923 in his work on Brownian motion [18], [19]. It has been extensively studied and applied in, most notably, stochastic calculus and analysis (see e.g. [20], [21], [22]) but it is related to a broad variety of subjects, among which our path integrals. In particular, the Wiener integral (integration w.r.t. Wiener measure) is a form of rigorous path integration, often called *functional integration*, which was already established well before the work of Feynman. As remarked in chapter 1, it was Mark Kac who discovered the connection between Feynman's path integral and Wiener's integral via the heat equation.

We shall adhere to a similar definition of the definition of Wiener measure, in particular conditional Wiener measure, as given in [6], but notably in the 1-dimensional case instead of the 3-dimensional one and without the restriction to time intervals which are symmetric around 0. Throughout the literature the definition is not entirely consistent regarding the starting point and the time interval, but this is a matter of preference. A more important difference between various literature sources has to do with the (lack of) normalization of the conditional Wiener measure, which we will discuss in more detail below. We begin by defining the relevant sets of paths.

Definition 2.2 (Set of Brownian paths). For fixed $t_a > 0$ and $a \in \mathbb{R}$, the set of continuous functions

$$\gamma : [t_a, \infty) \to \mathbb{R}$$

such that $\gamma(t_a) = a$ is denoted by X_a. Additionally, for fixed $t_b > t_a$ and $b \in \mathbb{R}$, the set of continuous functions

$$\gamma : [t_a, \infty) \to \mathbb{R}$$

such that $\gamma(t_a) = a$ and $\gamma(t_b) = b$ is denoted by X_{ab}. Elements of X_a and X_{ab} are called Brownian paths.

Next, let us define *cylinder subsets* on sets of paths X_a and X_{ab}.

Definition 2.3 (Cylinder subsets). Cylinder subsets of X_a are sets of the form

$$\{\gamma \in X_a : \ \gamma(t_j) \in I_j \ (j = 1, \ldots, n)\} \subseteq X_a \ .$$

with I_j closed or open intervals in $\mathbb{R}$ and $t_a < t_1 < \cdots < t_n$. Analogously, cylinder subsets of X_{ab} are sets of the form

$$\{\gamma \in X_{ab} : \ \gamma(t_j) \in I_j \ (j = 1, \ldots, n)\} \subseteq X_{ab} \ ,$$

with I_j closed or open intervals in $\mathbb{R}$ and $t_a < t_1 < \cdots < t_n < t_b$.

We shall henceforth refer to cylinder subsets of either set as *cylinder sets* or simply *cylinders*. This should cause no confusion, as it will be clear from the context which set we mean. Using the notion of cylinders, we can define a special collection of subsets on X_a and on X_{ab}. Such a collection is called a *σ-algebra*.

Definition 2.4 (σ-algebra of Brownian events). The collection of subsets of X_a that can be obtained from cylinders $C \subseteq X_a$ by the operations of countable unions, countable intersections and complement, is called the σ-algebra of Brownian events on X_a, and is denoted by $\mathcal{F}_a$. Similarly, the collection of subsets of X_{ab} that can be obtained from cylinders $C \subseteq X_{ab}$ by the operations of countable unions, countable intersections and complement, is called the σ-algebra of Brownian events on X_{ab}, and is denoted by $\mathcal{F}_{ab}$. Elements of $\mathcal{F}_a$ and $\mathcal{F}_{ab}$, which are subsets of X_a, respectively X_{ab}, are called Brownian events.

Thus, a Brownian event is a set of Brownian paths. This terminology, which is at this point still mysterious, shall be clarified in section 2.4.2. Those familiar with measure theory will note that $\mathcal{F}_a$ and $\mathcal{F}_{ab}$ are the σ-algebra generated by the collection of cylinders on X_a and X_{ab}, respectively. In particular, $\mathcal{F}_a$ contains X_a and $\mathcal{F}_{ab}$ contains X_{ab}. Moreover, from the definition it is clear that $\mathcal{F}_a$ and $\mathcal{F}_{ab}$ are closed under taking a countable union or intersection of elements, and under taking complements.

Having established a σ-algebra on X_a and on X_{ab}, we can define a measure on the measurable spaces $(X_a, \mathcal{F}_a)$ and $(X_{ab}, \mathcal{F}_{ab})$. This will be the *Wiener measure*.

Definition 2.5 (Wiener measure). Let the set function w be given on cylinder sets $C \subseteq X_a$ by

$$w(C) = \int_{I_1} \cdots \int_{I_n} \prod_{j=0}^{n-1} \left[\frac{1}{\sqrt{2\pi(t_{j+1} - t_j)}} \exp\left(-\frac{(x_{j+1} - x_j)^2}{2(t_{j+1} - t_j)} \right) \right] dx_1 \ldots dx_n \ ,$$

where $t_0 := t_a$, $x_0 := a$. Moreover, let w' be given on cylinder sets $C \subseteq X_{ab}$ by

$$w'(C) = \int_{I_1} \cdots \int_{I_n} \prod_{j=0}^{n} \left[\frac{1}{\sqrt{2\pi(t_{j+1} - t_j)}} \exp\left(-\frac{(x_{j+1} - x_j)^2}{2(t_{j+1} - t_j)} \right) \right] dx_1 \ldots dx_n \ ,$$

where $t_0 := t_a$, $t_{n+1} := t_b$, $x_0 := t_a$, $x_{n+1} = b$. The extension of w to the σ-algebra $\mathcal{F}_a$ on X_a is called Wiener measure on X_a. Similarly, the extension of w' to the σ-algebra $\mathcal{F}_{ab}$ on X_{ab} is called conditional[2] Wiener measure on X_{ab}. Wiener measure shall be denoted by W, whereas conditional Wiener measure shall be denoted by W'.

[2]The "condition" being that the end point is now also fixed.

Note that this definition relies on the existence of a unique extension of w and w' to the whole σ-algebra $\mathcal{F}_a$, respectively $\mathcal{F}_{ab}$. A proof of this is rather tedious and requires more advanced measure theory, so instead of providing it here we refer to [6], [23]. Furthermore, the version of the conditional Wiener measure which we provide here is the *unnormalized* variant, which is the version most commonly seen in literature which is written from a predominantly physical point of view. The normalized variant, where there is an additional division by a normalization constant in the definition of w', is more often seen in purely mathematical context. We will see later that the unnormalized version is indeed relevant for our work, and we will explain the fundamental difference in interpretation between the versions.

Through definition 2.2 up to 2.5, we have constructed a set of paths, a σ-algebra on the set of paths, and a measure acting on the σ-algebra. Thus, we have constructed the triplets $(X_a, \mathcal{F}_a, W)$ and $(X_{ab}, \mathcal{F}_{ab}, W')$, which are called measure spaces. An important remark which should be kept in mind is that in this context, the use of the term "space" does **not** allude to the concept of a vector space in any way. In fact, it is readily seen from definition 2.2 that, for example, $v, w \in X_a \not\Rightarrow v + w \in X_a$ under the usual addition operation in the space of continuous functions. We postpone giving a precise meaning of $(X_a, \mathcal{F}_a, W)$ and $(X_{ab}, \mathcal{F}_{ab}, W')$ to section 2.4.2.

2.2.2 Free path integral as a Wiener integral

Let us shift our attention back from the construction of the Wiener measure back to the path integral. We note that the terms in the limit in definition 2.1 look remarkably similar to the definition of conditional Wiener measure on cylinder sets. Indeed, they are in fact closely related, as we will now show. Denote the terms in the limit in definition 2.1 by

$$K_0^{(N)}(a, b; t_a, t_b) := \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N} \frac{(x_{j+1} - x_j)^2}{2\varepsilon}\right) dx \ , \tag{2.15}$$

so that $K_0(a, b; t_a, t_b) = \lim\limits_{N\to\infty} K_0^{(N)}(a, b; t_a, t_b)$. Consider the family of cylinders

$$C_N := \{\gamma \in X_{ab} : \ \gamma(t_j) \in \mathbb{R} \ (j = 1, \ldots, N)\} \ , \tag{2.16}$$

for $N \in \mathbb{N}_+$, with t_a and t_b independent of N, so that the number of "intermediate points" increases with N. By definition 2.5 we have for the family of cylinders (2.16) that

$$W'(C_N) = \int\limits_{\mathbb{R}^N} \prod_{j=0}^{N} \left[\frac{1}{\sqrt{2\pi(t_{j+1} - t_j)}} \exp\left(-\frac{(x_{j+1} - x_j)^2}{2(t_{j+1} - t_j)}\right)\right] dx_1 \ldots dx_N \ . \tag{2.17}$$

Assuming that for all j we have $t_{j+1} - t_j = \frac{t_b - t_a}{N+1} = \varepsilon$, this reduces to

$$W'(C_N) = \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N} \frac{(x_{j+1} - x_j)^2}{2\varepsilon}\right) dx = K_0^{(N)}(a, b; t_a, t_b) \ . \tag{2.18}$$

Thus, we find

$$K_0(a, b; t_a, t_b) = \lim_{N\to\infty} W'(C_N) \ . \tag{2.19}$$

Next, observe that the cylinders C_N are actually different ways of writing the exact same set every time, namely the set X_{ab} of all continuous paths from a to b over time $[t_a, t_b]$. Indeed, the constraint of intermediate points $\gamma(t_j)$ to the interval I_j is not a true constraint when $I_j = \mathbb{R}$. The only reason to introduce these arbitrary intermediate points is to get the integral denoting the

Wiener measure to appear in exactly the same form as the integral $K_0^{(N)}$. In light of the above, we conclude

$$K_0(a,b;t_a,t_b) = W'(X_{ab}) = \int\limits_{X_{ab}} dW' \ , \tag{2.20}$$

the right-hand side denoting the Wiener integral over X_{ab} (the right equality follows directly from the definition of integration w.r.t. a measure). This is precisely the result known as the Feynman-Kac formula for $V = 0$ (see (2.2.9) on page 34 of [15]), which establishes a connection between the free path integral and the Wiener integral. Equation (2.20) shows that definition 2.1, which defines the path integral in terms of ordinary Riemann integrals, actually leads to an equivalent formulation of Feynman's path integral in terms of a *well-defined* Wiener integral. The Wiener integral can be seen as a rigorous path integral, since the set X_{ab} over which we integrate is by definition a set of paths, and the measure W' is defined on collections of these paths. This is another reason why our way of defining the free path integral is very natural and intuitive. Finally, we can extend (2.20) to obtain an even stronger result, which really drives the point home that definition 2.1 preserves the desired properties of the heuristic path integral. It follows straightforwardly from definition 2.5 that

$$W'(X_{ab}) = \frac{1}{\sqrt{2\pi(t_b - t_a)}} \exp\left(-\frac{(b-a)^2}{2(t_b - t_a)}\right) \ . \tag{2.21}$$

This can be seen by realising that

$$\begin{aligned} W'(X_{ab}) &= W'\left(\left\{\gamma \in X_{ab} : \ \gamma\left(t_a + \frac{t_b - t_a}{2}\right) \in \mathbb{R}\right\}\right) \\ &= \frac{1}{2\pi\varepsilon} \int\limits_{\mathbb{R}} \exp\left(-\frac{(b-x_1)^2 + (x_1 - a)^2}{t_b - t_a}\right) dx_1 \end{aligned} \tag{2.22}$$

and evaluating the integral (we will not do the explicit evaluation here, since a more general case will be treated in section 2.3). Hence, we obtain

Result 2.1 (1-dimensional free path integral).

$$K_0(a,b;t_a,t_b) = W'(X_{ab}) = \int\limits_{X_{ab}} dW' = \frac{1}{\sqrt{2\pi(t_b - t_a)}} \exp\left(-\frac{(b-a)^2}{2(t_b - t_a)}\right) \ .$$

Result 2.1 is the main result so far. It presents the free path integral both as a rigorous Wiener integral as well as in closed form. To conclude this section, we remark that some authors set (2.21) as part of the definition of conditional Wiener measure, for example Glimm and Jaffe [6]. We have chosen not to do this because it is not strictly necessary and would needlessly obscure the definition.

2.3 Computing the free path integral

By recognizing in our definition of the free path integral a limit of Wiener integrals, and subsequently using properties of the Wiener measure, we derived a closed form for the free path integral, namely result 2.1. In this section, we show that we can rigorously manipulate the path integral when it is defined as in definition 2.1, in order to arrive at the same closed form as given by result 2.1 without involving Wiener measure.

Consider again the 1-dimensional free path integral, furnished with the appropriate normalization factor in the limit as explained in section 2.1:

$$K_0(a,b;t_a,t_b) = \lim_{N\to\infty}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right) dx\ . \tag{2.23}$$

We shall outline an approach[3] to evaluate the right-hand side limit to an expression in closed form. We remark that this is essentially a more rigorous version of the method illustrated in [24]. Only the most important steps and results shall be given here, while detailed computations can be found in the appendix. We start by introducing the change of variables

$$y_{i+1} = x_{i+1} - x_i \qquad (i = 0,\ldots,N-1)\ , \tag{2.24}$$

and introducing the auxiliary variable

$$y_{N+1} = x_{N+1} - x_N = b - x_N\ . \tag{2.25}$$

For the Jacobian $\partial y/\partial x$ of the change of variables (2.24), we have

$$\left(\frac{\partial y}{\partial x}\right)_{ij} = \frac{\partial y_i}{\partial x_j} = \begin{cases} 1 & \text{if } j = i \\ -1 & \text{if } j = i-1 \\ 0 & \text{otherwise}\ , \end{cases} \tag{2.26}$$

hence $\det(\partial y/\partial x) = 1$, which gives

$$\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right) dx = \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}\right) dy_1\ldots dy_N\ . \tag{2.27}$$

Although we only integrate over $y_1,\ldots,y_N$, we effectively integrate over all permitted values of all of the $N+1$ new variables, since y_{N+1} is automatically fixed by choosing $y_1,\ldots,y_N$. Thus, only N of the $N+1$ new variables are free variables. In particular, we have the linear dependency

$$\sum_{j=0}^{N} y_{j+1} = b - a\ , \tag{2.28}$$

which we can exploit to make the integration over y_{N+1} explicit. Instead of integrating over $y_1,\ldots,y_N$ as in (2.27), we may integrate over $y_1,\ldots,y_{N+1}$ by adding a δ-function in the integrand which restricts the choice for the $(N+1)$-th integration variable once the other N have been fixed. This gives

$$\begin{aligned} &\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right) dx \\ &= \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{N+1}} \exp\left(-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}\right) \delta\left(\sum_{j=0}^{N} y_{j+1} - (b-a)\right) dy\ , \end{aligned} \tag{2.29}$$

where $dy := dy_1\ldots dy_{N+1}$. Using the inverse Fourier transform of the Dirac δ-function, we can write

[3] Inspired by private communication with supervisor Luc Florack.

$$\delta\left(\sum_{j=0}^{N} y_{j+1}-(b-a)\right) = \frac{1}{2\pi}\int\limits_{\mathbb{R}} \exp\left[i\xi\left(\sum_{j=0}^{N} y_{j+1}-(b-a)\right)\right]\underbrace{\hat{\delta}(\xi)}_{=1}d\xi$$
$$= \frac{1}{2\pi}\int\limits_{\mathbb{R}} \exp\left[i\xi\left(\sum_{j=0}^{N} y_{j+1}-(b-a)\right)\right]d\xi\ , \tag{2.30}$$

hence

$$\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}}\int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right)dx$$
$$= \frac{1}{2\pi}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}}\int\limits_{\mathbb{R}}\int\limits_{\mathbb{R}^{N+1}} \exp\left[-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}+i\xi\left(\sum_{j=0}^{N} y_{j+1}-(b-a)\right)\right]dyd\xi\ , \tag{2.31}$$

where we changed the order of integration. The right-hand side of (2.31) can be evaluated in closed form, giving

$$\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}}\int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right)dx = \frac{1}{\sqrt{2\pi(t_b-t_a)}}\exp\left(-\frac{(b-a)^2}{2(t_b-t_a)}\right)\ , \tag{2.32}$$

and consequently

$$K_0(a,b;t_a,t_b) = \lim_{N\to\infty}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}}\int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\frac{(x_{j+1}-x_j)^2}{2\varepsilon}\right)dx$$
$$= \frac{1}{\sqrt{2\pi(t_b-t_a)}}\exp\left(-\frac{(b-a)^2}{2(t_b-t_a)}\right)\ . \tag{2.33}$$

The step-by-step computation can be found in appendix A. By virtue of computation, and in particular without involving Wiener measure, we have again found the closed form which we already established in section 2.2. Thus, definition 2.1 is robust, because the result found by performing rigorous manipulations to the Riemann integrals within the limit is entirely consistent with the result found by relating the path integral to the Wiener integral. For the n-dimensional analogue of equation (2.33), see result 3.3, which is obtained as a special case of the main result in chapter 3.

2.4 Interpreting the free path integral

So far, this chapter has explored the free path integral from a strictly mathematical point of view. Although mathematically rigorous treatment of path integrals is of particular interest, this is in fact only a part of the story. Feynman introduced the concept of a path integral not as a well-defined mathematical object, but rather as a tool in theoretical physics. Thus, with the mathematical results from the previous sections and the path integral's physical roots in mind, the next question which arises is as follows. How can we interpret the mathematical result 2.1 in physical context? The answer will be given in this section.

2.4.1 Diffusion

Recall that, according to the original idea of Feynman, the path integral is meant to represent the solution to the Schrödinger equation (see equation 1.2). Noting that the Hamiltonian Euclidean path integral (3.7) arises from Feynman's quantum mechanical path integral by introducing imaginary time, viz. $t \to -it$, one can argue that the Hamiltonian Euclidean path integral should then represent the solution of the equation that arises from making the substitution $t \to -it$ in the Schrödinger equation [5]. Similarly, our Lagrangian Euclidean path integral (1.4) should represent the solution to the same equation but with inverted potential V in the case where $V \neq 0$. The equation that one obtains when substituting $t \to -it$ in the Schrödinger equation is in fact the heat equation. Thus, in order to mirror Feynman's interpretation of his heuristic path integral, we would like the Euclidean path integral, when defined properly, to represent the solution to the heat equation (a priori this is just an informal identification which has no mathematical meaning). In particular, definition 2.1 should somehow be related to the solution of the 1-dimensional heat equation with $V = 0$, i.e. the 1-dimensional diffusion equation for constant diffusion coefficient $D = 1/2$,

$$\frac{\partial u(q,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 u(q,t)}{\partial q^2} \ . \tag{2.34}$$

Fortunately, our definition of the free path integral does just that.

The fundamental solution of the diffusion equation (2.34) is the solution subject to the initial condition

$$u(q,0) = \delta(q) \ , \tag{2.35}$$

where δ is the Dirac δ-function. It is well known that the solution to this initial value problem is given by

$$u(q,t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{q^2}{2t}\right) \ . \tag{2.36}$$

The right-hand side is often called the *heat kernel* or *diffusion kernel*. Obtaining this solution is outside the scope of the present work; details can be found in any introductory textbook on partial differential equations, see for example [25]. The fundamental solution u given by (2.36) is rather interesting, because we have

$$K_0(a,b;t_a,t_b) = \frac{1}{\sqrt{2\pi(t_b - t_a)}} \exp\left(-\frac{(b-a)^2}{2(t_b - t_a)}\right) = u(b-a, t_b - t_a) \ , \tag{2.37}$$

which is to say that apparently, the free path integral is the fundamental solution of the diffusion equation, i.e. the diffusion kernel, evaluated at time coordinate $t_b - t_a$ and space coordinate $b - a$. With this result we arrive at the original, heuristic identification of the Euclidean path integral with the heat equation, which has now been made rigorous in the case $V = 0$ by virtue of definition 2.1.

Equation (2.37) can be used to give physical meaning to the mathematically rigorous path integral. Since we now recognize it as the diffusion/heat kernel, we can interpret the path integral through the physical meaning of this kernel. The meaning of the kernel is probabilistic. Indeed, one may recognize in the right-hand side of (2.36) the probability density function (pdf) of a Gaussian random variable with mean 0 and variance t. Mathematically, a pdf f represents the probability that a random variable Y following that distribution falls in a certain range of values (a,b), viz.

$$\mathbb{P}(a < Y < b) = \int_a^b f(y)dy \ . \tag{2.38}$$

In statistical physics, one often encounters the following informal reformulation of the above. If dy is an infinitely small positive number, $f(y)dy$ represents the probability that Y is contained in the infinitesimal volume element $(y, y + dy)$, viz.

$$\mathbb{P}(y < Y < y + dy) = f(y)dy \ . \tag{2.39}$$

Thus, for fixed t we identify

$$\mathbb{P}(q < Q < q + dq) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{q^2}{2t}\right) dq \tag{2.40}$$

where Q is a random variable with pdf $u(\cdot, t)$, i.e. a Gaussian with mean 0 variance t. In the context of diffusion, the physical meaning of the left hand side of 2.40 is the probability that a single particle, subject to diffusion governed by (2.34) and starting in position $q_0 = 0$ at time $t_0 = 0$, is found in the infinitesimal volume element $(q, q+dq)$ at time $t > 0$. Note that the starting position in the origin is a result of the initial condition (2.35) (recall that the Dirac δ-function has an "infinite spike" at 0, and is equal to 0 everywhere else). Consider now the version of the diffusion kernel that we are interested in, namely (2.37). Although (2.37) expresses our kernel in terms of the standard kernel (2.36), there is a more instructive way of looking at our diffusion kernel. In fact,

$$p(q, t) := \frac{1}{\sqrt{2\pi(t - t_a)}} \exp\left(-\frac{(q - a)^2}{2(t - t_a)}\right) \qquad (t > t_a) \tag{2.41}$$

is the solution of the diffusion equation (2.34) subject to the alternative initial condition

$$u(q, t_a) = \delta(q - a) \ , \tag{2.42}$$

which describes a particle subject to diffusion, now starting at position a at time t_a. The right-hand side of (2.41) is again a pdf, namely of a Gaussian random variable Z with mean a and variance $t - t_a$, and thus we identify

$$\mathbb{P}(b < Z < b + db) = \frac{1}{\sqrt{2\pi(t_b - t_a)}} \exp\left(-\frac{(b - a)^2}{2(t_b - t_a)}\right) db = K_0(a, b; t_a, t_b)db \ , \tag{2.43}$$

with the left-hand side denoting the probability that the particle is found in the volume element $(b, b + db)$ at time $t_b > t_a$. Equation (2.43) connects the free path integral to the physical phenomenon of diffusion, highlighting the probabilistic interpretation of the path integral. In particular, (2.43) relates, in some sense, the probability that the particle ends up "in" b at time t_b to integration, or more suggestively *summation*, over all possible paths which the particle can traverse to go from its starting point a at time t_a to b at time t_b (a more precise relation will be given in section 2.4.2). It should however be kept in mind that (2.43) is just an informal way of writing the pdf, which is more suggestive than its mathematically rigorous counterpart,

Result 2.2 (1-dimensional free path integral as pdf).

$$\mathbb{P}(b_1 < Z < b_2) = \frac{1}{\sqrt{2\pi(t_b - t_a)}} \int_{b_1}^{b_2} \exp\left(-\frac{(b - a)^2}{2(t_b - t_a)}\right) db = \int_{b_1}^{b_2} K_0(a, b; t_a, t_b)db \ ,$$

where the left hand side denotes the probability that the particle is found in (b_1, b_2) at time t_b. We already suggested in section 2.1 that the proper choice of normalization constant $1/Z_N$ enabled a probabilistic interpretation of the path integral, and result 2.2 shows exactly how this works. In particular, we obtain the result

$$\int_{\mathbb{R}} K_0(a, b; t_a, t_b)db = 1 \tag{2.44}$$

from result 2.2 with $b_1 = -\infty$ and $b_2 = \infty$. This means that the probability of finding the particle in $(-\infty, \infty)$ at time t_b is equal to 1, which is to say that the particle has to be *somewhere*. This is precisely the interpretation of the requirement (2.13) according to which we chose the normalization constant, but now applied to the path integral K_0 itself, rather than the N-dimensional Riemann integrals. Furthermore, result 2.2 together with equation (2.20) shows that we can apparently interpret $W'(X_{ab})$ as a pdf in b, which is a quite elegant result. (This result can obviously also be established by just looking at the conditional Wiener measure, outside the context of path integrals.)

2.4.2 Brownian motion

Another way to look at the physical meaning of the free path integral is to interpret it in the context of Brownian motion, a phenomenon which is conceptually not quite the same as diffusion but closely related to it. Of course, we already hinted at Brownian motion by coining terms such as "Brownian paths" to refer to the paths over which we integrate, and by introducing the Wiener integral. In this section, we shall make the connection between the free path integral and Brownian motion precise, in order to yield another physical interpretation of the mathematically rigorous free path integral.[4]

The physical phenomenon of Brownian motion was studied scientifically for the first time by the botanist Robert Brown, which explains the name. Brown looked at pollen submerged in water through a microscope, and observed that the pollen were seemingly randomly moving through the water. At the time, Brown explained his observation as some phenomenon inherent to the pollen themselves, and not caused by external factors such as the current in the fluid or evaporation [26]. In 1905, Albert Einstein was the first to give a convincing explanation of Brownian motion. He argued that the peculiar movement of the pollen was caused by continuous collisions between the pollen and individual water molecules. Einstein presented a model for Brownian motion according to this theory, marking one of his first major scientific achievements, and published some additional papers on the theory of Brownian motion after the first paper [27]. At the time, Einsteins explanation was regarded as strong evidence for the existence of molecules and atoms, which was still a contested subject. Today, Einstein's explanation is widely accepted, and Brownian motion as such is a well-known phenomenon. In particular, Brownian motion has been extensively studied from a mathematical point of view within the field of probability theory and stochastic calculus (see e.g. [28], [29], [20]), and as such it is recognized to have a wide range of applications in, among others, (mathematical) physics and chemistry.

From now on, we shall focus on what is sometimes called the *mathematical Brownian motion* [20]. This refers to the mathematical model of the physical Brownian motion, that is, the mathematical model for random movements of particles submerged in fluid due to collisions with the fluid particles. (We shall not be so precise with the terminology, and simply use the term *Brownian motion* for both the physical manifestation and the model thereof.) Mathematically, Brownian motion is represented by a particular continuous stochastic process, called the *Wiener process*. A continuous stochastic process is essentially a family of random variables $\{X(t)\}$ with a continuous time index $t \in [t_0, \infty)$ for some $t_0 \geq 0$. Thus, at every fixed point in time $t \in [t_0, \infty)$, $X(t)$ is a variable which takes a random value. The Wiener process $\{\mathcal{W}(t)\}$, which describes the Brownian motion, is such a family of random variables, with some special properties that distinguish it from general stochastic processes. The concept of a stochastic process is however not of great interest for the current discussion, so for a more detailed introduction we refer to [21], [22], and chapter 1

[4] Readers who are familiar with the subject matter may find the distinction between Brownian motion and diffusion somewhat artificial. There is a degree of truth in this, but the distinction is made to illustrate how different formulations of the free path integral naturally lead to different angles of interpretation. The free path integral written as an exponential function points directly at the diffusion equation/a Gaussian pdf, whereas the formulation as a Wiener integral naturally leads to the mathematical formulation of Brownian motion. Furthermore, a separate treatment makes the text more accessible to those who are unfamiliar with the subject matter.

of [29]. The key point is that such a stochastic process needs some probabilistic environment to live in. Indeed, to have a notion of random variables, we must first have a notion of probabilities. This is provided by a *probability space*.

Definition 2.6 (**Probability space**). A probability space is a measure space $(\Omega, \mathcal{F}, P)$ where the measure P satisfies

$$P(\Omega) = 1 \ .$$

In this case, P is called a probability measure.

Since we have by definition that P is in addition non-negative and that, as a property of a measure, the measure of any set in $\mathcal{F}$ cannot exceed $P(\Omega)$, a probability measure maps every element of the σ-algebra to a number in $[0, 1]$. In a probability space, the set Ω is often called the *sample space*. The elements of the σ-algebra $\mathcal{F}$ are referred to as *events*. This way, the sample space Ω can be thought of as a set of "elementary events", which make up the subsets of Ω in $\mathcal{F}$, i.e. the events. Furthermore, when we think of elements of $\mathcal{F}$ as events, we can interpret $P(A)$ for $A \in \mathcal{F}$ as the probability that event A happens, because we have $P : \mathcal{F} \to [0, 1]$. With this, it is immediately clear why we require $P(\Omega) = 1$. The sample space Ω consists of all elementary events which we consider, so Ω should be assigned probability 1: events which are not included in the sample space (in the sense of being a subset) simply cannot happen. One could think of Ω as the "universe", outside of which nothing exists. This very brief summary is the essence of the measure theoretic approach to probability theory. There is a lot more to it, and some more details will emerge later, but for a thorough introduction we refer again to [16], in particular chapter 10, as well as chapter 1 of [29]. Having introduced the concept of a probability space, we state the following theorem.

Theorem 2.1. *The measure space* $(X_a, \mathcal{F}_a, W)$ *is a probability space.*

Proof. Let $t_1 > t_a$. We can write X_a in terms of a cylinder as

$$X_a = \{\gamma \in X_a : \ \gamma(t_1) \in \mathbb{R}\} \ .$$

By definition of the Wiener measure on cylinders (see definition 2.5), we have

$$W(X_a) = W\left(\{\gamma \in X_a : \ \gamma(t_1) \in \mathbb{R}\}\right) = \frac{1}{\sqrt{2\pi(t_1 - t_a)}} \int\limits_{\mathbb{R}} \exp\left(-\frac{(x-a)^2}{2(t_1 - t_a)}\right) dx \ .$$

The integral on the right-hand side is a standard Gaussian integral, which evaluates to

$$\int\limits_{\mathbb{R}} \exp\left(-\frac{(x-a)^2}{2(t_1 - t_a)}\right) dx = \sqrt{2\pi(t_1 - t_a)} \ .$$

Hence,

$$W(X_a) = \frac{1}{\sqrt{2\pi(t_1 - t_a)}} \cdot \sqrt{2\pi(t_1 - t_a)} = 1 \ .$$

□

Thus, through definitions 2.2 up to 2.5 we have actually constructed a probability space, and this is precisely the probability space in which the Wiener process describing Brownian motion lives. For this reason, we have the following terminology.

Definition 2.7 (**Probability space of Brownian motion**). The probability space $(X_a, \mathcal{F}_a, W)$ is called the probability space of Brownian motion.

This also explains the terminology in the definitions given in section 2.2.1. A more in-depth construction of this probability space starting from elementary measure theory can be found in [20], whereof the construction that we have outlined in section 2.2.1 is a condensed version.

Thus, the paths $\gamma \in X_a$ are paths which a particle undergoing Brownian motion may traverse, and the Wiener measure W of a set $A \in \mathcal{F}_a$ of such paths is the probability that the particle actually traverses one of these paths. In particular, we have $X_{ab} \subset X_a$, so that the Wiener measure assigns a probability $W(X_{ab})$ to the set of paths which go from a to b over time interval $[t_a, t_b]$, which is the probability that a Brownian particle starting in a at time t_a is found in b at time t_b. Note that this is not at all the same as $W'(X_{ab})$, the conditional Wiener measure applied to the same set of paths. Indeed, we saw in section 2.4.1 that $W'(X_{ab})$ is to be interpreted as a pdf in b, not as a probability. (In particular, $(X_{ab}, \mathcal{F}_{ab}, W')$ is **not** a probability space. Herein lies the difference between the normalized conditional Wiener measure and our unnormalized version, which we already mentioned. The normalized variant *is* a probability measure on $(X_{ab}, \mathcal{F}_{ab})$, but does not have the interpretation as a pdf.) Since $W'(X_{ab})$ is not a probability, we cannot directly interpret the free path integral as the probability of the set of Brownian paths X_{ab} through result 2.1, but we can express $W(X_{ab})$ in terms of the free path integral in a natural way as follows.

We determine $W(X_{ab})$ by expressing X_{ab} in terms of cylinder subsets of X_a, since we know the value of W for such cylinders by definition 2.3. Define

$$C_N := \left\{ \gamma \in X_a : \ \gamma(t_b) \in \left(b - \frac{1}{N}, b + \frac{1}{N} \right) \right\} . \tag{2.45}$$

We then have

$$X_{ab} = \bigcap_{N \in \mathbb{N}_+} C_N \ . \tag{2.46}$$

Since the sequence $\{C_N\}$ is decreasing, which is to say that $C_{N+1} \subseteq C_N$ for all $N \in \mathbb{N}_+$, we can apply an elementary theorem (proposition 1.2.5 on page 10 of [16]) to find

$$W(X_{ab}) = W\left(\bigcap_{N \in \mathbb{N}_+} C_N \right) \stackrel{*}{=} \lim_{N\to\infty} W(C_N) = \lim_{N\to\infty} \int_{b-\frac{1}{N}}^{b+\frac{1}{N}} \frac{1}{\sqrt{2\pi(t_b - t_a)}} \exp\left(\frac{(x-a)^2}{2(t_b - t_a)} \right) dx \ , \tag{2.47}$$

where we used the theorem in step $(*)$. We now instantly recognize the integrand as $K_0(a, x; t_a, t_b)$, and thus we obtain

Result 2.3 (**Free path integral and Wiener measure**).

$$W(X_{ab}) = \lim_{N\to\infty} \int_{b-\frac{1}{N}}^{b+\frac{1}{N}} K_0(a, x; t_a, t_b) dx \ .$$

This is the connection between on one hand the free path integral, and on the other hand the physical phenomenon of Brownian motion. We remark that we can also extend result 2.2 with a formulation in terms the Wiener measure, which connects Brownian motion and diffusion. Indeed, we have

Result 2.4 (**Brownian motion and diffusion**).

$$W\left(\{ \gamma \in X_a : \ \gamma(t_b) \in (b_1, b_2) \} \right) = \int_{b_1}^{b_2} K_0(a, x; t_a, t_b) dx = \mathbb{P}(b_1 < Z < b_2) \ .$$

(Note that result 2.3 is just the limiting case of result 2.4, where we shrink the interval (b_1, b_2) to which the path is confined at time t_b to a single point b.) Apparently, the position at time t_b of a particle undergoing Brownian motion starting from point a at time t_a is described by a Gaussian random variable Z with mean a and variance $t_b - t_a$, which is also the description of a particle undergoing diffusion as we saw in section 2.4.1. This means that Brownian motion and diffusion are essentially two sides of the same coin, both characterized by the free path integral as pdf.

To finalize the discussion, we introduce one more interpretation of result 2.1. This will not be a very useful interpretation for the free path integral, but we shall introduce it here since it will be used later on in chapter 3, where we discuss more complicated path integrals. This interpretation has to do with the measure theoretic meaning of the integral

$$\int_{X_{ab}} dW' \ . \tag{2.48}$$

We saw that it is, by definition, equal to $W'(X_{ab})$, but it can also be seen from a different perspective. To this end, consider the space $(X_{ab}, \mathcal{F}_{ab}, W')$. We saw that this is not a probability space, since W' is unnormalized. Suppose however that we were instead working with the normalized version W'_{norm}, i.e. the probability space $(X_{ab}, \mathcal{F}_{ab}, W'_{\text{norm}})$. In that case, we would have (as a general measure theoretic definition) that

$$\mathbb{E}[Z] = \int_{X_{ab}} Z dW'_{\text{norm}} \tag{2.49}$$

for a random variable Z in the probability space $(X_{ab}, \mathcal{F}_{ab}, W'_{\text{norm}})$ (which is simply a "nice" function on X_{ab}). Thus, if $(X_{ab}, \mathcal{F}_{ab}, W')$ would be a probability space, we could express the expected value of any random variable as an integral with respect to the measure W'. In particular, this would mean that we can express (2.48) as the expected value of the "random variable" 1. Unfortunately, we cannot do this in our case, since we are working with the unnormalized W' which is not a probability measure.

Nonetheless, we define in our case of unnormalized W' the functional

$$E_{ab}[Z] := \int_{X_{ab}} Z dW' \ . \tag{2.50}$$

We can interpret this as a sort of "unnormalized expectation" in the space $(X_{ab}, \mathcal{F}_{ab}, W')$[5], i.e. the "expectation" with respect to the unnormalized measure. It may seem rather artificial to introduce such an unnormalized expectation, but E_{ab} has a more natural interpretation in the context of the larger space $(X_a, \mathcal{F}_a, W)$ (which is also the reason why this object is used often throughout the literature on path integrals, see e.g. [17]). The true expected value of a random variable in the probability space of Brownian motion follows elegantly from E_{ab}. For a general function f on X_a, we have (see e.g. [30])

$$\int_{X_a} f dW = \int_{\mathbb{R}} \int_{X_{ab}} f dW' db \ , \tag{2.51}$$

from which it follows that

$$\mathbb{E}[Z] = \int_{X_a} Z dW = \int_{\mathbb{R}} \int_{X_{ab}} Z dW' db = \int_{\mathbb{R}} E_{ab}[Z] db \tag{2.52}$$

[5]This is somewhat dubious terminology, since we are not in a probability space and thus have no notion of expected value, but it is the simplest way to think about this object.

for a random variable Z in $(X_a, \mathcal{F}_a, W)$. It is important to realize that the expectation of Z is an object which lives in the large space $(X_a, \mathcal{F}_a, W)$, whereas E_{ab} lives for every $b \in \mathbb{R}$ in the space $(X_{ab}, \mathcal{F}_{ab}, W')$. Thus, equation (2.52) says that in order to compute the expected value of a random variable in the probability space of Brownian motion with starting point a, we can evaluate the unnormalized expectation $E_{ab}[Z]$ over every group of paths X_{ab} with a certain, fixed endpoint b, and then add up these unnormalized expectations for every possible endpoint $b \in \mathbb{R}$. Equation (2.52) allows us to view $E_{ab}[Z]$ as a true conditional expectation in $(X_a, \mathcal{F}_a, W)$ [31]. The difference between this interpretation and that of an unnormalized expectation is that the view as an unnormalized expectation implies that we are only looking at $(X_{ab}, \mathcal{F}_{ab}, W')$ as our "universe", with no notion of $(X_{ab}, \mathcal{F}_{ab})$ being contained in a larger space $(X_a, \mathcal{F}_a)$, whereas the view as a conditional expectation implies that we consider $(X_a, \mathcal{F}_a, W)$ to be the universe. In other words, one interpretation assumes that we only *know* paths in X_{ab}, whereas the other interpretation assumes that we know all paths in X_a but only *look at* those which are in X_{ab}. We shall use the terms *unnormalized expectation* and *conditional expectation* interchangeably, but one should keep this conceptual difference in mind at all times and realize that we are only speaking of a true expectation in the probabilistic sense in the latter case.

Although all this is quite elegant, the unnormalized expectation is not very useful for the free path integral: we just have

$$K_0(a, b; t_a, t_b) = \int_{X_{ab}} dW' = E_{ab}[1] \ , \tag{2.53}$$

which is a rather uninteresting result. Again, the reason for introducing it here is for use later on in chapter 3, where we will see more interesting results.

2.4.3 Boltzmann distribution

So far, we have interpreted the free path integral in the light of diffusion and Brownian motion. There is one more angle from which we can approach the free path integral, and this is the Boltzmann distribution. This approach is related to the preceding section. In sections 2.4.1 and 2.4.2, we characterized the free path integral as a pdf for diffusion as well as a Brownian particle. In this section, we will show that the path integral also has a different probabilistic interpretation, through a more direct but also less rigorous approach.

The Boltzmann distribution[6] (often called the Gibbs distribution or canonical distribution), after Ludwig Boltzmann, is a probability distribution which gives, for a physical system and every one of its possible states, the probability that the system is in that particular state. This probability is a function of the energy of the state and the temperature of the system. We will resort to a concise non-technical explanation here; a detailed introduction from a statistical physics point of view can be found in [32], [33]. Usually, one writes the distribution as

$$p_i \propto \exp\left(-\frac{E_i}{k_B T}\right) \ , \tag{2.54}$$

where p_i is the probability of state i, E_i its energy, k_B the Boltzmann constant, and T the absolute temperature of the system. Alternatively, we can write

$$p_i = \frac{1}{Q} \exp\left(-\frac{E_i}{k_B T}\right) \ , \tag{2.55}$$

where the normalization denominator Q is the *(canonical) partition function*[7] [32], which, loosely speaking, ensures that summation (in the discrete case) or integration (in the continuous case) of

[6]Not to be confused with the Maxwell-Boltzmann distribution.
[7]Often written as Z.

the probability over all possible states evaluates to 1. For the moment, however, let us focus on the form (2.54). A logical question is whether we can relate the exponent in (2.54) to the exponent in the integrand of the free path integral (2.1). To this end, let us start by analyzing the exponent

$$-\int_{t_a}^{t_b} \frac{\dot{\gamma}(t)^2}{2} dt \ . \tag{2.56}$$

Clearly, we are going to have to write this in terms of some kind of energy in order to get to the Boltzmann distribution. Observe that the integrand in (2.56), is actually the kinetic energy $E_{k,\gamma}$ of a unit-mass particle traversing the path γ at time t:

$$E_{k,\gamma}(t) = \frac{\dot{\gamma}(t)^2}{2} \ . \tag{2.57}$$

At first glance, it seems rather unfortunate then that we still have the integral over $[t_a, t_b]$. However, remembering that in the Boltzmann distribution the exponent contains the energy of state i, we identify the path γ of the particle as the state of the system, inspired by the fact that we integrate over these paths γ and the obvious observation that a particle traverses precisely one path of all the possible paths that it can traverse (i.e. it makes sense to view the paths as the states, since a system can only be in one state at a time). We then define the energy of the state, that is, the "energy" of a path γ, as

$$\int_{t_a}^{t_b} E_{k,\gamma}(t) dt = S_0(t_a, t_b)[\gamma] \ , \tag{2.58}$$

which is just the free action along the path between time t_a and t_b. Defining a state and its energy in this way, the integrand $\exp\left(-S_0(t_a, t_b)[\gamma]\right)$ of the free path integral is almost the of the same form as the right-hand side of (2.54), except for the absence of the physical constants k_B and T. However, we may arbitrarily include these constants explicitly instead of implicitly within the function γ, by virtue of a time scaling $t \to k_B T t$ (i.e. a change of variable $u = \frac{t}{k_B T}$). With this time scaling, we get

$$K_0(a, b; t_a, t_b) = \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\frac{S_0(u_a, u_b)[\tilde{\gamma}]}{k_B T}\right) \mathcal{D}\gamma \equiv \int_{\tilde{\gamma}(u_a)=a}^{\tilde{\gamma}(u_b)=b} \exp\left(-\frac{S_0(u_a, u_b)[\tilde{\gamma}]}{k_B T}\right) \mathcal{D}\tilde{\gamma} \ , \tag{2.59}$$

where $\tilde{\gamma}(u) := \gamma(t)$, $u_a := \frac{t_a}{k_b T}$ and $u_b := \frac{t_b}{k_b T}$. Note that equivalence between the path integrals follows from the fact that we do not change the paths themselves, but only reparametrize them. The integrand of the last path integral in (2.59) is now precisely of the form as the right-hand side in (2.54). The consequence of this identification is that, remarkably, we can interpret the free path integral even without a rigorous definition. According to equation (2.59), the free path integral represents an "integration" of, up to a proportionality constant, the probability of a reparametrized path $\tilde{\gamma}$, over all possible reparametrized paths $\tilde{\gamma}$ from a to b on the scaled time interval $[u_a, u_b]$. As such, the free path integral can be interpreted as, up to a proportionality constant, the probability that any of the admissible reparametrized paths $\tilde{\gamma}$ materializes, or equivalently, up to a proportionality constant the probability that any of the paths $\gamma \in X_{ab}$ materializes (since the admissible $\tilde{\gamma}$ are just reparametrized versions of the original admissible paths $\gamma \in X_{ab}$). This falls right in place with the results we obtained in section 2.4.2, where we saw that the free path integral is equal to $W'(X_{ab})$ which is a probability up to a proportionality constant (namely the normalization constant that is missing in our W', which would turn it into the normalized conditional Wiener measure and thus a probability instead of a pdf).

Although we chose to define the path as the state of the system, it bears mentioning that this is not the only possible choice. An alternative is to consider the state as a function of time, by recognizing the position of the particle at a fixed time t as the state at that point in time. In this case, we may interpret the integral (2.56) as a "summation" of the energy of the state at time t over all $t \in [t_a, t_b]$, which in turn allows for an interpretation of the integrand of the free path integral as a product of multiple Boltzmann distributions (one for every point in time between t_a and t_b). This definition of the state is not necessarily less natural, but it is somewhat more cumbersome to work out the details in this case as opposed to the way in which we proceeded above. To appreciate why this alternative approach may be insightful, note that the idea resembles the definition of the free path integral 2.1. In fact, it really *is* the same procedure, only backwards: write for the integral (2.56) its Riemann sum approximation, write the resulting exponential of a sum as a product of exponentials and recognize this as a product of Boltzmann distributions, and take the continuum limit. In the end, the interpretation of the result will be the same as what we found by defining the state, in a time-independent fashion, as the whole path.

Chapter 3

The path integral for quadratic potentials

Now that we understand how to define, work with and interpret the 1-dimensional free path integral, we have the basis which is necessary to start exploring the path integral for nonzero potential functions. In this chapter, we will consider a particularly interesting and instructive class of potentials. Our point of departure will be the 1-dimensional Euclidean path integral (1.4) with a quadratic potential function V, viz.

$$V(\gamma, t) \equiv V(\gamma) := \frac{\omega^2 \gamma(t)^2}{2} \tag{3.1}$$

with $\omega \in \mathbb{R}_+$. This gives the path integral

$$K_\omega(a, b; t_a, t_b) := \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(- \int\limits_{t_a}^{t_b} \frac{\dot{\gamma}(t)^2 - \omega^2 \gamma(t)^2}{2} dt \right) \mathcal{D}\gamma \ . \tag{3.2}$$

In the light of application to diffusion MRI, we are mainly interested in quadratic potentials. As we pointed out in chapter 1, the water molecules in diffusion MRI are obstructed by axons. A good description of diffusion MRI must therefore take into account that the particles cannot move arbitrarily, and this is precisely what we achieve by adding a quadratic potential function. The quadratic potential acts as a *potential barrier*, which essentially restricts the region in which the particles can move. Moreover, the quadratic potential function (3.1) is an interesting case beyond the specific purpose of diffusion MRI since it is the potential function of the simple harmonic oscillator (for unit-mass $m = 1$ and frequency $\nu = \omega/2\pi$), which is highly interesting to physics as this potential occurs frequently in nature. Thus, on one hand this potential function is a case of serious interest both in the context of diffusion MRI as well as in a general physical context. On the other hand, it is one of the few cases of nonzero potential functions which we can treat analytically. For these reasons, it is the logical next step after exploring the free path integral. Once we have seen the details in the 1-dimensional case, we will make the generalization to the n-dimensional case. This in turn will automatically generalize the results for the 1-dimensional free path integral as well.

3.1 Defining the Euclidean path integral

As with the free path integral, the first question is how to define the right-hand side of equation (3.2). We saw in section 2.1 that requirement (2.3) dictates a natural definition of the free path integral. This holds true for the Euclidean path integral with *any* potential. Recall that for the general form (1.4) in 1 dimension, we require

$$K_V(a,b;t_a,t_b) = \int_{\mathbb{R}} K_V(a,c;t_a,t_c)K_V(c,b;t_c,t_b)dc \tag{3.3}$$

for all a, b and $t_a < t_c < t_b$. Analogous to the special case $V = 0$, we can use (3.3) to define the Euclidean path integral in general, for any potential V. The procedure is essentially the same as in section 2.1. By considering an arbitrarily fine partition of the time interval, and thus arbitrarily many intermediate points, we obtain

$$K_V(a,b;t_a,t_b) = \lim_{N\to\infty} \int_{\mathbb{R}^N} \prod_{j=0}^{N} K_V(x_j,x_{j+1};\varepsilon)dx \tag{3.4}$$

with

$$K_V(x_j,x_{j+1};\varepsilon) = \int_{\gamma(t_j)=x_j}^{\gamma(t_{j+1}=x_{j+1}} \exp\left(-\int_{t_j}^{t_{j+1}} \frac{\dot\gamma(t)^2}{2} - V(\gamma,t)dt\right)\mathcal{D}\gamma\ . \tag{3.5}$$

As argued in section 2.1, in the limit $N \to \infty$ we restrict the path at arbitrarily many points in time so that the freedom of the path integration in (3.5) effectively vanishes, allowing us to omit it. We can approximate the integrand by

$$\exp\left(-\int_{t_j}^{t_{j+1}} \frac{\dot\gamma(t)^2}{2} - V(\gamma,t)dt\right) \approx \exp\left(-\frac{(x_{j+1}-x_j)^2}{2\varepsilon} + \varepsilon V(x_{j+1},t_{j+1})\right)\ , \tag{3.6}$$

which is arbitrarily accurate for $N \to \infty$, to arrive at the generalization of definition 2.1.

Definition 3.1 (**Euclidean path integral**). The 1-dimensional Euclidean path integral (1.4) is defined as

$$\begin{aligned} K_V(a,b;t_a,t_b) &:= \lim_{N\to\infty} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int_{\mathbb{R}^N} \prod_{j=0}^{N} \exp\left(-\frac{(x_{j+1}-x_j)^2}{2\varepsilon} + \varepsilon V(x_{j+1},t_{j+1})\right)dx \\ &= \lim_{N\to\infty} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\left[\frac{(x_{j+1}-x_j)^2}{2\varepsilon} - \varepsilon V(x_{j+1},t_{j+1})\right]\right)dx \end{aligned}$$

where $\varepsilon = \varepsilon(N) := \frac{t_b - t_a}{N+1} > 0$, $x_0 := a$, $x_{N+1} := b$ and $dx := dx_1 \dots dx_N$.

Note that we have already fixed the normalization term $1/(2\pi\varepsilon)^{(N+1)/2}$ in the definition. Because we must have consistency with definition 2.1 of the free path integral when setting $V = 0$ in the above, this is clearly the only option for the normalization term (unless we allow a normalization term which depends on V, but this makes no sense). Definition 3.1 is the common definition of the general Euclidean path integral in the literature, see for example [14], [15]. It is also Feynman's proposed definition for his path integral [1] with the complex factor $i/\hbar$ in the exponent replaced by -1, which is precisely how our Lagrangian version of the Euclidean path integral (1.4) arises from Feynman's formulation of the path integral (1.1).

3.2 Computing the path integral for quadratic potentials

Having defined the Euclidean path integral in full generality, we can now use this definition to find a closed form of the path integral for the quadratic potential function (3.1), in the same vein as the computation for the free path integral in section 2.3. This will prove to be rather cumbersome, but it is the most straightforward (and possibly the only) way of obtaining a closed-form expression for K_ω. The reason is that, unlike for the free path integral, we do not know if it is possible to express K_ω in terms of a Wiener integral. We can say what the exact form of K_ω as a Wiener integral must be if it exists, as we will see in section 3.4, but even with the closed form of K_ω known it is difficult to prove that K_ω is actually equal to this Wiener integral (if this is true at all). It seems even more difficult to prove this result a priori, without a closed form. Moreover, even *if* we were able to prove that K_ω can be written as this Wiener integral without computing its closed form, this characterization would not immediately yield a closed form as with the free path integral. The only conclusion which we would directly be able to draw is that K_ω is a solution to a certain second degree nonlinear PDE, which is difficult to solve, and this would still not give a fully closed form since we have no initial data specified (though we may be able to obtain these in some other way). All this will become more concrete in section 3.4. The important message for now is that the most sensible way to proceed is by performing a direct computation.

In order to compute K_ω, we shall first compute *another* path integral, which is almost the same as K_ω except for the sign in front of the quadratic potential. Though mathematically rather subtle, this is in fact a fundamental difference from a physical point view, as we will explain in a moment. It is a matter of preference whether one computes K_ω or this auxiliary path integral, since there is a simple replacement of the constant ω which allows one to toggle between the two. Thus, the closed form of one of them immediately gives the closed form of the other. We choose to start from the auxiliary path integral because the computation is simpler in this case. The path integral in question is

$$K_{i\omega}(a,b;t_a,t_b) := \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\dot\gamma(t)^2+\omega^2\gamma(t)^2}{2}dt\right)\mathcal{D}\gamma\ . \tag{3.7}$$

Observe that this is just the path integral which we obtain by replacing ω in the right-hand side of (3.2) by $\pm i\omega$, where i is the imaginary unit. This explains the subscript $i\omega$ in the above. (Although we restricted ω in (3.2) to be a positive real number, which makes sense from a physical point of view, the extension to a purely imaginary frequency does not give any problems from a mathematical point of view. From the physical point of view, this may be seen as an analytic continuation of sorts, much like the transformation to purely imaginary time in the path integral.) Furthermore, it is the path integral corresponding to the Hamiltonian (1.12) as opposed to the Lagrangian (1.8) for the quadratic potential (3.1). This relates the path integrals K_ω and $K_{i\omega}$ to the duality between Lagrangian and Hamiltonian formalism in physics, K_ω belonging to the former and $K_{i\omega}$ to the latter. Accordingly, we will see that the closed forms of K_ω and $K_{i\omega}$ look very similar but are of a completely different nature.

This being said, let us focus on computing $K_{i\omega}$ for now. The computation will be along the lines of [14], most notably the idea of expanding the paths around the classical path is inspired hereupon. Consider the term

$$\int\limits_{t_a}^{t_b} \frac{\dot\gamma(t)^2+\omega^2\gamma(t)^2}{2}dt \tag{3.8}$$

in the exponent in (3.7). We observe that this is the standard action functional

$$S(t_a,t_b)[\gamma] = \int_{t_a}^{t_b} \mathcal{L}(\gamma,\dot\gamma,t)dt = \int_{t_a}^{t_b} \frac{\dot\gamma(t)^2}{2} - V(\gamma,t)dt \tag{3.9}$$

for the inverted potential $V(\gamma,t) = -\frac{\omega^2\gamma(t)^2}{2}$. Hence, the classical equation of motion is

$$\ddot\gamma(t) = -\frac{d}{d\gamma}\left(-\frac{\omega^2\gamma(t)^2}{2}\right) = \omega^2\gamma(t)\ , \tag{3.10}$$

which is to say that the classical path of the particle is the solution of the boundary value problem

$$\begin{cases} \ddot\gamma = \omega^2\gamma \\ \gamma(t_a) = a \\ \gamma(t_b) = b\ . \end{cases} \tag{3.11}$$

It is well known that the general solution of the differential equation is given by $\gamma(t) = A\sinh(\omega t + \phi)$, thus we set

$$\gamma_{\mathrm{cl}}(t) := A\sinh(\omega t+\phi) \tag{3.12}$$

with $A,\phi\in\mathbb{R}$ such that they enforce the boundary conditions. The integral (3.8) can be explicitly evaluated for $\gamma = \gamma_{\mathrm{cl}}$. The computation is tedious but straightforward, and can be found in appendix B. We find

$$\int_{t_a}^{t_b} \frac{\dot\gamma_{\mathrm{cl}}(t)^2 + \omega^2\gamma_{\mathrm{cl}}(t)^2}{2}dt = \frac{\omega}{2}\frac{(a^2+b^2)\cosh(\omega(t_b-t_a)) - 2ab}{\sinh(\omega(t_b-t_a))}\ . \tag{3.13}$$

Consider now an arbitrary path $\gamma\in X_{ab}$. We may expand this path around the classical path, viz.

$$\gamma(t) = \gamma_{\mathrm{cl}}(t) + \gamma_{\mathrm{d}}(t)\ . \tag{3.14}$$

Since $\gamma(t_a) = \gamma_{\mathrm{cl}}(t_a) = a$ and $\gamma(t_b) = \gamma_{\mathrm{cl}}(t_b) = b$, we find $\gamma_{\mathrm{d}}(t_a) = \gamma_{\mathrm{d}}(t_b) = 0$, hence $\gamma_{\mathrm{d}}\in X_{00}$ (cf. definition 2.2). This way of writing γ is useful because of the following lemma.

Lemma 3.1. *For all $\gamma\in X_{ab}$, we have*

$$\int_{t_a}^{t_b} \frac{\dot\gamma(t)^2+\omega^2\gamma(t)^2}{2}dt = \int_{t_a}^{t_b} \frac{\dot\gamma_{\mathrm{cl}}(t)^2+\omega^2\gamma_{\mathrm{cl}}(t)^2}{2}dt + \int_{t_a}^{t_b} \frac{\dot\gamma_{\mathrm{d}}(t)^2+\omega^2\gamma_{\mathrm{d}}(t)^2}{2}dt$$

where γ_{cl} is the classical path and $\gamma_{\mathrm{d}} := \gamma - \gamma_{\mathrm{cl}}$.

Proof. We have

$$\int_{t_a}^{t_b} \frac{\dot\gamma(t)^2+\omega^2\gamma(t)^2}{2}dt = \int_{t_a}^{t_b} \frac{\left[\dot\gamma_{\mathrm{cl}}(t)+\dot\gamma_{\mathrm{d}}(t)\right]^2 + \omega^2\left[\gamma_{\mathrm{cl}}(t)+\gamma_{\mathrm{d}}(t)\right]^2}{2}dt = \int_{t_a}^{t_b} \frac{\dot\gamma_{\mathrm{cl}}(t)^2+\omega^2\gamma_{\mathrm{cl}}(t)^2}{2}dt$$
$$+ \int_{t_a}^{t_b} \frac{\dot\gamma_{\mathrm{d}}(t)^2+\omega^2\gamma_{\mathrm{d}}(t)^2}{2}dt + \int_{t_a}^{t_b} \dot\gamma_{\mathrm{cl}}(t)\dot\gamma_{\mathrm{d}}(t) + \omega^2\gamma_{\mathrm{cl}}(t)\gamma_{\mathrm{d}}(t)dt\ .$$

Integration by parts gives

$$\int_{t_a}^{t_b} \dot{\gamma}_{\text{cl}}(t)\dot{\gamma}_{\text{d}}(t) + \omega^2\gamma_{\text{cl}}(t)\gamma_{\text{d}}(t)dt = \left[\dot{\gamma}_{\text{cl}}(t)\gamma_{\text{d}}(t)\right]_{t_a}^{t_b} - \int_{t_a}^{t_b} \ddot{\gamma}_{\text{cl}}(t)\gamma_{\text{d}}(t)dt + \int_{t_a}^{t_b} \omega^2\gamma_{\text{cl}}(t)\gamma_{\text{d}}(t)dt \ .$$

The first term vanishes because $\gamma_{\text{d}}(t_a) = \gamma_{\text{d}}(t_b) = 0$, and the second and third term cancel each other since γ_{cl} satisfies the equation of motion $\ddot{\gamma} = \omega^2\gamma$. Thus,

$$\int_{t_a}^{t_b} \dot{\gamma}_{\text{cl}}(t)\dot{\gamma}_{\text{d}}(t) + \omega^2\gamma_{\text{cl}}(t)\gamma_{\text{d}}(t)dt = 0 \ ,$$

which completes the proof. □

Combining lemma 3.1 with (3.13), we can write the integrand of (3.7) as

$$\begin{aligned} &\exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}(t)^2 + \omega^2\gamma(t)^2}{2}dt\right) \\ &= \exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cosh(\omega(t_b-t_a)) - 2ab}{\sinh(\omega(t_b-t_a))} - \int_{t_a}^{t_b} \frac{\dot{\gamma}_{\text{d}}(t)^2 + \omega^2\gamma_{\text{d}}(t)^2}{2}dt\right) \\ &= \exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cosh(\omega(t_b-t_a)) - 2ab}{\sinh(\omega(t_b-t_a))}\right)\exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}_{\text{d}}(t)^2 + \omega^2\gamma_{\text{d}}(t)^2}{2}dt\right) \ , \end{aligned} \tag{3.15}$$

hence

$$\begin{aligned} &K_{i\omega}(a,b;t_a,t_b) \\ &= \exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cosh(\omega(t_b-t_a)) - 2ab}{\sinh(\omega(t_b-t_a))}\right)\int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}_{\text{d}}(t)^2 + \omega^2\gamma_{\text{d}}(t)^2}{2}dt\right)\mathcal{D}\gamma \ . \end{aligned} \tag{3.16}$$

Note that we are allowed to take the constant term out of the path integral since we can take constant terms outside the Riemann integral and limit in definition 3.1. Assuming that we may integrate over the paths $\gamma_{\text{d}} \in X_{00}$ instead of the paths $\gamma \in X_{ab}$, we obtain

$$\begin{aligned} &K_{i\omega}(a,b;t_a,t_b) \\ &= \exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cosh(\omega(t_b-t_a)) - 2ab}{\sinh(\omega(t_b-t_a))}\right)\int_{\gamma(t_a)=0}^{\gamma(t_b)=0} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}(t)^2 + \omega^2\gamma(t)^2}{2}dt\right)\mathcal{D}\gamma \\ &= \exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cosh(\omega(t_b-t_a)) - 2ab}{\sinh(\omega(t_b-t_a))}\right)K_{i\omega}(0,0;t_a,t_b) \ . \end{aligned} \tag{3.17}$$

We remark that the measure $\mathcal{D}\gamma$ is not well-defined, hence a change of variables is in principle not allowed. (More precisely, it is not clear how to interpret a change of variable with respect to this non-existent measure. We may assume that certain changes of variables are allowed, but this could lead to inconsistencies since there is no reason why a change of variable should work from a mathematical point of view. We will see an example of this at the end of section 4.2. Thus, one should remain cautious when performing such manipulations.) However, it is reasonable to assume that the change of variable works in this particular case, since we only "shift" the paths γ to get the paths γ_d. Equation (3.17) reduces the problem of computing the path integral $K_{i\omega}$ for general a and b to computing it for $a = b = 0$.

By definition 3.1, we have

$$\begin{aligned} K_{i\omega}(0,0;t_a,t_b) &:= \lim_{N\to\infty} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^N} \exp\left(-\sum_{j=0}^{N}\left[\frac{(x_{j+1}-x_j)^2}{2\varepsilon} + \varepsilon\cdot\frac{\omega^2 x_{j+1}^2}{2}\right]\right) dx \\ &= \lim_{N\to\infty} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^N} \exp\left(-\frac{1}{2\varepsilon}\sum_{j=0}^{N}\left[(x_{j+1}-x_j)^2 + \varepsilon^2\omega^2 x_{j+1}^2\right]\right) dx \end{aligned} \tag{3.18}$$

with $x_0 = x_{N+1} = 0$. Define the symmetric tridiagonal $N \times N$ matrix

$$A_N := \begin{pmatrix} 2+\varepsilon^2\omega^2 & -1 & & & \\ -1 & 2+\varepsilon^2\omega^2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2+\varepsilon^2\omega^2 & -1 \\ & & & -1 & 2+\varepsilon^2\omega^2 \end{pmatrix} . \tag{3.19}$$

Then, for $x_0 = x_{N+1} = 0$, we have

$$\sum_{j=0}^{N}\left[(x_{j+1}-x_j)^2 + \varepsilon^2\omega^2 x_{j+1}^2\right] = x^T A_N x \tag{3.20}$$

with $x := (x_1, \ldots, x_N)^T$. It is readily seen from equation (3.20) that $x^T A_N x > 0$ for all $x \neq 0$, so A_N is in fact symmetric positive-definite. Hence, there exists an $N \times N$ orthogonal matrix R with $\det R = 1$ (a rotation matrix) such that

$$\Delta = R^T A_N R , \tag{3.21}$$

where $\Delta := \operatorname{diag}(\lambda_1, \ldots, \lambda_N)$ with $\lambda_1, \ldots, \lambda_N > 0$ the eigenvalues of A_N. Set $x = Ry$. Then $x^T = y^T R^T$, and for $x_0 = x_{N+1} = 0$ we find

$$\begin{aligned} &\int\limits_{\mathbb{R}^N} \exp\left(-\frac{1}{2\varepsilon}\sum_{j=0}^{N}\left[(x_{j+1}-x_j)^2 + \varepsilon^2\omega^2 x_{j+1}^2\right]\right) dx = \int\limits_{\mathbb{R}^N} \exp\left(-\frac{1}{2\varepsilon} x^T A_N x\right) dx \\ &= \int\limits_{\mathbb{R}^N} \exp\left(-\frac{1}{2\varepsilon} y^T R^T A_N R y\right) dy = \int\limits_{\mathbb{R}^N} \exp\left(-\frac{1}{2\varepsilon} y^T \Delta y\right) dy \\ &= \int\limits_{\mathbb{R}^N} \exp\left(-\frac{1}{2\varepsilon}\sum_{j=1}^{N}\lambda_j y_j^2\right) dy = \prod_{j=1}^{N} \int\limits_{\mathbb{R}} \exp\left(-\frac{\lambda_j}{2\varepsilon}\cdot y_j^2\right) dy_j \overset{*}{=} \prod_{j=1}^{N}\sqrt{\frac{2\pi\varepsilon}{\lambda_j}} \overset{**}{=} \frac{\sqrt{2\pi\varepsilon}^N}{\sqrt{\det A_N}} , \end{aligned} \tag{3.22}$$

where we have used the standard Gaussian integral (2.10) in $(*)$ and the fact that $\det A_N = \lambda_1 \ldots \lambda_N$ in $(**)$. Substituting this in (3.18), we obtain

$$K_{i\omega}(0,0;t_a,t_b) = \lim_{N\to\infty} \frac{1}{\sqrt{2\pi\varepsilon \det A_N}} = \frac{1}{\sqrt{2\pi(t_b-t_a)}} \lim_{N\to\infty} \sqrt{\frac{N+1}{\det A_N}} \ . \tag{3.23}$$

It is possible to show that

$$\lim_{N\to\infty} \frac{\det A_N}{N+1} = \frac{\sinh(\omega(t_b-t_a))}{\omega(t_b-t_a)} \ , \tag{3.24}$$

see appendix C for details. Consequently,

$$K_{i\omega}(0,0;t_a,t_b) = \frac{1}{\sqrt{2\pi(t_b-t_a)}} \sqrt{\frac{\omega(t_b-t_a)}{\sinh(\omega(t_b-t_a))}} = \sqrt{\frac{\omega}{2\pi\sinh(\omega(t_b-t_a))}} \ . \tag{3.25}$$

Plugging this result into equation (3.17), we find

$$K_{i\omega}(a,b;t_a,t_b) = \sqrt{\frac{\omega}{2\pi\sinh(\omega(t_b-t_a))}} \exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cosh(\omega(t_b-t_a)) - 2ab}{\sinh(\omega(t_b-t_a))}\right) \ . \tag{3.26}$$

Recall that we obtain $K_{i\omega}$ from K_ω by replacing ω in the right-hand side of (3.2) by $\pm i\omega$. Similarly, we obtain K_ω from $K_{i\omega}$ by replacing ω in the right-hand side of (3.7) by $\pm i\omega$. This means that we can obtain K_ω in closed form by doing the same replacement in the right-hand side of (3.26). We then obtain

$$K_\omega(a,b;t_a,t_b) = \sqrt{\frac{\pm i\omega}{2\pi\sinh(\pm i\omega(t_b-t_a))}} \exp\left(\mp\frac{i\omega}{2}\frac{(a^2+b^2)\cosh(\pm i\omega(t_b-t_a)) - 2ab}{\sinh(\pm i\omega(t_b-t_a))}\right) \tag{3.27}$$

Using the identities $\sinh(x) = -i\sin(ix)$ and $\cosh(x) = \cos(ix)$, we find

$$\begin{aligned}
&\sqrt{\frac{\pm i\omega}{2\pi\sinh(\pm i\omega(t_b-t_a))}} \exp\left(\mp\frac{i\omega}{2}\frac{(a^2+b^2)\cosh(\pm i\omega(t_b-t_a)) - 2ab}{\sinh(\pm i\omega(t_b-t_a))}\right) \\
&= \sqrt{\frac{\mp\omega}{2\pi\sin(\mp\omega(t_b-t_a))}} \exp\left(\pm\frac{\omega}{2}\frac{(a^2+b^2)\cos(\mp\omega(t_b-t_a)) - 2ab}{\sin(\mp\omega(t_b-t_a))}\right) \\
&= \sqrt{\frac{\omega}{2\pi\sin(\omega(t_b-t_a))}} \exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cos(\omega(t_b-t_a)) - 2ab}{\sin(\omega(t_b-t_a))}\right) \ ,
\end{aligned} \tag{3.28}$$

hence

Result 3.1 (1-dimensional path integral with quadratic potential).

$$K_\omega(a,b;t_a,t_b) = \sqrt{\frac{\omega}{2\pi\sin(\omega(t_b-t_a))}} \exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cos(\omega(t_b-t_a)) - 2ab}{\sin(\omega(t_b-t_a))}\right) \ .$$

Thus, we see that the difference between Lagrangian and Hamiltonian formalism manifests in the closed form of the path integral through the difference between standard trigonometric functions and their hyperbolic counterparts. Looking at the closed form of K_ω, we see that the expression is in fact only defined for combinations of ω and $t_b - t_a$ such that $\omega(t_b-t_a) + 2k\pi \in (0,\pi)$ for some $k \in \mathbb{Z}$. If this is not the case, the sine in the square root is nonpositive, so that the expression is ill-defined. This may seem like a severe restriction, but from a physical point of view it is not so. Let us assume that we freely pick $\omega > 0$, and that we subsequently enforce the requirement on

$\omega(t_b - t_a)$ by restricting the size of the time interval $t_b - t_a$ (it does indeed not make sense to assume the contrary, namely that we pick $t_b - t_a$ and then restrict ω). Then, without loss of generality, we can replace the assumption that $\omega(t_b - t_a) + 2k\pi \in (0, \pi)$ for some k by the assumption that $\omega(t_b - t_a) \in (0, \pi)$, due to 2π-periodicity of K_ω. Now observe that, when freely choosing $\omega > 0$, the latter is equivalent to requiring $t_b - t_a \in (0, T/2)$, where $T = 2\pi/\omega$ is the period of the harmonic oscillator with frequency ω. This means that the closed form of K_ω is well-defined for all times t_b which occur within the first half of any period of the oscillator (not including the starting time and the half-period time). However, there is essentially no difference between the behaviour of the harmonic oscillator during the first half of its periodic motion and the second half. More precisely, the behaviour of the harmonic oscillator for times $t_b - t_a \in (T/2, T)$, for which the closed form we obtained is not defined, can be deduced from its behaviour for $t_b - t_a \in (0, T/2)$, for which the closed form is well-defined. The case for any $t_b - t_a > T$ such that $t_b - t_a \neq kT/2$ $(k = 3, 4, \dots)$ is equivalent to either some $t_b - t_a \in (0, T/2)$ or some $t_b - t_a \in (T/2, T)$ due to 2π-periodicity of K_ω. Thus, we conclude that it is from a physical point of view *almost* sufficient to be able to evaluate K_ω for $t_b - t_a \in (0, T/2)$ in closed form, which result 3.1 allows us to do. The remaining question is how to deal with $t_b - t_a = kT/2$ $(k \in \mathbb{N}_+)$. Furthermore, from a mathematical point of view it is desirable to find a generalized closed form which works for all $\omega, t_b - t_a > 0$, if this is possible. These are difficult problems which we shall not discuss further, but it may be worthwhile to investigate them. From now on, we shall implicitly assume that the time interval satisfies $t_b - t_a \in (0, T/2)$. Looking again at (3.26), we see that the expression for $K_{i\omega}$ requires no such restrictions on $\omega(t_b - t_a)$. Apparently, a Lagrangian formulation of the Euclidean path integral is restrictive in this sense, whereas a Hamiltonian formulation is not. Note also that, in the case where both K_ω and $K_{i\omega}$ are well-defined, their behaviour differs significantly. The sine and cosine in result 3.1 are bounded, periodic functions, whereas the hyperbolic sine and hyperbolic cosine in (3.26) are unbounded and not periodic. These observations illustrate that there is indeed a clear conceptual difference between the Lagrangian and Hamiltonian formulation of physics.

On a final note, we remark that it is readily seen that result 3.1 is consistent with result 2.1 for the free path integral, viz.

$$\lim_{\omega \downarrow 0} K_\omega(a, b; t_a, t_b) = K_0(t_a, t_b; a, b) \ . \tag{3.29}$$

Indeed, with the help of the standard limit

$$\lim_{x \downarrow 0} \frac{\sin(x)}{x} = 1 \ , \tag{3.30}$$

we find

$$\begin{aligned}
&\lim_{\omega \downarrow 0} K_\omega(a, b; t_a, t_b) \\
&= \lim_{\omega \downarrow 0} \sqrt{\frac{1}{2\pi(t_b - t_a)} \frac{\omega(t_b - t_a)}{\sin(\omega(t_b - t_a))}} \exp\left(-\frac{\omega(t_b - t_a)}{\sin(\omega(t_b - t_a))} \frac{(a^2 + b^2)\cos(\omega(t_b - t_a)) - 2ab}{2(t_b - t_a)}\right) \\
&= \frac{1}{\sqrt{2\pi(t_b - t_a)}} \exp\left(-\frac{a^2 + b^2 - 2ab}{2(t_b - t_a)}\right) = \frac{1}{\sqrt{2\pi(t_b - t_a)}} \exp\left(-\frac{(b - a)^2}{2(t_b - t_a)}\right) \\
&= K_0(a, b; t_a, t_b) \ .
\end{aligned} \tag{3.31}$$

3.3 Generalization to n dimensions

So far, we have worked with the 1-dimensional path integral only. Although this is instructive and convenient to introduce the main ideas, we ideally want to work with 3-dimensional path integrals or even arbitrary, n-dimensional ones in the context of physical applications, in particular diffusion MRI. To this end, we would like to generalize the results of chapter 2 as well as section 3.2. In this section, we will provide a definition for the n-dimensional Euclidean path integral and explicitly compute the result for a quadratic potential, analogous to the 1-dimensional case as discussed in the preceding section. With this, we immediately obtain a generalization of the results of chapter 2, since this is a special case of the quadratic potential.

In this section, the path integral of interest will be the n-dimensional Euclidean path integral (1.5) for the quadratic potential function

$$V(\gamma, t) \equiv V(\gamma) := \frac{\gamma^T(t)\Omega\gamma(t)}{2} \; , \tag{3.32}$$

where $\Omega \in \mathbb{R}^{n\times n}$ is symmetric and positive semi-definite. The role of Ω is comparable to that of the parameter ω in (3.1). Thus, the path integral that we will be considering is

$$K_\Omega(a, b; t_a, t_b) := \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\|\dot\gamma\|^2 - \gamma^T\Omega\gamma}{2} dt \right) \mathcal{D}\gamma \; , \tag{3.33}$$

with $t_a, t_b \in \mathbb{R}_+ \cup \{0\}$, $t_b > t_a$ and $a, b \in \mathbb{R}^n$. Recall that in the 1-dimensional case, the quadratic potential creates a potential barrier which restricts the area in which particles can move. The effect is the same in the general n-dimensional case, but now the restriction may differ per direction. Thus, by choosing a suitable matrix Ω one can give the particle very little freedom in one direction and a lot in others, which is a good way to model axons obstructing diffusion in certain directions in diffusion MRI.

The definition of the general n-dimensional Euclidean path integral (1.5) for an arbitrary potential V can be derived in a similar fashion as definition 3.1, using requirement (2.2). Throughout the following, a double subscript will be used to denote components of indexed vectors: $x_{k,l} \in \mathbb{R}$ is the l-th component of $x_k \in \mathbb{R}^n$. A symbol with a single subscript may denote either an indexed vector or an indexed real number/a component of a vector without index, where the exact type will be clear from the context.

Definition 3.2 (**n-dimensional Euclidean path integral**)**.** The n-dimensional Euclidean path integral (1.5) is defined as

$$\begin{aligned} K_V(a, b; t_a, t_b) &:= \lim_{N\to\infty} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\|x_{j+1} - x_j\|^2}{2\varepsilon} + \varepsilon V(x_{j+1}, t_{j+1}) \right) dx \\ &= \lim_{N\to\infty} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \exp\left(-\sum_{j=0}^{N} \left[\frac{\|x_{j+1} - x_j\|^2}{2\varepsilon} - \varepsilon V(x_{j+1}, t_{j+1}) \right] \right) dx \end{aligned}$$

where $\varepsilon = \varepsilon(N) := \frac{t_b - t_a}{N+1} > 0$, $x_0 := a$, $x_{N+1} := b$ and $dx := dx_1 \ldots dx_N$, $dx_i := dx_{i,1} \ldots dx_{i,n}$.

Definition 3.2 is clearly a generalization of definition 3.1, and it is obtained in the exact same fashion as the generalization to higher dimensions of the definition of Feynman's path integral with factor $i/\hbar$ in the exponent (see equation (2.2.20) on page 36 of [15]). Note that the normalization factor in front is raised to the power n compared to the 1-dimensional case, cf. definition 3.1. This is a result of the fact that we now have to integrate for every intermediate point $x_j \in \mathbb{R}^n$ over n coordinates. The normalization constant is determined in the same way as for the 1-dimensional free path integral, namely by requiring for the case $V = 0$ that

$$\frac{1}{Z_N}\int\limits_{\mathbb{R}^n}\int\limits_{\mathbb{R}^{nN}}\prod_{j=0}^{N}\exp\left(-\frac{\left\|x_{j+1}-x_j\right\|^2}{2\varepsilon}\right)dxdb = 1\ . \tag{3.34}$$

This is equivalent to requiring

$$\frac{1}{Z_N}\int\limits_{\mathbb{R}^n}\int\limits_{\mathbb{R}^{nN}}\prod_{j=0}^{N}\prod_{i=1}^{n}\exp\left(-\frac{(x_{j+1,i}-x_{j,i})^2}{2\varepsilon}\right)dxdb = 1\ . \tag{3.35}$$

After a change of variables $y_{j+1,i} = x_{j+1,i} - x_{j+1,i}$ the left-hand side can be seen to be a product of $n(N+1)$ Gaussian integrals, so from equation (2.12) it follows that the correct normalization term is indeed $Z_N = (2\pi\varepsilon)^{n(N+1)/2}$, resulting from a term $1/\sqrt{2\pi\varepsilon}$ in front of each of the $n(N+1)$ Gaussian integrals. Assuming that the normalization factor does not depend on V, we conclude that this is the correct normalization factor for general V by virtue of consistency with the case $V = 0$.

Let us now turn to finding a closed form of the path integral (3.33). By definition 3.2, we have

$$K_\Omega(a,b;t_a,t_b) = \lim_{N\to\infty}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}}\int\limits_{\mathbb{R}^{nN}}\prod_{j=0}^{N}\exp\left(-\frac{\left\|x_{j+1}-x_j\right\|^2}{2\varepsilon}+\varepsilon\cdot\frac{x_{j+1}^T\Omega x_{j+1}}{2}\right)dx\ . \tag{3.36}$$

Consider the integral terms within the limit on the right-hand side. The idea is to evaluate the integral not per group of components $x_{j,1},\dots,x_{j,n}$ (i.e. per vector x_j), but per group of components $x_{1,i},\dots,x_{N,i}$. This is in general not possible, but it works under our assumption that Ω is symmetric positive semi-definite. Since Ω is symmetric positive semi-definite, we can write

$$\Lambda = U^T\Omega U\ , \tag{3.37}$$

where U is an orthogonal matrix with $\det U = 1$ and $\Lambda := \operatorname{diag}(\lambda_1,\dots,\lambda_n)$ with $\lambda_1,\dots,\lambda_n \geq 0$ the eigenvalues of Ω. We set $x_j = Uy_j$. Then $x_j^T = y_j^T U^T$, and since $\det U = 1$ we have

$$\begin{aligned}
&\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}}\int\limits_{\mathbb{R}^{nN}}\prod_{j=0}^{N}\exp\left(-\frac{\left\|x_{j+1}-x_j\right\|^2}{2\varepsilon}+\varepsilon\cdot\frac{x_{j+1}^T\Omega x_{j+1}}{2}\right)dx\\
&=\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}}\int\limits_{\mathbb{R}^{nN}}\prod_{j=0}^{N}\exp\left(-\frac{\left\|Uy_{j+1}-Uy_j\right\|^2}{2\varepsilon}+\varepsilon\cdot\frac{y_{j+1}^T U^T\Omega U y_{j+1}}{2}\right)dy\\
&\overset{*}{=}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}}\int\limits_{\mathbb{R}^{nN}}\prod_{j=0}^{N}\exp\left(-\frac{\left\|y_{j+1}-y_j\right\|^2}{2\varepsilon}+\varepsilon\cdot\frac{y_{j+1}^T\Lambda y_{j+1}}{2}\right)dy\\
&=\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}}\int\limits_{\mathbb{R}^{nN}}\prod_{j=0}^{N}\exp\left(-\sum_{i=1}^{n}\left[\frac{(y_{j+1,i}-y_{j,i})^2}{2\varepsilon}-\varepsilon\cdot\frac{\lambda_i y_{j+1,i}^2}{2}\right]\right)dy\ ,
\end{aligned} \tag{3.38}$$

where step $(*)$ follows from the fact that orthogonal matrices are length-preserving, in the sense that $\|Uv\| = \|v\|$. Note that we can switch the product over the vector index j and the sum over the vector component index i around, viz.

$$\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\sum_{i=1}^{n}\left[\frac{(y_{j+1,i}-y_{j,i})^2}{2\varepsilon} - \varepsilon\cdot\frac{\lambda_i y_{j+1,i}^2}{2}\right]\right) dy$$
$$= \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \prod_{i=1}^{n} \exp\left(-\sum_{j=0}^{N}\left[\frac{(y_{j+1,i}-y_{j,i})^2}{2\varepsilon} - \varepsilon\cdot\frac{\lambda_i y_{j+1,i}^2}{2}\right]\right) dy \tag{3.39}$$

$$= \prod_{i=1}^{n}\left[\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{N}} \exp\left(-\sum_{j=0}^{N}\left[\frac{(y_{j+1,i}-y_{j,i})^2}{2\varepsilon} - \varepsilon\cdot\frac{\lambda_i y_{j+1,i}^2}{2}\right]\right) dy_{1,i}\dots dy_{N,i}\right] . \tag{3.40}$$

The advantage of this is that we now have a constant parameter λ_i in the "potential term" $-\varepsilon\lambda_i y_{j+1,i}^2/2$ within the summation in the exponent, instead of one which depends on the summation index. Observe that each of the terms in the product (3.40) is in the limit a 1-dimensional path integral which we have already computed, namely the free path integral K_0 if $\lambda_i = 0$, or the path integral for the quadratic potential K_ω with $\omega = \sqrt{\lambda_i}$ if $\lambda_i > 0$. Thus, we have

$$\lim_{N\to\infty}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{N}} \exp\left(-\sum_{j=0}^{N}\left[\frac{(y_{j+1,i}-y_{j,i})^2}{2\varepsilon} - \varepsilon\cdot\frac{\lambda_i y_{j+1,i}^2}{2}\right]\right) dy_{1,i}\dots dy_{N,i}$$
$$= K_{\sqrt{\lambda_i}}(y_{0,i}, y_{N+1,i}; t_a, t_b) = K_{\sqrt{\lambda_i}}\left(\left[U^T a\right]_i, \left[U^T b\right]_i; t_a, t_b\right) . \tag{3.41}$$

Consequently,

Result 3.2 (*n*-**dimensional path integral with quadratic potential**).

$$K_\Omega(a,b;t_a,t_b) = \lim_{N\to\infty}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|x_{j+1}-x_j\right\|^2}{2\varepsilon} + \varepsilon\cdot\frac{x_{j+1}^T\Omega x_{j+1}}{2}\right) dx$$
$$= \lim_{N\to\infty}\prod_{i=1}^{n}\left[\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{N}} \exp\left(-\sum_{j=0}^{N}\left[\frac{(y_{j+1,i}-y_{j,i})^2}{2\varepsilon} - \varepsilon\cdot\frac{\lambda_i y_{j+1,i}^2}{2}\right]\right) dy_{1,i}\dots dy_{N,i}\right]$$
$$= \prod_{i=1}^{n}\left[\lim_{N\to\infty}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{N}} \exp\left(-\sum_{j=0}^{N}\left[\frac{(y_{j+1,i}-y_{j,i})^2}{2\varepsilon} - \varepsilon\cdot\frac{\lambda_i y_{j+1,i}^2}{2}\right]\right) dy_{1,i}\dots dy_{N,i}\right]$$
$$= \prod_{i=1}^{n} K_{\sqrt{\lambda_i}}\left(\left[U^T a\right]_i, \left[U^T b\right]_i; t_a, t_b\right) .$$

Thus, it turns out that the n-dimensional path integral with a quadratic potential function is a product of n 1-dimensional path integrals with potential functions that depend on the eigenvalues of Ω. We again have to take care of the fact that the closed form of the 1-dimensional path integral K_ω is only defined for certain $\omega(t_b - t_a)$, as we saw in section 3.2. For the general n-dimensional case we must therefore restrict the length of the time interval $t_b - t_a$ based on the eigenvalues of the matrix Ω (which will allow us to pick any symmetric, positive semi-definite potential matrix $\Omega \in \mathbb{R}^{n\times n}$, as desired). If λ_1 is the largest positive eigenvalue, we assume henceforth that $t_b - t_a \in (0, \pi/\sqrt{\lambda_1})$ (note that in the case $\lambda_1 = \dots = \lambda_n = 0$ we need not restrict the time interval at all). Indeed, in this case we have for all positive eigenvalues λ_i that $t_b - t_a \in (0, \pi/\sqrt{\lambda_i})$, or equivalently $\sqrt{\lambda_i}(t_b - t_a) \in (0, \pi)$, meaning that all 1-dimensional path integrals $K_{\sqrt{\lambda_i}}$ in result 3.2 have a well-defined closed form. By result 2.1 and result 3.1, we get

$$K_{\sqrt{\lambda_i}}\left(\left[U^T a\right]_i, \left[U^T b\right]_i; t_a, t_b\right)$$
$$= \begin{cases} \frac{1}{\sqrt{2\pi(t_b-t_a)}} \exp\left(-\frac{\left[\left(U^T b\right)_i - \left(U^T a\right)_i\right]^2}{2(t_b-t_a)}\right) & \text{if } \lambda_i = 0 \\ \sqrt{\frac{\sqrt{\lambda_i}}{2\pi\sin(\sqrt{\lambda_i}(t_b-t_a))}} \exp\left(-\frac{\sqrt{\lambda_i}}{2}\frac{\left[\left(U^T a\right)_i^2 + \left(U^T b\right)_i^2\right]\cos(\sqrt{\lambda_i}(t_b-t_a)) - 2\left(U^T a\right)_i\left(U^T b\right)_i}{\sin(\sqrt{\lambda_i}(t_b-t_a))}\right) & \text{if } \lambda_i > 0 \ . \end{cases} \tag{3.42}$$

As discussed in section 3.2, the physical behaviour for $t_b - t_a$ such that $t_b - t_a \in (\pi/\sqrt{\lambda_i}, 2\pi/\sqrt{\lambda_i})$ for some $\lambda_i > 0$ can be deduced from the case $t_b - t_a \in (0, \pi/\sqrt{\lambda_1})$, and the rest follows by 2π-periodicity except for the case where $t_b - t_a = k\pi/\sqrt{\lambda_i}$ for some $\lambda_i > 0$ and some $k \in \mathbb{N}_+$.

Note that result 3.2 is consistent with the 1-dimensional case K_ω. Indeed, K_ω can be seen as K_Ω with Ω the "1×1 matrix" ω^2, which gives $\lambda_1 = \omega^2 > 0$, and then the general expression in result 3.2 reduces to K_ω. If Ω is positive-definite, which is to say that $\lambda_1, \ldots, \lambda_n > 0$, the closed form given by result 3.2 contains the determinant of Ω:

$$\begin{aligned} K_\Omega(a, b; t_a, t_b) &= \prod_{i=1}^n \left[\sqrt{\frac{\sqrt{\lambda_i}}{2\pi\sin(\sqrt{\lambda_i}(t_b - t_a))}}\right. \\ &\left.\cdot \exp\left(-\frac{\sqrt{\lambda_i}}{2}\frac{\left[\left(U^T a\right)_i^2 + \left(U^T b\right)_i^2\right]\cos(\sqrt{\lambda_i}(t_b - t_a)) - 2\left(U^T a\right)_i\left(U^T b\right)_i}{\sin(\sqrt{\lambda_i}(t_b - t_a))}\right)\right] \\ &= \sqrt{\frac{\sqrt{\det\Omega}}{(2\pi)^n\prod_{i=1}^n \sin(\sqrt{\lambda_i}(t_b - t_a))}} \\ &\cdot \exp\left(-\sum_{i=1}^n \frac{\sqrt{\lambda_i}}{2}\frac{\left[\left(U^T a\right)_i^2 + \left(U^T b\right)_i^2\right]\cos(\sqrt{\lambda_i}(t_b - t_a)) - 2\left(U^T a\right)_i\left(U^T b\right)_i}{\sin(\sqrt{\lambda_i}(t_b - t_a))}\right) \ . \end{aligned} \tag{3.43}$$

Unfortunately, it is even in this special case troublesome to simplify the closed form of K_Ω further.

As we already pointed out in the beginning of this chapter, the generalization to the n-dimensional case for quadratic potential functions automatically provides a generalization to the n-dimensional case for the free path integral. The n-dimensional free path integral is given by (1.5) with $V = 0$, but that is just K_Ω for $\Omega = O$, with O the all-zero $n \times n$ matrix. The eigenvalues of O are all 0, which means that the n-dimensional free path integral K_O evaluates by result 3.2 to

Result 3.3 (**n-dimensional free path integral**).

$$\begin{aligned} K_O(a, b; t_a, t_b) &= \prod_{i=1}^n K_0(a_i, b_i; t_a, t_b) = \prod_{i=1}^n \left[\frac{1}{\sqrt{2\pi(t_b - t_a)}} \exp\left(-\frac{\left[\left(U^T b\right)_i - \left(U^T a\right)_i\right]^2}{2(t_b - t_a)}\right)\right] \\ &= \frac{1}{\sqrt{2\pi(t_b - t_a)}^n} \exp\left(-\frac{1}{2(t_b - t_a)}\sum_{i=1}^n \left[\left(U^T b\right)_i - \left(U^T a\right)_i\right]^2\right) \\ &= \frac{1}{\sqrt{2\pi(t_b - t_a)}^n} \exp\left(-\frac{\left\|U^T (b - a)\right\|^2}{2(t_b - t_a)}\right) \stackrel{*}{=} \frac{1}{\sqrt{2\pi(t_b - t_a)}^n} \exp\left(-\frac{\|b - a\|^2}{2(t_b - t_a)}\right) \ . \end{aligned}$$

Step $(*)$ follows by orthogonality of U^T. From the closed form, it is immediately apparent that K_O is invariant under rotations of a and b, meaning that

$$K_O(a,b;t_a,t_b) = K_O(Ra,Rb;t_a,t_b) \tag{3.44}$$

for any orthogonal matrix R with $\det R = 1$. This is due to the fact that orthogonal matrices preserve length, as mentioned earlier.

Although K_Ω is in general not invariant under rotations of a and b, it can be easily shown that we have

$$K_\Omega(Ra,Rb;t_a,t_b) = K_{R^T\Omega R}(a,b;t_a,t_b) \tag{3.45}$$

for any orthogonal matrix R with $\det R = 1$. This can be seen by considering the terms in the limit (3.36), namely

$$\int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|x_{j+1}-x_j\right\|^2}{2\varepsilon} + \varepsilon\cdot\frac{x_{j+1}^T\Omega x_{j+1}}{2}\right) dx\ , \tag{3.46}$$

where $x_0 = Ra$ and $x_N = Rb$, and setting $x_j = Ry_j$. This gives $y_0 = a$, $y_{N+1} = b$ and

$$\begin{aligned}&\int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|x_{j+1}-x_j\right\|^2}{2\varepsilon} + \varepsilon\cdot\frac{x_{j+1}^T\Omega x_{j+1}}{2}\right) dx \\ &= \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|y_{j+1}-y_j\right\|^2}{2\varepsilon} + \varepsilon\cdot\frac{y_{j+1}^T R^T\Omega R y_{j+1}}{2}\right) dy\ .\end{aligned} \tag{3.47}$$

Consequently,

Result 3.4 (rotations).

$$\begin{aligned}K_\Omega(Ra,Rb;t_a,t_b) &= \lim_{N\to\infty}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|x_{j+1}-x_j\right\|^2}{2\varepsilon} + \varepsilon\cdot\frac{x_{j+1}^T\Omega x_{j+1}}{2}\right) dx_j \\ &= \lim_{N\to\infty}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|y_{j+1}-y_j\right\|^2}{2\varepsilon} + \varepsilon\cdot\frac{y_{j+1}^T R^T\Omega R y_{j+1}}{2}\right) dy_j = K_{R^T\Omega R}(a,b;t_a,t_b)\ .\end{aligned}$$

This is a rather intuitive result: when considering a particle moving through space from point a to point b under the influence of a potential field, rotating these points would effectively be the same as keeping the original points a and b and rotating the potential field in the opposite way, which corresponds to replacing Ω with $R^T\Omega R$ in the path integral. Usually, for a given matrix Ω we do not have $\Omega = R^T\Omega R$ for all rotation matrices R, but there may be nontrivial rotations $R \neq I$ for which this equality holds, in which case the path integral K_Ω is invariant under that particular rotation. In the special case $\Omega = \alpha I$ with $\alpha \in \mathbb{R}$, we do have $\Omega = R^T\Omega R$ for all rotation matrices R, so $K_{\alpha I}$ is truly rotation invariant. Furthermore, we also see from this result that the free path integral K_O is rotation invariant.

We remark that substituting $\Omega \to R\Omega R^T$ in the result above yields

$$K_{R\Omega R^T}(Ra,Rb;t_a,t_b) = K_\Omega(a,b;t_a,t_b)\ . \tag{3.48}$$

Apparently, a rotation of a and b may be undone by rotating the potential field in the same way. Again, we see that there is effectively no difference between rotating a and b, and rotating the potential field, as expected.

3.4 Interpreting the path integral for quadratic potentials

Having evaluated the n-dimensional path integral quadratic potential functions, we will now focus again on the 1-dimensional case. In this section, we will investigate how to physically interpret the path integral for quadratic potentials, as we did for the free path integral in section 2.4. This is done by looking at the 1-dimensional case for the sake of simplicity. All this theory may be generalized to n dimensions, from which analogous interpretations for the n-dimensional path integrals follow (both for the free path integral and for those with quadratic potential functions), but doing so here would only obscure the discussion and distract from the main focus of this section. With this out of the way, let us take a closer look at the physical meaning of (3.2).

Our point of departure will be a generalization of the result which we found in section 2.2.2, namely equation (2.20). As it turns out, it is possible to represent certain Euclidean path integrals as Wiener integrals, similar to the free path integral in (2.20), under some assumptions on the potential function V. This is a fundamental and well-known result in the theory of path integrals, functional integration and stochastic calculus & analysis, known as the *Feynman-Kac formula*. The Feynman-Kac formula can be found in a multitude of forms throughout literature on the aforementioned subjects, some more transparent than others. Although the details and the proof are outside the scope of this work, we shall provide one form of the Feynman-Kac formula in full, namely the variant which can be found in [15], [6] for the 1-dimensional case (see theorem 3.2.3 on page 48 of [6]).

Theorem 3.1 (**Feynman-Kac formula**). *Let $V = V(\gamma)$ be a continuous, real-valued function on $\mathbb{R}$ which is bounded from below, and let $H = -\frac{1}{2}\Delta + V$ be essentially self-adjoint. Then*

$$\int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}(t)^2}{2} + V\left(\gamma(t)\right) dt\right) \mathcal{D}\gamma = \int_{X_{ab}} \exp\left(-\int_{t_a}^{t_b} V\left(\gamma(t)\right) dt\right) dW' \ ,$$

where the path integral on the left-hand side is defined by definition 3.1.

Proof. See the proof of theorem 3.2.3 on page 48 of [6]. □

We will not delve into the definition of (essential) self-adjointness, but those interested may consult any introductory textbook on functional analysis, for example [34]. The proof of theorem 3.1 is rather technical and uses both advanced functional analysis and measure theory, and moreover it is not particularly insightful for the present discussion, which is why have omitted it. What is important, is that we can apply the Feynman-Kac formula to (3.7). The quadratic potential function (3.1) is continuous, real-valued and nonnegative i.e. bounded from below. Since the quadratic potential function is a polynomial (in γ) and bounded from below, it is essentially self-adjoint [6]. Thus, we can apply theorem 3.1 to obtain

$$K_{i\omega}(a, b; t_a, t_b) = \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}(t)^2 + \omega^2\gamma(t)^2}{2} dt\right) \mathcal{D}\gamma = \int_{X_{ab}} \exp\left(-\int_{t_a}^{t_b} \frac{\omega^2\gamma(t)^2}{2} dt\right) dW' \ . \tag{3.49}$$

It is rather unfortunate that the path integrals for which the Feynman-Kac formula is given are of the Hamiltonian type, with an inverted sign in front of the potential when compared to our Lagrangian Euclidean path integral (1.4). This makes it impossible to directly apply the Feynman-Kac formula to the path integral that we are interested in, namely K_ω given by (3.2): to get the left-hand side in the Feynman-Kac formula to be equal to K_ω, we would have to set $V = -\omega^2\gamma^2/2$, which is a function that is bounded from above instead of bounded from below. Likewise, it would be tempting to apply the Feynman-Kac formula for $V = \omega^2\gamma^2/2$ as we did above and then substitute $\omega \to \pm i\omega$ in (3.49), but this also boils down to changing the sign of the potential function, which we are not allowed to do for our quadratic potential. Although there are cases of unbounded potential functions for which the equality of the Feynman-Kac formula still holds [35], these are special cases which are difficult to prove and scarcely covered in the literature. This is another manifestation of the fundamental difference between Hamiltonian and Lagrangian formalism in physics, as we already pointed out in section 3.2. The Feynman-Kac formula states a rigorous formulation of the Hamiltonian Euclidean path integral in terms of a Wiener integral for a broad and general class of potential functions, but when restating the formula in terms of a Lagrangian Euclidean path integral (our Euclidean path integral (1.4)), one obtains restrictions on the potential which are a lot more severe: the requirement of boundedness from below in the Hamiltonian formulation changes to the way more stringent requirement of boundedness from above in the Lagrangian formulation, as the example of the quadratic potential illustrates.

To demonstrate the usefulness of the Feynman-Kac formula when applicable, let us consider (3.49). Writing $K_{i\omega}$ as a Wiener integral, we are again looking at the probability space of Brownian motion which we introduced introduced in section 2.4.2, see definition 2.7. Recalling equation (2.50), we see that

$$K_{i\omega}(a,b;t_a,t_b) = \int\limits_{X_{ab}} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\omega^2\gamma(t)^2}{2} dt\right) dW' = E_{ab}\left[\exp\left(-\int\limits_{t_a}^{t_b} \frac{\omega^2\gamma(t)^2}{2} dt\right)\right] . \tag{3.50}$$

Thus, the path integral $K_{i\omega}$ can be interpreted as a conditional expectation in the probability space $(X_a, \mathcal{F}_a, W)$ of the functional

$$\exp\left(-\int\limits_{t_a}^{t_b} \frac{\omega^2\gamma(t)^2}{2} dt\right) , \tag{3.51}$$

where the exponent can be seen as minus the contribution of the potential V to the Hamiltonian (1.12) along the segment $\gamma|_{[t_a,t_b]}$. This conditional expectation can be seen as taking the average of the functional over only those Brownian paths which start in a at time t_a and are in b at time t_b. Equation (3.50) together with (2.52) implies

$$\mathbb{E}\left[\exp\left(-\int\limits_{t_a}^{t_b} \frac{\omega^2\gamma(t)^2}{2} dt\right)\right] = \int\limits_{\mathbb{R}} K_{i\omega}(a,b;t_a,t_b) db , \tag{3.52}$$

with $\mathbb{E}$ the expected value in the probability space $(X_a, \mathcal{F}_a, W)$, which can be seen as taking the average of the functional over *all* Brownian paths which start in a at time t_a. This explanation of $K_{i\omega}$ is rather elegant. Despite the fact that its closed form (3.26) is not very revealing, the Feynman-Kac formula provides a simple way of interpreting the path integral. This example clearly shows the usefulness of the Feynman-Kac formula, and it serves as a motivation to look into the possibility of proving an analogous result for the path integral of interest K_ω. We will not attempt to rigorously prove such a result here, but we will argue why it is reasonable to expect that the analogue of (3.49) holds for K_ω.

To this end, let us depart slightly from the mathematical rigour that has otherwise been the focus of this work so far, and suppose that the analogue of equation (3.49) holds for K_ω. That is, suppose we have

$$K_\omega(a,b;t_a,t_b) = \int\limits_{X_{ab}} \exp\left(\int\limits_{t_a}^{t_b} \frac{\omega^2\gamma(t)^2}{2} dt\right) dW' = E_{ab}\left[\exp\left(\int\limits_{t_a}^{t_b} \frac{\omega^2\gamma(t)^2}{2} dt\right)\right] . \quad \textbf{(supposition)} \tag{3.53}$$

(Note that this is the only Wiener integral to which K_ω can possibly be equal. Equality between K_ω and any other Wiener integral would be inconsistent with the Feynman-Kac formula upon inverting the potential.) In this case, the path integral is the average of the functional

$$\exp\left(\int\limits_{t_a}^{t_b} \frac{\omega^2\gamma(t)^2}{2} dt\right) \tag{3.54}$$

over the paths $\gamma \in X_{ab}$ (so again a conditional expectation in $(X_a, \mathcal{F}_a, W)$), where the exponent is minus the contribution of the potential energy V to the action functional

$$S(t_a,t_b)[\gamma] := \int\limits_{t_a}^{t_b} \mathcal{L}(\gamma,\dot\gamma,t) dt \tag{3.55}$$

with the Lagrangian $\mathcal{L}$ given by (1.8). This is in itself a rather elegant interpretation of K_ω, but it does not yet provide much of an argument as to why (3.53) should hold in the first place. We will now address this question. In [17], it is shown that the functional

$$W(q,t) := E_{0q}\left[\exp\left(-\int\limits_0^t U\left(\gamma(\tau)\right) d\tau\right)\right] \tag{3.56}$$

satisfies the partial differential equation

$$\frac{\partial W(q,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 W(q,t)}{\partial q^2} - U(q)W(q,t) , \tag{3.57}$$

which is a generalization of the diffusion/heat equation (2.34). Note that the (q,t)-dependence of (3.56) manifests in the fact that the conditional expectation is taken over those paths $\gamma \in X_{0q}$ which start in 0 at time 0 and are in q at time t. In particular, this means that

$$\psi(q,t) := E_{0q}\left[\exp\left(\int\limits_0^t \frac{\omega^2\gamma^2}{2} d\tau\right)\right] = \int\limits_{X_{0q}} \exp\left(\int\limits_0^t \frac{\omega^2\gamma^2}{2} d\tau\right) dW' \tag{3.58}$$

satisfies

$$\frac{\partial \psi(q,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 \psi(q,t)}{\partial q^2} + \frac{\omega^2 q^2}{2}\psi(q,t) . \tag{3.59}$$

We claim that this may be generalized to an arbitrary starting time $t_a \geq 0$ and starting point $a \in \mathbb{R}$, so that

$$\psi(q,t) := E_{aq}\left[\exp\left(\int\limits_{t_a}^t \frac{\omega^2\gamma^2}{2} d\tau\right)\right] = \int\limits_{X_{aq}} \exp\left(\int\limits_{t_a}^t \frac{\omega^2\gamma^2}{2} d\tau\right) dW' \tag{3.60}$$

satisfies (3.59) for $t > t_a$. Under our assumption (3.53), this means that

$$\frac{\partial K_\omega(a,q;t_a,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 K_\omega(a,q;t_a,t)}{\partial q^2} + \frac{\omega^2 q^2}{2} K_\omega(a,q;t_a,t) \ . \tag{3.61}$$

In other words, if we can indeed write K_ω as a Wiener integral through (3.53), then (3.61) holds. This prompts the question whether we can invert this line of reasoning, and somehow make use of the PDE to prove (3.53). Since we have a closed form for K_ω, we can check independently of assumption (3.53) whether K_ω satisfies the PDE. By virtue of computation with the closed form given by result 3.1, one can verify that (3.61) holds for $t - t_a \in (0, T/2)$ (see appendix D for details). Thus, both the path integral K_ω and the function (3.60) satisfy the *same* partial differential equation, which is an indication that these 2 objects are related to each other, though not necessarily in the assumed way (3.53). To prove (3.53), one could introduce an initial condition which uniquely fixes the solution of the PDE, and subsequently show that both the path integral K_ω as well as the function (3.60) satisfy this initial condition, which implies that they must be equal by uniqueness of the solution. The most promising approach seems to furnish the PDE with the initial condition

$$\psi(q,t_a) = \delta(q-a) \ . \tag{3.62}$$

Although we have strictly speaking only defined the path integral for $t_b > t_a$ (which in this case means $t > t_a$), we can consider the limit $t \downarrow t_a$ of the closed form given by result 3.1 to determine the behaviour of $K_\omega(a,q;t_a,t)$ "at $t = t_a$". Considering the cases $q = a$ and $q \neq a$ separately, we conjecture that the behaviour at $t = t_a$ is described by a δ-function, in the sense of a distributional limit (see [36] for more on distributions and distributional limits). We have

$$K_\omega(a,q;t_a,t) = \sqrt{\frac{\omega}{2\pi \sin(\omega(t-t_a))}} \exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right) \ . \tag{3.63}$$

For $q = a$, we get 0 for the numerator and for the denominator in the exponent as $t \downarrow t_a$, so we can apply L'Hôpital's rule to find that the exponent goes to 0, so that the exponential goes to 1. Clearly, the factor under the square root in front tends to infinity as $t \downarrow t_a$, so that

$$\lim_{t \downarrow t_a} K_\omega(a,a;t_a,t) = \infty \ . \tag{3.64}$$

On the other hand, for $q \neq a$ the numerator in the exponent is nonzero as $t \downarrow t_a$, whereas the denominator goes to 0, so that the exponent tends to minus infinity and the exponential decreases to 0. Consequently,

$$\lim_{t \downarrow t_a} K_\omega(a,q;t_a,t) = 0 \tag{3.65}$$

for $q \neq a$. The 2 cases together lead to the following conjecture.

Conjecture 3.1.

$$\lim_{t \downarrow t_a} K_\omega(a,q;t_a,t) = \delta(q-a) \ .$$

One should realize that this conjecture is not a statement about a limit of t-parametrized functions $K_\omega(a,q;t_a,t)$ of q, but rather a limit of *tempered distributions associated with* $K_\omega(a,q;t_a,t)$. Indeed, by definition of the distributional limit, conjecture 3.1 is equivalent to

$$\lim_{t \downarrow t_a} \int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi(q)dq = \int_{\mathbb{R}} \delta(q-a)\phi(q)dq = \delta_a(\phi) = \phi(a) \tag{3.66}$$

for all test functions $\phi \in \mathscr{S}(\mathbb{R})$. Note that for each $t > t_a$ the integral within the limit on the left-hand side is, unlike the "integral" of the δ-function, an ordinary Riemann integral, since the function $K_\omega(a,q;t_a,t)$ of q is well-defined for all $t > t_a$ (i.e. it is a true function of q for all fixed

$t > t_a$ and only needs to be treated as a generalized function in the limit $t \downarrow t_a$). Thus, to prove conjecture 3.1, one would have to show

$$\lim_{t\downarrow t_a} \int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi(q)dq = \phi(a) \tag{3.67}$$

for all $\phi \in \mathscr{S}(\mathbb{R})$. Unfortunately, it turns out that this is deceptively hard to prove, but we will argue why we expect this to be true. To start, we can Taylor expand the test function around a, viz.

$$\phi(q) = \phi(a) + \phi'(\xi(q))(q-a) \ , \tag{3.68}$$

with $a < \xi(q) < q$. This gives

$$\begin{aligned}\int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi(q)dq &= \int_{\mathbb{R}} K_\omega(a,q;t_a,t)\left[\phi(a) + \phi'(\xi(q))(q-a)\right]dq \\ &= \phi(a)\int_{\mathbb{R}} K_\omega(a,q;t_a,t)dq + \int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi'(\xi(q))(q-a)dq \ ,\end{aligned} \tag{3.69}$$

and

$$\begin{aligned}&\lim_{t\downarrow t_a}\int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi(q)dq \\ &= \phi(a)\lim_{t\downarrow t_a}\int_{\mathbb{R}} K_\omega(a,q;t_a,t)dq + \lim_{t\downarrow t_a}\int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi'(\xi(q))(q-a)dq \ .\end{aligned} \tag{3.70}$$

A straightforward computation (see appendix E) reveals that

$$\lim_{t\downarrow t_a}\int_{\mathbb{R}} K_\omega(a,q;t_a,t)dq = 1 \ , \tag{3.71}$$

so we find

$$\lim_{t\downarrow t_a}\int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi(q)dq = \phi(a) + \lim_{t\downarrow t_a}\int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi'(\xi(q))(q-a)dq \ . \tag{3.72}$$

Thus, it remains to show that the integral on the right-hand side vanishes in the limit. To start, we can bound the remainder term in the Taylor expansion by virtue of "rapid decay" of Schwartz functions, so that

$$\left|\phi'(\xi(q))\right| < M \tag{3.73}$$

for some $M \in \mathbb{R}_+$. Thus,

$$\begin{aligned}&\left|\int_{\mathbb{R}} K_\omega(a,q;t_a,t)\phi'(\xi(q))(q-a)dq\right| \leq \int_{\mathbb{R}}\left|K_\omega(a,q;t_a,t)\phi'(\xi(q))(q-a)\right|dq \\ &< M\int_{\mathbb{R}}|q-a|\,K_\omega(a,q;t_a,t)dq\end{aligned} \tag{3.74}$$

The problem is to show that the latter integral vanishes in the limit. The integrand is

$$|q-a|\,K_\omega(a,q;t_a,t) = |q-a|\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right) \tag{3.75}$$

for $t-t_a$ sufficiently small. Since $\cos(\omega(t-t_a))\uparrow 1$ as $t\downarrow t_a$, the integrand looks very much like

$$|q-a|\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\exp\left(-\frac{\omega}{2}\frac{(a-q)^2}{\sin(\omega(t-t_a))}\right) \tag{3.76}$$

for sufficiently small $t-t_a$, which can be seen to vanish in the limit by a substitution of variables

$$z = \sqrt{\frac{\omega}{2\sin(\omega(t-t_a))}}(a-q)\ . \tag{3.77}$$

Alas, this is obviously not *quite* the case, since $t-t_a$ in the integrand is small but fixed. To be precise, we have

$$\cos(\omega(t-t_a)) = 1+R \tag{3.78}$$

with $R=\mathcal{O}\left((t-t_a)^2\right)$ and $R<0$ since $\cos(\omega(t-t_a))$ approaches 1 from below. Hence, what we in fact get for $t-t_a$ sufficiently small, is

$$|q-a|\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\exp\left(-\frac{\omega}{2}\frac{(a-q)^2}{\sin(\omega(t-t_a))}\right)\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)R}{\sin(\omega(t-t_a))}\right) \tag{3.79}$$

Since the remainder term R is negative, the total exponent of the latter exponential becomes positive, so within the integral (for small but fixed $t-t_a$) this exponent can still grow unboundedly for $q\to\pm\infty$, which means that we cannot simply bound this exponential by a constant. Of course, for small $t-t_a$ (i.e. small R) the growth of this latter exponential is slower than the decay towards 0 of the first exponential as $q\to\pm\infty$. Because of this, we expect that the integral vanishes in the limit, but due to the unboundedness of the remainder exponential regardless of how small $t-t_a$ gets, this is not easily proven.

Assuming that conjecture 3.1 does indeed hold, $K_\omega(a,q;t_a,t)$ is the unique solution of the PDE (3.61) under initial condition (3.62). If we can additionally show that the function ϕ given by (3.60) satisfies (3.62), then we have proven (3.53). One may observe from result 2.1 that in the case $q\neq a$, the "size" $W'(X_{aq})$ of the set X_{aq} tends to 0 as $t\downarrow t_a$. From this, it can be argued that the expected value of the functional over the paths in X_{aq} should decrease to 0, since this is just an integral w.r.t W' over the set X_{aq}. One may analogously reason that in the case $q=a$, the size $W'(X_{aq})$ gets larger and larger as $t\downarrow t_a$, causing the expected value of the functional over these paths to grow. These may (or may not) be perfectly valid heuristics, but making this train of thought rigorous would be a more advanced exercise in stochastic analysis. To conclude, it seems quite reasonable to expect that conjecture 3.1 holds and that our function (3.60) satisfies (3.62), which in turn would mean that (3.53) holds, but rigorously proving this is an undertaking too ambitious for the present work. Nonetheless, the arguments presented here show that (3.53) is more than plausible.

We remind the reader that amidst this speculation we have established a connection between K_ω and a generalized form of the heat equation, which holds regardless of whether (3.53) and conjecture 3.1 are true or not. As mentioned above, we have

Result 3.5 (path integral with quadratic potential & heat-type equation).

$$\frac{\partial K_\omega(a,q;t_a,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 K_\omega(a,q;t_a,t)}{\partial q^2} + \frac{\omega^2 q^2}{2}K_\omega(a,q;t_a,t)$$

for $t-t_a\in(0,T/2)$.

This just follows from the closed form of K_ω which was found in a rigorous fashion in section 3.2. Hence, we obtain an interpretation of the path integral for a quadratic potential as a solution of a heat-type equation, just as the free path integral satisfies a heat equation, which we established in section 2.4.1. If conjecture 3.1 holds, we have the stronger result that K_ω satisfies the PDE (3.59) subject to the initial condition (3.62), which would be the complete analogue of the result for the free path integral that we saw in section 2.4.1. This is another reason why one may expect conjecture 3.1 to hold.

On a final note, we point out another interesting observation about K_ω. Recall that the free path integral can be interpreted as a probability density function, as seen in section 2.4.1. One may ask whether this generalizes to the case with a quadratic potential. It turns out that this is not the case. Indeed, in appendix E we show that

$$\int_{\mathbb{R}} K_\omega(a, b; t_a, t_b)db = \frac{1}{\sqrt{\cos(\omega(t_b - t_a))}} \exp\left(\frac{\omega}{2}\frac{a^2\sin(\omega(t_b - t_a))}{\cos(\omega(t_b - t_a))}\right) \neq 1 \tag{3.80}$$

for $t_b - t_a$ sufficiently small, which means that K_ω is not a pdf. Although the path integral for a quadratic potential should still have a probabilistic meaning, it can apparently not be interpreted as a pdf. Observe that in the case of an inverted potential, the Feynman-Kac formula (theorem 3.1) indeed tells us that the path integral is a conditional expectation of some functional over a certain set of paths, rather than a pdf. The same interpretation for our path integral of interest K_ω is hypothesized in (3.53).

Chapter 4

The anisotropic path integral

So far, we have worked exclusively with Euclidean path integrals

$$K_\Omega(a,b;t_a,t_b) = \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\|\dot{\gamma}\|^2 - \gamma^T\Omega\gamma}{2} dt\right) \mathcal{D}\gamma \ , \tag{4.1}$$

with $\Omega \in \mathbb{R}^{n\times n}$ symmetric and positive semi-definite. These are path integrals of the *isotropic* type. The term isotropic pertains to the fact that the kinetic energy term in the action functional is

$$\|\dot{\gamma}\|^2 = \dot{\gamma}^T I \dot{\gamma} \ , \tag{4.2}$$

with I the $n \times n$ identity matrix. This form of the kinetic term is common in literature on path integrals. In the light of certain applications, in particular diffusion MRI, it is interesting to consider another, more general type of kinetic term, namely

$$\dot{\gamma}^T M \dot{\gamma} \ , \tag{4.3}$$

where $M \in \mathbb{R}^{n\times n}$ is symmetric and positive-definite. This form of the kinetic term describes a moving particle with a certain preferred direction, which is captured by the matrix M. In particular, it describes *anisotropic* diffusion, which is diffusion where the particles move easier in some directions than in others. The diffusion in diffusion MRI is an example this, since the axons act as barriers for the diffusing water molecules. Replacing the standard kinetic term in the path integral by the more general one leads to the *anisotropic path integral*[8],

$$K_{M,\Omega}(a,b;t_a,t_b) := \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\dot{\gamma}^T M\dot{\gamma} - \gamma^T\Omega\gamma}{2} dt\right) \mathcal{D}\gamma \ , \tag{4.4}$$

where $\Omega \in \mathbb{R}^{n\times n}$ is symmetric and positive semi-definite. Although this may seem quite different from the Euclidean, isotropic path integrals we discussed so far, it is not so. In fact, once we have an appropriate definition of (4.4), it is rather simple to reduce the anisotropic path integral to a case of the Euclidean path integral with quadratic potential, the type which we discussed in chapter 3. Note that the particular choice $M = I$ is allowed, so that the anisotropic path integral is a generalization of the Euclidean path integral with quadratic potential.

[8]Since the term *anisotropic* pertains, strictly speaking, only to the form of the kinetic term, one may take the term *anisotropic path integral* to refer to such a path integral for an arbitrary potential V. We choose to restrict our attention to zero or quadratic potentials and henceforth refer to this as the anisotropic path integral.

4.1 Defining the anisotropic path integral

Before computing the anisotropic path integral, we need to give a proper definition to (4.4). It is logical to define it analogously to the Euclidean path integral, for which we established definition 3.1. Clearly, we cannot proceed directly in the same way due to the matrix M in the potential term. To deal with this, observe that there is an orthogonal matrix $V \in \mathbb{R}^{n\times n}$ with $\det V = 1$ and a diagonal matrix $\Delta \in \mathbb{R}^{n\times n}$ such that

$$M = V\Delta V^T \ , \tag{4.5}$$

since M is symmetric. In particular, $\Delta = \operatorname{diag}(\mu_1, \dots, \mu_n)$ with $\mu_1, \dots, \mu_n$ the eigenvalues of M. Since M is positive-definite, we have $\mu_1, \dots, \mu_n > 0$. Define

$$\sqrt{\Delta} := \operatorname{diag}(\sqrt{\mu_1}, \dots, \sqrt{\mu_n}) \ . \tag{4.6}$$

Note that $\sqrt{\Delta}^2 = \Delta$. We then have

$$\begin{aligned}
K_{M,\Omega}(a,b;t_a,t_b) &= \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot\gamma^T M \dot\gamma - \gamma^T\Omega\gamma}{2} dt\right)\mathcal{D}\gamma \\
&= \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot\gamma^T V\Delta V^T \dot\gamma - \gamma^T\Omega\gamma}{2} dt\right)\mathcal{D}\gamma = \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot\gamma^T V\sqrt{\Delta}\sqrt{\Delta} V^T \dot\gamma - \gamma^T\Omega\gamma}{2} dt\right)\mathcal{D}\gamma \\
&= \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\left(\sqrt{\Delta}V^T\dot\gamma\right)^T \sqrt{\Delta}V^T\dot\gamma - \gamma^T\Omega\gamma}{2} dt\right)\mathcal{D}\gamma \\
&= \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\left\|\sqrt{\Delta}V^T\dot\gamma\right\|^2 - \gamma^T\Omega\gamma}{2} dt\right)\mathcal{D}\gamma \ .
\end{aligned} \tag{4.7}$$

This looks almost the same as the Euclidean path integral for a quadratic potential (3.33), except that we have an additional term $\sqrt{\Delta}V^T$ in the norm. Comparing with definition 3.2, it is now clear that we have to add the factor $\sqrt{\Delta}V^T$ in the approximation of the kinetic term in a limit definition of (4.4). This implies another problem, namely the fact that we need a different normalization term than the one in definition 3.2. This results from the added factor $\sqrt{\Delta}V^T$ in the approximation of the kinetic term in the limit, which means that we need a change of variables to obtain a product of Gaussian integrals, picking up a multiplicative constant in front of the integrals along the way.

To make this more precise and determine the correct normalization constant, define

$$K_{M,\Omega}(a,b;t_a,t_b) := \lim_{N\to\infty} C_N \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|\sqrt{\Delta}V^T\left(x_{j+1}-x_j\right)\right\|^2}{2\varepsilon} + \varepsilon\cdot\frac{x_{j+1}^T\Omega x_{j+1}}{2}\right) dx \ , \tag{4.8}$$

with C_N the to-be-determined normalization constant, $\varepsilon := \frac{t_b - t_a}{N+1}$, $x_0 := a$, $x_{N+1} := b$ and $dx := dx_1 \dots dx_N$ as before. As for the Euclidean path integral we assume that C_N does not depend on Ω, but it may depend on M (we will see later that this is in fact necessary). Note that this is indeed the analogue of definition 3.2, with the additional factor $\sqrt{\Delta}V^T$ in the approximation of the kinetic term and a new normalization constant. We determine the normalization constant in a similar fashion as for the Euclidean path integral, namely by requiring for the potential-free case $\Omega = O$ that

$$C_N \int_{\mathbb{R}} \int_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(- \frac{\left\| \sqrt{\Delta}V^T \left(x_{j+1} - x_j\right) \right\|^2}{2\varepsilon} \right) dx db = 1 \;, \tag{4.9}$$

and applying the assumption that C_N does not depend on Ω to extend the obtained normalization constant to the general case by virtue of consistency. Set $y_j = \sqrt{\Delta}V^T x_j$. We then have $x_j = V\sqrt{\Delta}^{-1} y_j$, and

$$\begin{aligned} &C_N \int_{\mathbb{R}^n} \int_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(- \frac{\left\| \sqrt{\Delta}V^T \left(x_{j+1} - x_j\right) \right\|^2}{2\varepsilon} \right) dx db \\ &= \frac{C_N}{\left[\det\left(\sqrt{\Delta}V^T\right)\right]^{N+1}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(- \frac{\left\| y_{j+1} - y_j \right\|^2}{2\varepsilon} \right) dy d\tilde{b} \end{aligned} \tag{4.10}$$

with $y_0 = \sqrt{\Delta}V^T a$, $y_{N+1} = \tilde{b} = \sqrt{\Delta}V^T b$ and $dy = dy_1 \dots dy_N$. Observe that

$$\det\left(\sqrt{\Delta}V^T\right) = \det\left(\sqrt{\Delta}\right) \det\left(V^T\right) = \det\sqrt{\Delta} = \sqrt{\mu_1} \dots \sqrt{\mu_n} = \sqrt{\mu_1 \dots \mu_n} = \sqrt{\det M} \;. \tag{4.11}$$

Plugging this results into (4.10) yields

$$\begin{aligned} &C_N \int_{\mathbb{R}^n} \int_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(- \frac{\left\| \sqrt{\Delta}V^T \left(x_{j+1} - x_j\right) \right\|^2}{2\varepsilon} \right) dx db \\ &= \frac{C_N}{\sqrt{\det M}^{N+1}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(- \frac{\left\| y_{j+1} - y_j \right\|^2}{2\varepsilon} \right) dy d\tilde{b} \;. \end{aligned} \tag{4.12}$$

The integral on the right-hand side of (4.12) corresponds to a Euclidean path integral. Recall from chapter 3 that

$$\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(- \frac{\left\| x_{j+1} - x_j \right\|^2}{2\varepsilon} \right) dx db = 1 \;, \tag{4.13}$$

where $x_{N+1} = b$, regardless of the starting point x_0. In particular,

$$\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(- \frac{\left\| y_{j+1} - y_j \right\|^2}{2\varepsilon} \right) dy d\tilde{b} = 1 \tag{4.14}$$

with $y_0 = \sqrt{\Delta}V^T a$ and $y_{N+1} = \tilde{b}$. Equivalently,

$$\frac{\sqrt{\det M}^{N+1} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}}}{\sqrt{\det M}^{N+1}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(- \frac{\left\| y_{j+1} - y_j \right\|^2}{2\varepsilon} \right) dy d\tilde{b} = 1 \;. \tag{4.15}$$

Comparing to equation (4.12) yields

$$\begin{aligned}
&C_N \int\limits_{\mathbb{R}} \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|\sqrt{\Delta} V^T\left(x_{j+1}-x_j\right)\right\|^2}{2\varepsilon}\right) dx db = 1 \\
\iff\ & C_N = \sqrt{\det M}^{N+1} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} = \left(\frac{\det M}{(2\pi\varepsilon)^n}\right)^{\frac{N+1}{2}} .
\end{aligned} \tag{4.16}$$

This leads to the following definition of the anisotropic path integral.

Definition 4.1 (**n-dimensional anisotropic path integral**)**.** The n-dimensional anisotropic path integral (4.4) is defined as

$$\begin{aligned}
K_{M,\Omega}(a,b;t_a,t_b) &:= \lim_{N\to\infty} \left(\frac{\det M}{(2\pi\varepsilon)^n}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{nN}} \prod_{j=0}^{N} \exp\left(-\frac{\left\|\sqrt{\Delta} V^T\left(x_{j+1}-x_j\right)\right\|^2}{2\varepsilon} + \varepsilon \cdot \frac{x_{j+1}^T \Omega x_{j+1}}{2}\right) dx \\
&= \lim_{N\to\infty} \left(\frac{\det M}{(2\pi\varepsilon)^n}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{nN}} \exp\left(-\sum_{j=0}^{N}\left[\frac{\left\|\sqrt{\Delta} V^T\left(x_{j+1}-x_j\right)\right\|^2}{2\varepsilon} - \varepsilon \cdot \frac{x_{j+1}^T \Omega x_{j+1}}{2}\right]\right) dx ,
\end{aligned}$$

where $\varepsilon = \varepsilon(N) := \frac{t_b - t_a}{N+1} > 0$, $x_0 := a$, $x_{N+1} := b$ and $dx := dx_1 \dots dx_N$, $dx_i := dx_{i,1} \dots dx_{i,n}$.

4.2 Computing the anisotropic path integral

With definition 4.1, it is straightforward to reduce the anisotropic path integral to a case of the Euclidean path integral for a quadratic potential. Set $y_j = \sqrt{\Delta} V^T x_j$, then $x_j = V \sqrt{\Delta}^{-1} y_j$ and

$$\begin{aligned}
&\left(\frac{\det M}{(2\pi\varepsilon)^n}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{nN}} \exp\left(-\sum_{j=0}^{N}\left[\frac{\left\|\sqrt{\Delta} V^T\left(x_{j+1}-x_j\right)\right\|^2}{2\varepsilon} - \varepsilon \cdot \frac{x_{j+1}^T \Omega x_{j+1}}{2}\right]\right) dx \\
&= \frac{1}{\left[\det\left(\sqrt{\Delta} V^T\right)\right]^N} \\
&\times \left(\frac{\det M}{(2\pi\varepsilon)^n}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{nN}} \exp\left(-\sum_{j=0}^{N}\left[\frac{\left\|y_{j+1}-y_j\right\|^2}{2\varepsilon} - \varepsilon \cdot \frac{y_{j+1}^T \left(\sqrt{\Delta}^{-1}\right)^T V^T \Omega V \sqrt{\Delta}^{-1} y_{j+1}}{2}\right]\right) dy \\
&\overset{(4.11)}{=} \frac{1}{\sqrt{\det M}^N} \left(\frac{\det M}{(2\pi\varepsilon)^n}\right)^{\frac{N+1}{2}} \int\limits_{\mathbb{R}^{nN}} \exp\left(-\sum_{j=0}^{N}\left[\frac{\left\|y_{j+1}-y_j\right\|^2}{2\varepsilon} - \varepsilon \cdot \frac{y_{j+1}^T \sqrt{\Delta}^{-1} V^T \Omega V \sqrt{\Delta}^{-1} y_{j+1}}{2}\right]\right) dy \\
&= \sqrt{\det M} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \exp\left(-\sum_{j=0}^{N}\left[\frac{\left\|y_{j+1}-y_j\right\|^2}{2\varepsilon} - \varepsilon \cdot \frac{y_{j+1}^T \sqrt{\Delta}^{-1} V^T \Omega V \sqrt{\Delta}^{-1} y_{j+1}}{2}\right]\right) dy .
\end{aligned} \tag{4.17}$$

Plugging this into definition 4.1, we find

$$\begin{aligned}
&K_{M,\Omega}(a,b;t_a,t_b)\\
&= \sqrt{\det M} \lim_{N\to\infty} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n(N+1)}{2}} \int\limits_{\mathbb{R}^{nN}} \exp\left(-\sum_{j=0}^{N}\left[\frac{\left\|y_{j+1}-y_j\right\|^2}{2\varepsilon} - \varepsilon\cdot\frac{y_{j+1}^T\sqrt{\Delta}^{-1}V^T\Omega V\sqrt{\Delta}^{-1}y_{j+1}}{2}\right]\right) dy\\
&= \sqrt{\det M} K_{\sqrt{\Delta}^{-1}V^T\Omega V\sqrt{\Delta}^{-1}}\left(\sqrt{\Delta}V^Ta, \sqrt{\Delta}V^Tb; t_a, t_b\right) .
\end{aligned} \tag{4.18}$$

For brevity, let us henceforth define

$$\Omega' := \sqrt{\Delta}^{-1}V^T\Omega V\sqrt{\Delta}^{-1} . \tag{4.19}$$

Then the result for the anisotropic path integral reads

$$K_{M,\Omega}(a,b;t_a,t_b) = \sqrt{\det M} K_{\Omega'}\left(\sqrt{\Delta}V^Ta, \sqrt{\Delta}V^Tb; t_a, t_b\right) . \tag{4.20}$$

Observe that the path integral $K_{\Omega'}$ falls within the scope of chapter 3, since Ω' is positive semi-definite as a result of Ω being positive semi-definite. Indeed, for $x \in \mathbb{R}^n$ we have

$$x^T\Omega' x = x^T\sqrt{\Delta}^{-1}V^T\Omega V\sqrt{\Delta}^{-1}x = \left(V\sqrt{\Delta}^{-1}x\right)^T \Omega \left(V\sqrt{\Delta}^{-1}x\right) \geq 0 . \tag{4.21}$$

Thus, the anisotropic path integral $K_{M,\Omega}$ essentially reduces to the Euclidean path integral with quadratic potential $K_{\Omega'}$. It should be kept in mind that, despite its name, the matrix Ω' depends on both Ω and M, through the matrices Δ and V from the diagonalization of M (4.5). Note that for $M = I$, the right-hand side of (4.20) reduces to $K_\Omega(a,b;t_a,t_b)$ as desired, since $\Delta = V = I$ in this case.

For the special case $\Omega = O$, which we call the *anisotropic free path integral*, we find

Result 4.1 (anisotropic free path integral).

$$\begin{aligned}
K_{M,O}(a,b;t_a,t_b) &= \sqrt{\det M} K_O\left(\sqrt{\Delta}V^Ta, \sqrt{\Delta}V^Tb; t_a, t_b\right)\\
&\overset{\text{res. 3.3}}{=} \frac{\sqrt{\det M}}{\sqrt{2\pi(t_b-t_a)}^n} \exp\left(-\frac{\left\|\sqrt{\Delta}V(b-a)\right\|^2}{2(t_b-t_a)}\right)\\
&= \frac{\sqrt{\det M}}{\sqrt{2\pi(t_b-t_a)}^n} \exp\left(-\frac{\left(\sqrt{\Delta}V(b-a)\right)^T\sqrt{\Delta}V(b-a)}{2(t_b-t_a)}\right)\\
&= \frac{\sqrt{\det M}}{\sqrt{2\pi(t_b-t_a)}^n} \exp\left(-\frac{(b-a)^TV^T\left(\sqrt{\Delta}\right)^T\sqrt{\Delta}V(b-a)}{2(t_b-t_a)}\right)\\
&= \frac{\sqrt{\det M}}{\sqrt{2\pi(t_b-t_a)}^n} \exp\left(-\frac{(b-a)^TV^T\Delta V(b-a)}{2(t_b-t_a)}\right) = \frac{\sqrt{\det M}}{\sqrt{2\pi(t_b-t_a)}^n} \exp\left(-\frac{(b-a)^TM(b-a)}{2(t_b-t_a)}\right) .
\end{aligned}$$

Note that the closed form of the anisotropic free path integral is completely different from the closed form of the Euclidean path integral for a quadratic potential. Indeed, the difference is readily seen by considering the 1-dimensional case of result 4.1 and comparing it to result 3.1.

The former contains no trigonometric functions whereas the latter does. It is quite interesting that the difference is so striking, for the following reason. The underlying phenomenon which is represented by the anisotropic free path integral is that of anisotropic diffusion, where the particles have a certain preferred direction in which they diffuse instead of an arbitrary direction as represented by the Euclidean free path integral (see section 2.4.1). On the other hand, the addition of a quadratic potential term to the Euclidean free path integral introduces a potential barrier, as we already discussed in chapter 3. There is a conceptual difference with true anisotropic diffusion, but in the end the effect is similar. In particular, both the path integral K_Ω and $K_{M,O}$ model the obstruction of diffusing water molecules by axons in diffusion MRI. One might therefore expect that the closed forms of these path integrals look similar, but this is apparently not the case.

For the general case of the anisotropic path integral, we have

$$\begin{aligned} K_{M,\Omega}(a,b;t_a,t_b) &= \sqrt{\det M}\, K_{\Omega'}\left(\sqrt{\Delta}V^T a, \sqrt{\Delta}V^T b; t_a, t_b\right) \\ &\overset{\text{res. }3.2}{=} \sqrt{\det M}\prod_{i=1}^{n} K_{\sqrt{\lambda_i}}\left(\left[U^T\sqrt{\Delta}V^T a\right]_i, \left[U^T\sqrt{\Delta}V^T b\right]_i; t_a, t_b\right)\ , \end{aligned} \tag{4.22}$$

where $\lambda_1,\ldots,\lambda_n \geq 0$ are the eigenvalues of Ω', and $U \in \mathbb{R}^{n\times n}$ the orthogonal matrix with $\det U = 1$ which satisfies

$$\operatorname{diag}(\lambda_1,\ldots,\lambda_n) = U^T\Omega' U\ . \tag{4.23}$$

For brevity, we henceforth define

$$W^T := U^T\sqrt{\Delta}V^T\ . \tag{4.24}$$

Then the general result for the anisotropic path integral reads

Result 4.2 (anisotropic path integral).

$$K_{M,\Omega}(a,b;t_a,t_b) = \sqrt{\det M}\prod_{i=1}^{n} K_{\sqrt{\lambda_i}}\left(\left[W^T a\right]_i, \left[W^T b\right]_i; t_a, t_b\right)\ .$$

In the same way as in section 3.3, we restrict the size of the time interval $t_b - t_a$ based on the eigenvalues of the matrix Ω'. If λ_1 is the largest positive eigenvalue, we henceforth assume that $t_b - t_a \in (0, \pi/\sqrt{\lambda_1})$. This ensures that all path integrals $K_{\sqrt{\lambda_i}}$ in result 4.2 have a well-defined closed form, namely

$$\begin{aligned} &K_{\sqrt{\lambda_i}}\left(\left[W^T a\right]_i, \left[W^T b\right]_i; t_a, t_b\right) \\ &\overset{(3.42)}{=} \begin{cases} \frac{1}{\sqrt{2\pi(t_b-t_a)}}\exp\left(-\frac{\left[\left(W^T b\right)_i - \left(W^T a\right)_i\right]^2}{2(t_b-t_a)}\right) & \text{if } \lambda_i = 0 \\ \sqrt{\frac{\sqrt{\lambda_i}}{2\pi\sin(\sqrt{\lambda_i}(t_b-t_a))}}\exp\left(-\frac{\sqrt{\lambda_i}}{2}\frac{\left[\left(W^T a\right)_i^2 + \left(W^T b\right)_i^2\right]\cos(\sqrt{\lambda_i}(t_b-t_a)) - 2\left(W^T a\right)_i\left(W^T b\right)_i}{\sin(\sqrt{\lambda_i}(t_b-t_a))}\right) & \text{if } \lambda_i > 0\ . \end{cases} \end{aligned} \tag{4.25}$$

It should go without saying that evaluating the anisotropic path integral is, computationally, a rather cumbersome affair for nontrivial cases with $n \geq 2$. One first has to diagonalize M to find the matrix Ω', and then one has to diagonalize this matrix Ω' to find its eigenvalues λ_i and the matrix W^T. Then, finally, one obtains a product of n one-dimensional path integrals, for which we have a closed expression (which is, unfortunately, quite complicated in the nontrivial case $\lambda_i > 0$). This being said, it is in principle feasible to evaluate the anisotropic path integral exactly in the special case of interest $n = 3$. For (much) higher dimensions, one may resort to numerical methods for finding eigenvalues and eigenvectors of matrices (see e.g. [37]).

After all this work to arrive at an appropriate definition of the anisotropic path integral and subsequently compute its closed form, one might ask if this could not have been done easier. After all, the essence of the computations is the change of variables $y_j = \sqrt{\Delta}V^T x_j$. With this in mind, it may be tempting to opt for a naive approach and carry out an analogous change of variables directly within the path integral by setting $\eta(t) = \sqrt{\Delta}V^T\gamma(t)$, treating it just as any other change of variables in a well-defined Riemann integral. Doing so, we would obtain

$$\begin{aligned}
K_{M,\Omega}(a,b;t_a,t_b) &\overset{(4.7)}{=} \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\left\|\sqrt{\Delta}V^T\dot{\gamma}\right\|^2 - \gamma^T\Omega\gamma}{2} dt\right)\mathcal{D}\gamma \\
&= \frac{1}{\det\left(\sqrt{\Delta}V^T\right)} \int_{\eta(t_a)=\sqrt{\Delta}V^T a}^{\eta(t_b)=\sqrt{\Delta}V^T b} \exp\left(-\int_{t_a}^{t_b} \frac{\left\|\dot{\eta}\right\|^2 - \eta^T\Omega'\eta}{2} dt\right)\mathcal{D}\eta \qquad \textbf{(incorrect)} \\
&= \frac{1}{\sqrt{\det M}} K_{\Omega'}\left(\sqrt{\Delta}V^T a, \sqrt{\Delta}V^T b; t_a, t_b\right) ,
\end{aligned}$$

which is clearly the wrong result, cf. equation (4.20). Of course, there is indeed no reason why this naive approach should work, since the measure $\mathcal{D}\gamma$ is not well-defined and thus cannot be subjected to formal manipulations such as a change of variables. Moreover, even in cases when the path integral as a whole can be defined in a reasonable way, such as definitions 2.1, 3.2 and 4.1, the result is vastly different from ordinary Riemann integration, not least because one is working with a limit of Riemann integrals whose dimension becomes arbitrarily large. Thus, one cannot assume Riemann integral-like behaviour of the path integral in these cases either. In general, one should be careful with formal manipulations to path integrals and always ask whether the desired manipulations are justifiable by the definition of the path integral in question.

4.3 Perturbing the anisotropic path integral

In this section, we shall present a method to treat an even more general class of path integrals analytically, expressing them in terms of anisotropic path integrals. This method is a generalization of a perturbative approach suggested by supervisor Luc Florack, but similar methods can be found in various literature sources as well (see e.g. [38] and the references therein). It differs from the techniques which we employed in the previous chapters, because we will not be able to provide a fully closed form of the more general type of path integrals. What we will be doing instead, is expressing them as an infinite series containing only anisotropic path integrals for which we have a closed form. We shall furthermore not be concerned with giving an appropriate definition of the complicated path integral as we did before. Rather, we will be performing manipulations with the path integral itself. We recall from section 4.2 that it is not straightforward to perform formal manipulations to the path integral, so we aim to keep this to a minimum and only perform "reasonable" manipulations. In particular, we will avoid manipulations to the heuristic measure in path space (i.e. change of variable in the path integral). For this perturbative approach, we will be using the "intermediate point requirement" (2.2) to split path integrals, on which we based all previous definitions of the path integrals, and in addition we will make some other, mild assumptions.

The path integral of interest is

$$K_{M,\Omega,V}(a,b;t_a,t_b) := \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}^T M\dot{\gamma} - \gamma^T\Omega\gamma}{2} - V(\gamma,t)dt\right)\mathcal{D}\gamma \ , \tag{4.26}$$

where $M \in \mathbb{R}^{n\times n}$ is symmetric and positive-definite, $\Omega \in \mathbb{R}^{n\times n}$ symmetric and positive semi-definite, and

$$\|V\|_\infty := \sup_{(x,t)\in\mathbb{R}^n\times[t_a,t_b]} \big|V(x,t)\big| \ll \frac{1}{t_b - t_a} \ . \tag{4.27}$$

Thus, we essentially consider the anisotropic path integral and add to its quadratic potential another, sufficiently small function V which may be interpreted as a perturbation of the quadratic potential. Note that this may be reduced to a Euclidean path integral with perturbed quadratic potential by setting $M = I$, or a "perturbed free path integral" (of either Euclidean or anisotropic type) by setting $\Omega = O$.

We shall assume that the length of the time interval $t_b - t_a$ is chosen such that the anisotropic path integral $K_{M,\Omega}(a,b;t_a,t_b)$ has a well-defined closed form through result 4.2 and equation (4.25), since we are going to express $K_{M,\Omega,V}$ in terms of $K_{M,\Omega}$. To start, we rewrite (4.26) as

$$K_{M,\Omega,V}(a,b;t_a,t_b) = \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}^T M\dot{\gamma} - \gamma^T\Omega\gamma}{2}dt\right)\exp\left(\int_{t_a}^{t_b} V(\gamma,t)dt\right)\mathcal{D}\gamma \tag{4.28}$$

and Taylor expand the exponential term containing the perturbation, viz.

$$\exp\left(\int_{t_a}^{t_b} V(\gamma,t)dt\right) = \sum_{k=0}^{\infty}\frac{1}{k!}\left(\int_{t_a}^{t_b} V(\gamma,t)dt\right)^k \ . \tag{4.29}$$

This yields

$$\begin{aligned} K_{M,\Omega,V}(a,b;t_a,t_b) &= \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}^T M\dot{\gamma} - \gamma^T\Omega\gamma}{2}dt\right)\sum_{k=0}^{\infty}\frac{1}{k!}\left(\int_{t_a}^{t_b} V(\gamma,t)dt\right)^k \mathcal{D}\gamma \\ &\overset{*}{=} \sum_{k=0}^{\infty}\frac{1}{k!}\int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}^T M\dot{\gamma} - \gamma^T\Omega\gamma}{2}dt\right)\left(\int_{t_a}^{t_b} V(\gamma,t)dt\right)^k \mathcal{D}\gamma \ , \end{aligned} \tag{4.30}$$

where step $(*)$ relies on the assumption that we may interchange the infinite summation and path integration. For convenience, let us define

$$K^{(k)}_{M,\Omega,V}(a,b;t_a,t_b) := \frac{1}{k!}\int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b} \frac{\dot{\gamma}^T M\dot{\gamma} - \gamma^T\Omega\gamma}{2}dt\right)\left(\int_{t_a}^{t_b} V(\gamma,t)dt\right)^k \mathcal{D}\gamma \ , \tag{4.31}$$

so that

$$K_{M,\Omega,V}(a,b;t_a,t_b) = \sum_{k=0}^{\infty} K^{(k)}_{M,\Omega,V}(a,b;t_a,t_b) \ . \tag{4.32}$$

This series expansion has a quite elegant interpretation. The path integrals in the series can be seen as the contribution to $K_{M,\Omega,V}$ of those paths that are "patched together" line segments. These paths are trajectories of scattering particles, comparable to Brownian motion: the particles start by travelling in a straight line from a to b, but on the way they collide with other particles and thus the direction of their straight path changes. The k-th term in the series expansion, that is, the path integral $K^{(k)}_{M,\Omega,V}$ then represents the contribution to $K_{M,\Omega,V}$ of those scattering trajectories along which the particle collides with another particle k times (giving a path which consists of $k+1$ line segments). This is shown in figure 4.1. Apparently, summing the contributions of all these scattering trajectories is equivalent to considering *all* paths $\gamma \in X_{ab}$ as per the original path integral $K_{M,\Omega,V}$, even though X_{ab} contains many more paths than just these scattering trajectories.

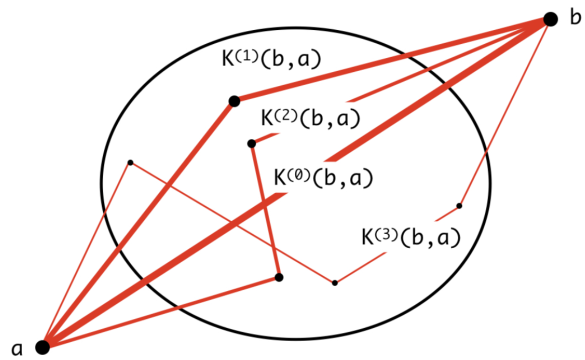

Figure 4.1: Example paths corresponding to the lowest order terms in the series expansion. (Original drawing by supervisor Luc Florack, used with permission.)

Note that

$$K^{(0)}_{M,\Omega,V}(a,b;t_a,t_b) = \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\dot\gamma^T M \dot\gamma - \gamma^T \Omega \gamma}{2} dt\right) \mathcal{D}\gamma = K_{M,\Omega}(a,b;t_a,t_b) \; . \tag{4.33}$$

For $k \geq 1$, we make each of the k integrals containing V within $K^{(k)}_{M,\Omega,V}$ distinct by introducing time variables $s_1, \dots, s_k$, which gives

$$K^{(k)}_{M,\Omega,V}(a,b;t_a,t_b) = \frac{1}{k!} \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\dot\gamma^T M \dot\gamma - \gamma^T \Omega \gamma}{2} dt\right) \left(\prod_{j=1}^{k} \int\limits_{t_a}^{t_b} V(\gamma(s_j), s_j) ds_j\right) \mathcal{D}\gamma \; . \tag{4.34}$$

We now assume that we may interchange the order of the integration over $s_1, \dots, s_k$ and the path integration, so that

$$K^{(k)}_{M,\Omega,V}(a,b;t_a,t_b) = \frac{1}{k!} \int\limits_{[t_a,t_b]^k} \int\limits_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int\limits_{t_a}^{t_b} \frac{\dot\gamma^T M \dot\gamma - \gamma^T \Omega \gamma}{2} dt\right) \left(\prod_{j=1}^{k} V(\gamma(s_j), s_j)\right) \mathcal{D}\gamma ds \; , \tag{4.35}$$

where $ds := ds_1 \ldots ds_k$. This is a quite natural assumption. In (4.34), one considers in the integrand of the path integral the effect of the k perturbation terms V along the whole path, and one "repeats" this for every path. In (4.35) on the other hand, one considers in the integrand of the time integral the effect of the k perturbation terms V at fixed times $s_1, \ldots, s_k$ for all paths combined, and one repeats this for every combination of times $s_1, \ldots, s_k$. In the end, one will have considered the effect of every single one of the k perturbation terms along every path (i.e. for every path at every moment in time) in both cases.

Note that we can restrict the integration domain to $t_a < s_1 < \cdots < s_k < t_b$ by dropping the factorial [38]:

$$K^{(k)}_{M,\Omega,V}(a,b;t_a,t_b) = \int_{t_a}^{t_b}\int_{t_a}^{s_k}\cdots\int_{t_a}^{s_2}\int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b}\frac{\dot\gamma^T M\dot\gamma - \gamma^T\Omega\gamma}{2}dt\right)\left(\prod_{j=1}^{k} V(\gamma(s_j),s_j)\right)\mathcal{D}\gamma ds\ . \tag{4.36}$$

The benefit of interchanging the order of integration is that we can now focus on the path integral

$$F^{(k)}_{M,\Omega,V}(a,b;t_a,t_b;s_1,\ldots,s_k) := \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{t_b}\frac{\dot\gamma^T M\dot\gamma - \gamma^T\Omega\gamma}{2}dt\right)\left(\prod_{j=1}^{k} V(\gamma(s_j),s_j)\right)\mathcal{D}\gamma \tag{4.37}$$

where the perturbation V only contributes at fixed times $s_1, \ldots, s_k$. Since $t_a < s_1 < \cdots < s_k < t_b$, we can conveniently apply the "intermediate point requirement" (2.2) to split the path integral over $[t_a,t_b]$ into a product of path integrals over $[t_a,s_1],[s_1,s_2],\ldots,[s_k,t_b]$. (Strictly speaking, we only stated that (2.2) should hold for the Euclidean path integral (1.5), but we simply require that this also holds for our path integral $F^{(k)}_{M,\Omega,V}$.) In doing so, the points $\gamma(s_j)$ will become parameters over which we integrate independently from the path integration, effectively making the path integrals over the smaller time intervals independent of the perturbation term. Defining $s_0 := t_a,\ x_0 := a,\ s_{k+1} := t_b,\ x_{k+1} := b$ and $dx := dx_1 \ldots dx_k$, we get

$$\begin{aligned}
F^{(k)}_{M,\Omega,V}(a,b;t_a,t_b;s_1,\ldots,s_k) &= \int_{\gamma(t_a)=a}^{\gamma(t_b)=b} \exp\left(-\int_{t_a}^{s_1}\frac{\dot\gamma^T M\dot\gamma - \gamma^T\Omega\gamma}{2}dt\right) V(\gamma(s_1),s_1)\times\ldots \\
&\cdots\times\exp\left(-\int_{s_{k-1}}^{s_k}\frac{\dot\gamma^T M\dot\gamma - \gamma^T\Omega\gamma}{2}dt\right) V(\gamma(s_k),s_k)\times\exp\left(-\int_{s_k}^{t_b}\frac{\dot\gamma^T M\dot\gamma - \gamma^T\Omega\gamma}{2}dt\right)\mathcal{D}\gamma \\
&= \int_{\mathbb{R}^{kn}}\left[\int_{\gamma(s_0)=x_0}^{\gamma(s_1)=x_1}\exp\left(-\int_{s_0}^{s_1}\frac{\dot\gamma^T M\dot\gamma - \gamma^T\Omega\gamma}{2}dt\right) V(\gamma(s_1),s_1)\mathcal{D}\gamma\times\ldots\right. \\
&\cdots\times\int_{\gamma(s_{k-1})=x_{k-1}}^{\gamma(s_k)=x_k}\exp\left(-\int_{s_{k-1}}^{s_k}\frac{\dot\gamma^T M\dot\gamma - \gamma^T\Omega\gamma}{2}dt\right) V(\gamma(s_k),s_k)\mathcal{D}\gamma \\
&\left.\times\int_{\gamma(s_k)=x_k}^{\gamma(s_{k+1})=x_{k+1}}\exp\left(-\int_{s_k}^{s_{k+1}}\frac{\dot\gamma^T M\dot\gamma - \gamma^T\Omega\gamma}{2}dt\right)\mathcal{D}\gamma\right] dx
\end{aligned}$$

$$= \int\limits_{\mathbb{R}^{kn}} \left[\int\limits_{\gamma(s_0)=x_0}^{\gamma(s_1)=x_1} \exp\left(-\int\limits_{s_0}^{s_1} \frac{\dot{\gamma}^T M \dot{\gamma} - \gamma^T \Omega \gamma}{2} dt \right) \mathcal{D}\gamma \right.$$

$$\left. \times \prod_{j=1}^{k} \left(V(x_j, s_j) \int\limits_{\gamma(s_j)=x_j}^{\gamma(s_{j+1})=x_{j+1}} \exp\left(-\int\limits_{s_j}^{s_{j+1}} \frac{\dot{\gamma}^T M \dot{\gamma} - \gamma^T \Omega \gamma}{2} dt \right) \mathcal{D}\gamma \right) \right] dx$$

$$= \int\limits_{\mathbb{R}^{kn}} K_{M,\Omega}(x_0, x_1; s_0, s_1) \prod_{j=1}^{k} \left[V(x_j, s_j) K_{M,\Omega}(x_j, x_{j+1}; s_j, s_{j+1}) \right] dx \ . \tag{4.38}$$

This gives

$$\begin{aligned} K^{(k)}_{M,\Omega,V}(a, b; t_a, t_b) &= \int\limits_{t_a}^{t_b} \int\limits_{t_a}^{s_k} \cdots \int\limits_{t_a}^{s_2} F^{(k)}_{M,\Omega,V}(a, b; t_a, t_b; s_1, \ldots, s_k) ds \\ = \int\limits_{t_a}^{t_b} \int\limits_{t_a}^{s_k} \cdots \int\limits_{t_a}^{s_2} \int\limits_{\mathbb{R}^{kn}} & K_{M,\Omega}(x_0, x_1; s_0, s_1) \prod_{j=1}^{k} \left[V(x_j, s_j) K_{M,\Omega}(x_j, x_{j+1}; s_j, s_{j+1}) \right] dx ds \ , \end{aligned} \tag{4.39}$$

and consequently

Result 4.3 (Perturbed anisotropic path integral).

$$K_{M,\Omega,V}(a, b; t_a, t_b) = \sum_{k=0}^{\infty} K^{(k)}_{M,\Omega,V}(a, b; t_a, t_b) = K_{M,\Omega}(a, b; t_a, t_b)$$

$$+ \sum_{k=1}^{\infty} \int\limits_{t_a}^{t_b} \int\limits_{t_a}^{s_k} \cdots \int\limits_{t_a}^{s_2} \int\limits_{\mathbb{R}^{kn}} K_{M,\Omega}(x_0, x_1; s_0, s_1) \prod_{j=1}^{k} \left[V(x_j, s_j) K_{M,\Omega}(x_j, x_{j+1}; s_j, s_{j+1}) \right] dx ds \ .$$

Note that $0 < s_{j+1} - s_j < t_b - t_a$ on the whole integration domain. Since we assumed that $t_b - t_a$ is chosen such that $K_{M,\Omega}(a, b; t_a, t_b)$ has a well-defined closed form (for all $a, b \in \mathbb{R}$), this implies that $K_{M,\Omega}(x_j, x_{j+1}; s_j, s_{j+1})$ is also well-defined in closed form through result 4.2 and equation (4.25) on the whole integration domain. In particular, the closed forms are integrable functions, hence the series expansion in result 4.3 is indeed well-defined. We have thus reduced the path integral $K_{M,\Omega,V}$ to a series of ordinary Riemann integrals. Convergence of the series is guaranteed by the restriction (4.27) on the magnitude of the perturbation. It should be clear that the approach presented here can in fact be applied to *any* perturbed potential, as long as the path integrals in the resulting series expansion (containing the unperturbed potential) are known in closed form.

Chapter 5

Summary of the main results & future research

Throughout the preceding chapters, we have discussed a variety of path integrals, computing them in closed form and interpreting them whenever possible. In this final chapter, we shall provide a compact overview of the most significant results. We will also point out relevant problems that were not (fully) solved in this work, which may serve as a starting point for future research.

5.1 Rigorous results

In chapter 2, we started by exploring the free path integral. We found that it can be written in closed form in various ways, which are all given by result 2.1:

$$K_0(a,b;t_a,t_b) = W'(X_{ab}) = \int\limits_{X_{ab}} dW' = \frac{1}{\sqrt{2\pi(t_b-t_a)}} \exp\left(-\frac{(b-a)^2}{2(t_b-t_a)}\right) \ . \tag{5.1}$$

We recognize the heat/diffusion kernel in the closed form, which is actually a probability density function in the end point b. Thus, the free path integral is a pdf, namely of a Gaussian random variable. A more explicit formulation of the free path integral as a pdf is given by result 2.2:

$$\mathbb{P}(b_1 < Z < b_2) = \frac{1}{\sqrt{2\pi(t_b-t_a)}} \int\limits_{b_1}^{b_2} \exp\left(-\frac{(b-a)^2}{2(t_b-t_a)}\right) db = \int\limits_{b_1}^{b_2} K_0(a,b;t_a,t_b) db \ , \tag{5.2}$$

where Z denotes a Gaussian random variable with mean a and variance $t_b - t_a$. $\mathbb{P}(b_1 < Z < b_2)$ is the probability that a particle undergoing diffusion starting in a at time t_a is found in some point $b \in (b_1, b_2)$ at time t_b. If we consider the probability density over an arbitrarily small interval, we find an expression of the probability which the Wiener measure assigns to the set of Brownian paths X_{ab} in terms of the free path integral, namely result 2.3:

$$W(X_{ab}) = \lim_{N\to\infty} \int\limits_{b-\frac{1}{N}}^{b+\frac{1}{N}} K_0(a,x;t_a,t_b) dx \ . \tag{5.3}$$

Finally, we extended result 2.2 to also include a formulation in terms of Wiener measure, given by result 2.4:

$$W\left(\{\gamma \in X_a : \gamma(t_b) \in (b_1, b_2)\}\right) = \int_{b_1}^{b_2} K_0(a, b; t_a, t_b) db = \mathbb{P}(b_1 < Z < b_2) . \tag{5.4}$$

Thus, the free path integral is the pdf for both diffusion and Brownian motion. In particular, this shows that diffusion and Brownian motion are similar in that they are both characterized by the same pdf.

In chapter 3, we looked at the important case of a path integral for a quadratic potential function. We saw that the Lagrangian formulation of the Euclidean path integral gives problems in this case, since the closed form of the path integral is not defined for all time intervals, which is not the case in the Hamiltonian formulation. Under the restriction $t_b - t_a \in (0, T/2)$, or equivalently $\omega(t_b - t_a) \in (0, \pi)$, we found the closed form for the 1-dimensional case which is given by result 3.1:

$$K_\omega(a, b; t_a, t_b) = \sqrt{\frac{\omega}{2\pi \sin(\omega(t_b - t_a))}} \exp\left(-\frac{\omega}{2} \frac{(a^2 + b^2)\cos(\omega(t_b - t_a)) - 2ab}{\sin(\omega(t_b - t_a))}\right) . \tag{5.5}$$

The general n-dimensional case was shown to reduce to a product of 1-dimensional path integrals in result 3.2:

$$K_\Omega(a, b; t_a, t_b) = \prod_{i=1}^{n} K_{\sqrt{\lambda_i}}\left(\left[U^T a\right]_i, \left[U^T b\right]_i; t_a, t_b\right) . \tag{5.6}$$

It follows that the n-dimensional case has a well-defined closed form through result 3.1 if $t_b - t_a \in (0, \pi/\sqrt{\lambda_1})$, where we assume λ_1 to be the largest nonzero eigenvalue of Ω (if all eigenvalues are 0, we simply have $\Omega = O$, in which case no restriction on the time interval is needed). As a special case of the n-dimensional case for a quadratic potential, we found the closed form of the general n-dimensional free path integral, given by result 3.3:

$$K_O(a, b; t_a, t_b) = \frac{1}{\sqrt{2\pi(t_b - t_a)}^n} \exp\left(-\frac{\|b - a\|^2}{2(t_b - t_a)}\right) . \tag{5.7}$$

Result 3.4 shows that the path integral for a quadratic potential behaves as desired under rotations of the potential field/the starting and end point:

$$K_\Omega(Ra, Rb; t_a, t_b) = K_{R^T \Omega R}(a, b; t_a, t_b) . \tag{5.8}$$

In particular, the free path integral is invariant under rotations of the starting and end point. We also obtained the interpretation of the 1-dimensional path integral with quadratic potential as solution to a heat-type equation through result 3.5:

$$\frac{\partial K_\omega(a, q; t_a, t)}{\partial t} = \frac{1}{2} \frac{\partial^2 K_\omega(a, q; t_a, t)}{\partial q^2} + \frac{\omega^2 q^2}{2} K_\omega(a, q; t_a, t) \tag{5.9}$$

for $t - t_a \in (0, T/2)$.

In chapter 4, we looked beyond the Euclidean path integral and introduced the anisotropic path integral. For the special case of the n-dimensional anisotropic free path integral, we found the closed form in result 4.1:

$$K_{M,O}(a, b; t_a, t_b) = \frac{\sqrt{\det M}}{\sqrt{2\pi(t_b - t_a)}^n} \exp\left(-\frac{(b - a)^T M (b - a)}{2(t_b - t_a)}\right) . \tag{5.10}$$

We found that the general n-dimensional anisotropic path integral reduces to a product of 1-dimensional Euclidean path integrals with quadratic potential as given by result 4.2:

$$K_{M,\Omega}(a,b;t_a,t_b) = \sqrt{\det M}\prod_{i=1}^{n} K_{\sqrt{\lambda_i}}\left(\left[W^T a\right]_i, \left[W^T b\right]_i; t_a, t_b\right) . \tag{5.11}$$

It follows that the general n-dimensional anisotropic path integral has a well-defined closed form through result 3.1 if $t_b - t_a \in (0, \pi/\sqrt{\lambda_1})$, where we assume λ_1 to be the largest nonzero eigenvalue of Ω' (again, if all eigenvalues are 0 we have $\Omega' = O$, and then we need not restrict the time interval). Finally, we looked at an even more general class of path integrals in the form of a perturbed anisotropic path integral. We obtained a series expansion in terms of the usual (unperturbed) anisotropic path integral in result 4.3:

$$\begin{aligned} &K_{M,\Omega,V}(a,b;t_a,t_b) = K_{M,\Omega}(a,b;t_a,t_b) \\ &+\sum_{k=1}^{\infty}\int_{t_a}^{t_b}\int_{t_a}^{s_k}\cdots\int_{t_a}^{s_2}\int_{\mathbb{R}^{kn}} K_{M,\Omega}(x_0,x_1;s_0,s_1)\prod_{j=1}^{k}\left[V(x_j,s_j)K_{M,\Omega}(x_j,x_{j+1};s_j,s_{j+1})\right]dxds\ . \end{aligned} \tag{5.12}$$

If we choose $t_b - t_a$ such that $K_{M,\Omega}(a,b;t_a,t_b)$ has a well-defined closed form as discussed above, then all anisotropic path integrals $K_{M,\Omega}(x_j, x_{j+1}; s_j, s_{j+1})$ in the Riemann integral are also well-defined in closed form, since $0 < s_{j+1} - s_j < t_b - t_a$ on the integration domain.

5.2 Future research

The most important problem which we encountered in this work, is the fact that our closed form for the 1-dimensional path integral with quadratic potential is only well-defined for certain time intervals $t_b - t_a$ (in particular, only for end times t_b which fall within the first half of a period of the harmonic oscillator). This is a direct consequence of the choice for a Lagrangian formulation of the Euclidean path integral instead of a Hamiltonian formulation. Although this restriction on the time interval is not necessarily very severe from a physical standpoint, it would be mathematically more pleasing if we can find a way to generalize the closed form to all time intervals $t_b - t_a > 0$. Indeed, if we look at the definition of the Euclidean path integral there is no clear reason why this should be restricted to certain time intervals in the 1-dimensional Lagrangian case of a quadratic potential. Thus, it would be worth investigating whether it is possible to extend the closed form of the Lagrangian 1-dimensional path integral with quadratic potential to general $t_b - t_a > 0$. In this case, we would also immediately be able to extend the closed forms for the general n-dimensional path integral with quadratic potential and anisotropic path integral, since these are defined in terms of the 1-dimensional path integral with quadratic potential.

Another significant problem is the interpretation of the path integral with quadratic potential in the Lagrangian case. For the Hamiltonian case, we have the Feynman-Kac formula which provides a clear way to interpret the path integral, but there seems to be no proof of a similar result for the Lagrangian formulation which we are interested in. Nonetheless, we expect that such a result does hold. We sketched a possible proof in section 3.4. To complete it, one would have to prove conjecture 3.1 and show that (3.60) satisfies (3.62) (in the sense of a distributional limit $t \downarrow t_a$). These claims need not be true, but if they are, it would be valuable to work them out in full rigor, since this would prove that we have an elegant formulation of the Lagrangian path integral with quadratic potential as a Wiener integral. Alternatively, one could try to come up with an entirely different proof. Although it would be a most unexpected result, a proof of the converse, namely that the Lagrangian path integral with quadratic potential **cannot** be represented as a Wiener integral, would also be a useful result. In any case, one may restrict attention to the Wiener integral in (3.53), since this is the only Wiener integral which the path integral can possibly be equal to by virtue of consistency with the Feynman-Kac formula.

Aside from these significant problems, it would be worthwhile to look into the closed form of the general n-dimensional path integral with quadratic potential and of the anisotropic path integral. It is desirable to simplify these expressions, if possible. In particular, we would like to obtain expressions in which the starting and end point are not included component-wise as in result 3.2 and 4.2, but rather as complete vectors through some sort of vector/matrix-vector multiplication as in the closed forms the n-dimensional free path integral and the anisotropic free path integral, i.e. result 3.3 and 4.1. It may be sensible to start with the relatively simple case where Ω is positive-definite, viz. (3.43), so that all 1-dimensional path integrals in the product are of the same form.

Appendix A

Computation of the free path integral

Consider the right hand side of equation (2.31),

$$\frac{1}{2\pi}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}}\int\limits_{\mathbb{R}}\int\limits_{\mathbb{R}^{N+1}}\exp\left[-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}+i\xi\left(\sum_{j=0}^{N}y_{j+1}-(b-a)\right)\right]dyd\xi\ . \tag{A.1}$$

Let us write

$$\begin{aligned}&\frac{1}{2\pi}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}}\int\limits_{\mathbb{R}}\int\limits_{\mathbb{R}^{N+1}}\exp\left[-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}+i\xi\left(\sum_{j=0}^{N}y_{j+1}-(b-a)\right)\right]dyd\xi\\&=\frac{1}{2\pi}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}}\int\limits_{\mathbb{R}}\exp\left(-i\xi(b-a)\right)\int\limits_{\mathbb{R}^{N+1}}\exp\left(-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}+i\xi\sum_{j=0}^{N}y_{j+1}\right)dyd\xi\ ,\end{aligned}\tag{A.2}$$

and focus on the innermost integral

$$\int\limits_{\mathbb{R}^{N+1}}\exp\left(-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}+i\xi\sum_{j=0}^{N}y_{j+1}\right)dy\ . \tag{A.3}$$

We may rewrite this as a product of 1-dimensional integrals and apply a change of variables to obtain

$$\begin{aligned}&\int\limits_{\mathbb{R}^{N+1}}\exp\left(-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}+i\xi\sum_{j=0}^{N}y_{j+1}\right)dy=\prod_{j=0}^{N}\int\limits_{\mathbb{R}}\exp\left(-\frac{y_{j+1}^2}{2\varepsilon}+i\xi y_{j+1}\right)dy_{j+1}\\&=\left(\int\limits_{\mathbb{R}}\exp\left(-\frac{y^2}{2\varepsilon}+i\xi y\right)dy\right)^{N+1}=\sqrt{2\varepsilon}^{N+1}\left(\int\limits_{\mathbb{R}}\exp\left(-u^2+\sqrt{2\varepsilon}i\xi u\right)du\right)^{N+1}\ .\end{aligned}\tag{A.4}$$

We rewrite the exponent in the latter integral as

$$-u^2+\sqrt{2\varepsilon}i\xi u=-\left(u-\sqrt{\frac{\varepsilon}{2}}i\xi\right)^2-\frac{\varepsilon\xi^2}{2}\ , \tag{A.5}$$

so that

$$\begin{aligned}
&\int_{\mathbb{R}^{N+1}} \exp\left(-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}+i\xi\sum_{j=0}^{N}y_{j+1}\right)dy \\
&=\sqrt{2\varepsilon}^{N+1}\exp\left(-\frac{\varepsilon(N+1)\xi^2}{2}\right)\left(\int_{\mathbb{R}}\exp\left[-\left(u-\sqrt{\frac{\varepsilon}{2}}i\xi\right)^2\right]du\right)^{N+1} .
\end{aligned} \tag{A.6}$$

We can now use a result from complex analysis which follows from the Cauchy integral theorem (see [39] for details about this theorem).

Lemma A.1.

$$\int_{\mathbb{R}} \exp\left(-(\omega+i\eta)^2\right)d\omega=\sqrt{\pi}$$

for all $\eta\in\mathbb{R}$.

Proof. Without loss of generality, we assume that $\eta>0$. Define for $R\in\mathbb{R}_+$ the parametrized curves in the complex plane $\gamma_{1,R}$, $\gamma_{2,R}$, $\gamma_{3,R}$ and $\gamma_{4,R}$ by

$$\gamma_{1,R}:\ [-R,R]\to\mathbb{C}:\ t\mapsto -t \tag{A.7}$$
$$\gamma_{2,R}:\ [0,\eta]\to\mathbb{C}:\ t\mapsto -R+it \tag{A.8}$$
$$\gamma_{3,R}:\ [-R,R]\to\mathbb{C}:\ t\mapsto t+i\eta \tag{A.9}$$
$$\gamma_{4,R}:\ [-\eta,0]\to\mathbb{C}:\ t\mapsto R-it\ . \tag{A.10}$$

(For $\eta<0$, we would need slightly different curves.) Define $\gamma_R:=\gamma_{1,R}\cup\gamma_{2,R}\cup\gamma_{3,R}\cup\gamma_{4,R}$. Observe that γ_R is for every R a Jordan curve. Moreover, $f(z):=\exp\left(-z^2\right)$ is holomorphic, so that we have

$$\int_{\gamma_R}\exp\left(-z^2\right)dz=0 \tag{A.11}$$

by Cauchy's theorem. This implies

$$\int_{\gamma_{3,R}}\exp\left(-z^2\right)dz=-\int_{\gamma_{1,R}}\exp\left(-z^2\right)dz-\int_{\gamma_{2,R}}\exp\left(-z^2\right)dz-\int_{\gamma_{4,R}}\exp\left(-z^2\right)dz\ . \tag{A.12}$$

Let us now study the separate integrals, in particular their behaviour as $R\to\infty$. Note that in the limit, the integral over $\gamma_{3,R}$ becomes the integral that we are interested in:

$$\int_{\gamma_{3,R}}\exp\left(-z^2\right)dz=\int_{-R}^{R}\exp\left(-(t+i\eta)^2\right)dt=\int_{-R}^{R}\exp\left(-(\omega+i\eta)^2\right)d\omega\overset{R\to\infty}{\longrightarrow}\int_{\mathbb{R}}\exp\left(-(\omega+i\eta)^2\right)d\omega\ . \tag{A.13}$$

The integral over $\gamma_{1,R}$ converges to a standard Gaussian integral:

$$\int_{\gamma_{1,R}}\exp\left(-z^2\right)dz=-\int_{-R}^{R}\exp\left(-t^2\right)dt\overset{R\to\infty}{\longrightarrow}-\int_{\mathbb{R}}\exp\left(-t^2\right)dt=-\sqrt{\pi}\ . \tag{A.14}$$

The integral over $\gamma_{2,R}$ vanishes in the limit, since

$$\int_{\gamma_{2,R}} \exp\left(-z^2\right) dz = i\int_0^\eta \exp\left(-\left(-R+it\right)^2\right) dt \tag{A.15}$$

and hence

$$\begin{aligned} &\left|\int_{\gamma_{2,R}} \exp\left(-z^2\right) dz\right| = \left|\int_0^\eta \exp\left(-\left(-R+it\right)^2\right) dt\right| \leq \int_0^\eta \left|\exp\left(-\left(-R+it\right)^2\right)\right| dt \\ &= \int_0^\eta \left|\exp\left(-R^2+t^2\right)\exp\left(2Rti\right)\right| dt = \int_0^\eta \exp\left(-R^2+t^2\right) dt \leq \int_0^\eta \exp\left(-R^2+\eta^2\right) dt \\ &= \eta \exp\left(-R^2+\eta^2\right) \overset{R\to\infty}{\longrightarrow} 0 \ . \end{aligned} \tag{A.16}$$

Analogously, one can show that the integral over $\gamma_{4,R}$ vanishes in the limit. Finally, we may pass to the limit $R \to \infty$ in (A.12) to obtain

$$\int_{\mathbb{R}} \exp\left(-\left(\omega+i\eta\right)^2\right) d\omega = \sqrt{\pi} \ . \tag{A.17}$$

□

Lemma A.1 together with (A.6) gives

$$\int_{\mathbb{R}^{N+1}} \exp\left(-\sum_{j=0}^{N} \frac{y_{j+1}^2}{2\varepsilon} + i\xi \sum_{j=0}^{N} y_{j+1}\right) dy = \sqrt{2\pi\varepsilon}^{N+1} \exp\left(-\frac{\varepsilon(N+1)\xi^2}{2}\right) \ . \tag{A.18}$$

Plugging in this result into (A.2), we find

$$\begin{aligned} &\frac{1}{2\pi}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \int_{\mathbb{R}}\int_{\mathbb{R}^{N+1}} \exp\left[-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon} + i\xi\left(\sum_{j=0}^{N} y_{j+1} - (b-a)\right)\right] dyd\xi \\ &= \frac{1}{2\pi}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}} \sqrt{2\pi\varepsilon}^{N+1} \int_{\mathbb{R}} \exp\left(-i\xi(b-a)\right) \exp\left(-\frac{\varepsilon(N+1)\xi^2}{2}\right) d\xi \\ &= \frac{1}{2\pi}\int_{\mathbb{R}} \exp\left(-\frac{\varepsilon(N+1)\xi^2}{2} - i\xi(b-a)\right) d\xi \ . \end{aligned} \tag{A.19}$$

We rewrite the exponent of the latter integral as

$$-\frac{\varepsilon(N+1)\xi^2}{2} - i\xi(b-a) = -\left(\sqrt{\frac{\varepsilon(N+1)}{2}}\xi + \frac{i(b-a)}{2}\sqrt{\frac{2}{\varepsilon(N+1)}}\right)^2 - \frac{(b-a)^2}{2\varepsilon(N+1)} \ , \tag{A.20}$$

which gives

$$\begin{aligned}&\frac{1}{2\pi}\int_{\mathbb{R}}\exp\left(-\frac{\varepsilon(N+1)\xi^2}{2}-i\xi(b-a)\right)d\xi\\&=\frac{1}{2\pi}\exp\left(-\frac{(b-a)^2}{2\varepsilon(N+1)}\right)\int_{\mathbb{R}}\exp\left[-\left(\sqrt{\frac{\varepsilon(N+1)}{2}}\xi+\frac{i(b-a)}{2}\sqrt{\frac{2}{\varepsilon(N+1)}}\right)^2\right]d\xi\ .\end{aligned}\tag{A.21}$$

After a change of variable, applying lemma (A.1) again and using that $\varepsilon(N+1)=t_b-t_a$, we obtain

$$\begin{aligned}&\frac{1}{2\pi}\int_{\mathbb{R}}\exp\left(-\frac{\varepsilon(N+1)\xi^2}{2}-i\xi(b-a)\right)d\xi\\&=\frac{1}{2\pi}\sqrt{\frac{2}{\varepsilon(N+1)}}\exp\left(-\frac{(b-a)^2}{2\varepsilon(N+1)}\right)\int_{\mathbb{R}}\exp\left[-\left(\xi+\frac{i(b-a)}{2}\sqrt{\frac{2}{\varepsilon(N+1)}}\right)^2\right]d\xi\\&=\frac{1}{2\pi}\sqrt{\frac{2}{\varepsilon(N+1)}}\exp\left(-\frac{(b-a)^2}{2\varepsilon(N+1)}\right)\sqrt{\pi}\\&=\frac{1}{\sqrt{2\pi(t_b-t_a)}}\exp\left(-\frac{(b-a)^2}{2(t_b-t_a)}\right)\ .\end{aligned}\tag{A.22}$$

Plugging this into (A.19) yields

$$\begin{aligned}&\frac{1}{2\pi}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N+1}{2}}\int_{\mathbb{R}}\int_{\mathbb{R}^{N+1}}\exp\left[-\sum_{j=0}^{N}\frac{y_{j+1}^2}{2\varepsilon}+i\xi\left(\sum_{j=0}^{N}y_{j+1}-(b-a)\right)\right]dyd\xi\\&=\frac{1}{\sqrt{2\pi(t_b-t_a)}}\exp\left(-\frac{(b-a)^2}{2(t_b-t_a)}\right)\ .\end{aligned}\tag{A.23}$$

Appendix B

Computation of the action integral for the classical path

In this appendix, we will compute

$$\int_{t_a}^{t_b} \frac{\dot{\gamma}_{\mathrm{cl}}(t)^2 + \omega^2 \gamma_{\mathrm{cl}}(t)^2}{2} dt \; , \tag{B.1}$$

with

$$\gamma_{\mathrm{cl}}(t) = A \sinh(\omega t + \phi) \; , \tag{B.2}$$

where $A, \phi \in \mathbb{R}$ are chosen such that $\gamma_{\mathrm{cl}}(t_a) = a, \gamma_{\mathrm{cl}}(t_b) = b$. Throughout our computations, we shall implicitly make use of the following identities for the hyperbolic sine and cosine:

$$\begin{aligned}
&\cosh^2(x) + \sinh^2(x) = \cosh(2x) \; , \\
&\cosh^2(x) - \sinh^2(x) = 1 \; , \\
&\sinh(2x) = 2\sinh(x)\cosh(x) \; , \\
&\sinh(x \pm y) = \sinh(x)\cosh(y) \pm \cosh(x)\sinh(y) \; , \\
&\cosh(x \pm y) = \cosh(x)\cosh(y) \pm \sinh(x)\sinh(y) \; , \\
&\sinh(-x) = -\sinh(x) \; .
\end{aligned} \tag{B.3}$$

Using the fact that

$$\frac{d}{dx}\sinh(x) = \cosh(x) \; , \tag{B.4}$$

it is straightforward to evaluate (B.1). We find

$$\begin{aligned}
&\int_{t_a}^{t_b} \frac{\dot{\gamma}_{\mathrm{cl}}(t)^2 + \omega^2 \gamma_{\mathrm{cl}}(t)^2}{2} dt = \int_{t_a}^{t_b} \frac{(\omega A \cosh(\omega t + \phi))^2 + \omega^2 (A \sinh(\omega t + \phi))^2}{2} dt \\
&= \frac{\omega^2 A^2}{2} \int_{t_a}^{t_b} \cosh^2(\omega t + \phi) + \sinh^2(\omega t + \phi) dt = \frac{\omega^2 A^2}{2} \int_{t_a}^{t_b} \cosh(2\omega t + 2\phi) dt \\
&= \frac{\omega^2 A^2}{2} \left[\frac{1}{2\omega} \sinh(2\omega t + 2\phi) \right]_{t_a}^{t_b} = \frac{\omega A^2}{4} \left[\sinh(2\omega t_b + 2\phi) - \sinh(2\omega t_a + 2\phi) \right] \; .
\end{aligned} \tag{B.5}$$

The difficulty is to write the result explicitly, that is, to write it solely in terms of t_a, t_b, a, b and ω. To this end, we shall not derive closed expressions for A and ϕ, but rather derive expressions for the terms $A^2 \sinh(2\omega t_b + 2\phi)$ and $A^2 \sinh(2\omega t_a + 2\phi)$ at once, following the approach in [14].

Recall the boundary conditions:

$$a = \gamma_{\text{cl}}(t_a) = A \sinh(\omega t_a + \phi) = A \left[\sinh(\omega t_a)\cosh(\phi) + \cosh(\omega t_a)\sinh(\phi)\right] \ , \tag{B.6}$$

$$b = \gamma_{\text{cl}}(t_b) = A \sinh(\omega t_b + \phi) = A \left[\sinh(\omega t_b)\cosh(\phi) + \cosh(\omega t_b)\sinh(\phi)\right] \ . \tag{B.7}$$

With these, we find

$$\begin{aligned} &b\cosh(\omega t_a) - a\cosh(\omega t_b) = A\left[\sinh(\omega t_b)\cosh(\phi)\cosh(\omega t_a) + \cosh(\omega t_b)\sinh(\phi)\cosh(\omega t_a)\right. \\ &\left. - \sinh(\omega t_a)\cosh(\phi)\cosh(\omega t_b) - \cosh(\omega t_a)\sinh(\phi)\cosh(\omega t_b)\right] \\ &= A\cosh(\phi)\left[\sinh(\omega t_b)\cosh(\omega t_a) - \sinh(\omega t_a)\cosh(\omega t_b)\right] = A\cosh(\phi)\sinh(\omega(t_b - t_a)) \end{aligned} \tag{B.8}$$

$$\iff A\cosh(\phi) = \frac{b\cosh(\omega t_a) - a\cosh(\omega t_b)}{\sinh(\omega(t_b - t_a))} \tag{B.9}$$

and

$$\begin{aligned} &b\sinh(\omega t_a) - a\sinh(\omega t_b) = A\left[\sinh(\omega t_b)\cosh(\phi)\sinh(\omega t_a) + \cosh(\omega t_b)\sinh(\phi)\sinh(\omega t_a)\right. \\ &\left. - \sinh(\omega t_a)\cosh(\phi)\sinh(\omega t_b) - \cosh(\omega t_a)\sinh(\phi)\sinh(\omega t_b)\right] \\ &= A\sinh(\phi)\left[\cosh(\omega t_b)\sinh(\omega t_a) - \cosh(\omega t_a)\sinh(\omega t_b)\right] = A\sinh(\phi)\sinh(\omega(t_a - t_b)) \end{aligned} \tag{B.10}$$

$$\iff A\sinh(\phi) = \frac{b\sinh(\omega t_a) - a\sinh(\omega t_b)}{\sinh(\omega(t_a - t_b))} = \frac{a\sinh(\omega t_b) - b\sinh(\omega t_a)}{\sinh(\omega(t_b - t_a))} \ . \tag{B.11}$$

We can now compute the terms $A^2 \sinh(2\omega t_b + 2\phi)$ and $A^2 \sinh(2\omega t_a + 2\phi)$ in closed form. For the first term, we find

$$\begin{aligned} &A^2\sinh(2\omega t_b + 2\phi) \\ &= 2A^2\sinh(\omega t_b + \phi)\cosh(\omega t_b + \phi) \overset{(B.7)}{=} 2Ab\cosh(\omega t_b + \phi) \\ &= 2Ab\left[\cosh(\omega t_b)\cosh(\phi) + \sinh(\omega t_b)\sinh(\phi)\right] \\ &\overset{(B.9),(B.11)}{=} 2b\cosh(\omega t_b)\cdot\frac{b\cosh(\omega t_a) - a\cosh(\omega t_b)}{\sinh(\omega(t_b - t_a))} \\ &+ 2b\sinh(\omega t_b)\cdot\frac{a\sinh(\omega t_b) - b\sinh(\omega t_a)}{\sinh(\omega(t_b - t_a))} \\ &= \frac{2b^2\left[\cosh(\omega t_b)\cosh(\omega t_a) - \sinh(\omega t_b)\sinh(\omega t_a)\right] - 2ab\left[\cosh^2(\omega t_b) - \sinh^2(\omega t_b)\right]}{\sinh(\omega(t_b - t_a))} \\ &= \frac{2b^2\cosh(\omega(t_b - t_a)) - 2ab}{\sinh(\omega(t_b - t_a))} \ . \end{aligned} \tag{B.12}$$

Likewise, we find for the second term

$$\begin{aligned} &A^2\sinh(2\omega t_a + 2\phi) \\ &= 2A^2\sinh(\omega t_a + \phi)\cosh(\omega t_a + \phi) \overset{(B.6)}{=} 2Aa\cosh(\omega t_a + \phi) \\ &= 2Aa\left[\cosh(\omega t_a)\cosh(\phi) + \sinh(\omega t_a)\sinh(\phi)\right] \end{aligned}$$

$$\overset{(B.9),(B.11)}{=} 2a\cosh(\omega t_a)\cdot\frac{b\cosh(\omega t_a)-a\cosh(\omega t_b)}{\sinh(\omega(t_b-t_a))}$$
$$+\,2a\sinh(\omega t_a)\cdot\frac{a\sinh(\omega t_b)-b\sinh(\omega t_a)}{\sinh(\omega(t_b-t_a))}$$
$$=\frac{-2a^2\left[\cosh(\omega t_a)\cosh(\omega t_b)-\sinh(\omega t_a)\sinh(\omega t_b)\right]+2ab\left[\cosh^2(\omega t_a)-\sinh^2(\omega t_a)\right]}{\sinh(\omega(t_b-t_a))}$$
$$=\frac{-2a^2\cosh(\omega(t_b-t_a))+2ab}{\sinh(\omega(t_b-t_a))}\ . \tag{B.13}$$

Combining (B.12) and (B.13) with (B.5), we obtain

$$\int_{t_a}^{t_b}\frac{\dot{\gamma}_{\mathrm{cl}}(t)^2+\omega^2\gamma_{\mathrm{cl}}(t)^2}{2}dt=\frac{\omega A^2}{4}\left[\sinh(2\omega t_b+2\phi)-\sinh(2\omega t_a+2\phi)\right]=\frac{\omega}{4}\frac{2b^2\cosh(\omega(t_b-t_a))-2ab}{\sinh(\omega(t_b-t_a))}$$
$$+\,\frac{\omega}{4}\frac{2a^2\cosh(\omega(t_b-t_a))-2ab}{\sinh(\omega(t_b-t_a))}=\frac{\omega}{2}\frac{(a^2+b^2)\cosh(\omega(t_b-t_a))-2ab}{\sinh(\omega(t_b-t_a))}\ . \tag{B.14}$$

Appendix C

Computation of the limit (3.24)

In this appendix we will show that

$$\lim_{N\to\infty} \frac{\det A_N}{N+1} = \frac{\sinh(\omega(t_b - t_a))}{\omega(t_b - t_a)} \ , \tag{C.1}$$

where A_N is given by (3.19). We will follow the proof sketched in [14]. Throughout all computations, we will implicitly use the identities (B.3). Define for $c \in \mathbb{R}$ the symmetric tridiagonal $N \times N$ matrix $M_N(c)$ by

$$M_N(c) := \begin{pmatrix} 2c & -1 & & & \\ -1 & 2c & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2c & -1 \\ & & & -1 & 2c \end{pmatrix} . \tag{C.2}$$

For this matrix, we have the following lemma.

Lemma C.1. *Let $c > 1$ and $u \in \mathbb{R}$ such that $c = \cosh(u)$. Then*

$$\det M_N(c) = \frac{\sinh((N+1)u)}{\sinh(u)} \ .$$

Proof. We proceed by induction. Observe that

$$\begin{aligned}
&\det M_1(c) = 2c = 2\cosh(u) = \frac{2\sinh(u)\cosh(u)}{\sinh(u)} = \frac{\sinh(2u)}{\sinh(u)} \ , \\
&\det M_2(c) = \det \begin{pmatrix} 2c & -1 \\ -1 & 2c \end{pmatrix} = 4c^2 - 1 = 4\cosh^2(u) - 1 = 3 - 4\left(1 - \cosh^2(u)\right) \\
&= 3 + 4\sinh^2(u) = \frac{4\sinh^3(u) + 3\sinh(u)}{\sinh(u)} \ .
\end{aligned}$$

Moreover, we have

$$\begin{aligned}
&\sinh(3u) = \sinh(2u)\cosh(u) + \cosh(2u)\sinh(u) = 2\sinh(u)\cosh^2(u) + \left(2\cosh^2(u) - 1\right)\sinh(u) \\
&= 4\sinh(u)\cosh^2(u) - \sinh(u) = 4\sinh(u)\left(1 + \sinh^2(u)\right) - \sinh(u) = 4\sinh^3(u) + 3\sinh(u) \ ,
\end{aligned}$$

hence

$$\det M_2(c) = \frac{\sinh(3u)}{\sinh(u)} \ .$$

Observe that we have the following recursive relation:

$$\det M_{N+1}(c) = 2c \det M_N(c) - \det M_{N-1}(c) \ . \tag{C.3}$$

This can be seen as follows. By expanding the determinant of $M_{N+1}(c)$ along the first row, we get

$$\det M_{N+1}(c) = 2c \det M_N(c) + \det B \ ,$$

where B is the $N \times N$ matrix which has $(-1, 0, \ldots, 0)^T$ as its first column, and as its other $N-1$ columns the rightmost $N-1$ columns of M_{N+1} starting from the second row. Expanding the determinant of B along its first column, we then get

$$\det B = -\det C \ ,$$

where C is the lower rightmost $(N-1) \times (N-1)$ block of B. But then, by our characterization of the $N-1$ rightmost columns of B, the columns of C are precisely the rightmost $N-1$ columns of M_{N+1} starting from its third row. This implies that C is the lower rightmost $(N-1) \times (N-1)$ block of M_{N+1}, hence $C = M_{N-1}(c)$, which gives the recursive relation.

Using the above observations, we shall give the induction proof. Clearly, the statement holds for $n = 1$ and $n = 2$. Assume now that the statement holds up to some $k \geq 2$, which is to say that it holds for $n = 1, 2, \ldots, k$. We can then use the recursion to obtain

$$\det M_{k+1}(c) = 2c \det M_k(c) - \det M_{k-1}(c) = 2c \cdot \frac{\sinh((k+1)u)}{\sinh(u)} - \frac{\sinh(ku)}{\sinh(u)}$$
$$= \frac{2\cosh(u)\sinh((k+1)u) - \sinh(ku)}{\sinh(u)} \ .$$

We have

$$\begin{aligned} \sinh((k+2)u) &= \sinh((k+1)u)\cosh(u) + \cosh((k+1)u)\sinh(u) \ , \\ \sinh(ku) &= \sinh((k+1)u)\cosh(u) - \cosh((k+1)u)\sinh(u) \ . \end{aligned}$$

Summing the left- and right-hand sides gives

$$\begin{aligned} &\sinh((k+2)u) + \sinh(ku) = 2\sinh((k+1)u)\cosh(u) \\ \iff\ &2\sinh((k+1)u)\cosh(u) - \sinh(ku) = \sinh((k+2)u) \ . \end{aligned}$$

Consequently,

$$\det M_{k+1}(c) = \frac{\sinh((k+2)u)}{\sinh(u)} \ ,$$

which completes the induction step. □

Using this lemma, the computation of the limit for the determinant of A_N is straightforward. Noting that we have $A_N = M_N(1 + \varepsilon^2\omega^2/2)$, we get

$$\frac{\det A_N}{N+1} = \frac{\sinh((N+1)u)}{(N+1)\sinh(u)} \tag{C.4}$$

with $\cosh(u) = 1 + \varepsilon^2\omega^2/2$, according to the lemma. We have, using $\varepsilon = (t_b - t_a)/(N+1)$, that

$$\begin{aligned} &\sinh^2(u) = \cosh^2(u) - 1 = \left(1 + \frac{\varepsilon^2\omega^2}{2}\right)^2 - 1 = \varepsilon^2\omega^2 + \frac{\varepsilon^4\omega^4}{4} \\ &\Longrightarrow\ (N+1)^2\sinh^2(u) = (t_b - t_a)^2\omega^2 + \varepsilon^2 \cdot \frac{(t_b - t_a)^2\omega^4}{4} \overset{(N\to\infty)}{\longrightarrow} (t_b - t_a)^2\omega^2 \\ &\Longrightarrow\ (N+1)\sinh(u) \overset{(N\to\infty)}{\longrightarrow} \omega(t_b - t_a)\ . \end{aligned} \tag{C.5}$$

Observe that $u = \operatorname{arcosh}\left(1 + \frac{\varepsilon^2\omega^2}{2}\right) > 0$, and moreover

$$u = \operatorname{arcosh}\left(1 + \frac{\varepsilon^2\omega^2}{2}\right) \overset{(N\to\infty)}{\longrightarrow} \operatorname{arcosh}(1) = 0 \implies \frac{\sinh(u)}{u} \overset{(N\to\infty)}{\longrightarrow} 1 \tag{C.6}$$

because of the standard limit $\lim_{x\to 0}\sinh(x)/x = 1$. In particular,

$$\frac{\sinh(u)}{u} > 0 \qquad (N \geq N^*) \tag{C.7}$$

for some $N^* \in \mathbb{N}_+$. Since $u > 0$, this implies $\sinh(u) > 0$ for $N \geq N^*$. We can therefore write

$$(N+1)u = (N+1)\sinh(u) \cdot \frac{u}{\sinh(u)} \qquad (N \geq N^*)\ , \tag{C.8}$$

and consequently, together with (C.5) and (C.6),

$$(N+1)u \overset{(N\to\infty)}{\longrightarrow} \omega(t_b - t_a)\ . \tag{C.9}$$

Combining (C.5) and (C.9) with (C.4), we conclude

$$\frac{\det A_N}{N+1} = \frac{\sinh((N+1)u)}{(N+1)\sinh(u)} \overset{(N\to\infty)}{\longrightarrow} \frac{\sinh(\omega(t_b - t_a))}{\omega(t_b - t_a)}\ . \tag{C.10}$$

Appendix D

Verification of the PDE (3.61)

Recall result 3.1:

$$K_\omega(a,b;t_a,t_b)=\sqrt{\frac{\omega}{2\pi\sin(\omega(t_b-t_a))}}\exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cos(\omega(t_b-t_a))-2ab}{\sin(\omega(t_b-t_a))}\right) \tag{D.1}$$

for $\omega(t_b-t_a)\in(0,\pi)$. We will now show that K_ω satisfies the PDE (3.59), that is,

$$\frac{\partial K_\omega(a,q;t_a,t)}{\partial t}=\frac{1}{2}\frac{\partial^2 K_\omega(a,q;t_a,t)}{\partial q^2}+\frac{\omega^2q^2}{2}K_\omega(a,q;t_a,t) \tag{D.2}$$

for $\omega(t-t_a)\in(0,\pi)$. We start by computing the time derivative. We have

$$\begin{aligned}\frac{\partial}{\partial t}\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}&=\frac{1}{2}\sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega}}\cdot\frac{\partial}{\partial t}\frac{\omega}{2\pi\sin(\omega(t-t_a))}\\&=-\frac{\omega^2}{2}\sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega}}\frac{\cos(\omega(t-t_a))}{2\pi\sin^2(\omega(t-t_a))}\ ,\end{aligned} \tag{D.3}$$

and

$$\begin{aligned}&\frac{\partial}{\partial t}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\&=\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\cdot\frac{\partial}{\partial t}\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\&=-\frac{\omega}{2}\frac{\sin(\omega(t-t_a))\cdot-\omega(a^2+q^2)\sin(\omega(t-t_a))-\left[(a^2+q^2)\cos(\omega(t-t_a))-2aq\right]\cdot\omega\cos(\omega(t-t_a))}{\sin^2(\omega(t-t_a))}\\&\cdot\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\&=\frac{\omega^2(a^2+q^2)\sin^2(\omega(t-t_a))+\omega^2(a^2+q^2)\cos^2(\omega(t-t_a))-2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))}\\&\cdot\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\&=\frac{\omega^2(a^2+q^2)-2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\ .\end{aligned} \tag{D.4}$$

Hence,

$$
\begin{aligned}
\frac{\partial K_\omega(a,q;t_a,t)}{\partial t} &= \frac{\partial}{\partial t}\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\cdot\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\
&+\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\cdot\frac{\partial}{\partial t}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\
&=-\frac{\omega^2}{2}\sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega}}\frac{\cos(\omega(t-t_a))}{2\pi\sin^2(\omega(t-t_a))}\cdot\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\
&+\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\cdot\frac{\omega^2(a^2+q^2)-2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\
&=\left[-\frac{\omega^2\cos(\omega(t-t_a))}{4\pi\sin^2(\omega(t-t_a))}\sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega}}+\frac{\omega^2(a^2+q^2)-2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))}\right.\\
&\left.\cdot\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\right]\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\,.
\end{aligned}
\tag{D.5}
$$

Next, we compute the second spatial derivative. We have

$$
\begin{aligned}
\frac{\partial K_\omega(a,q;t_a,t)}{\partial q} &= \sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\cdot\frac{\partial}{\partial q}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\
&=\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\
&\cdot\frac{\partial}{\partial q}\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\\
&=-\frac{\omega}{2}\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\cdot\frac{2q\cos(\omega(t-t_a))-2a}{\sin(\omega(t-t_a))}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\,,
\end{aligned}
\tag{D.6}
$$

and thus

$$
\begin{aligned}
\frac{\partial^2 K_\omega(a,q;t_a,t)}{\partial q^2} &= -\frac{\omega}{2}\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\left[\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\right.\\
&\left.\cdot\frac{\partial}{\partial q}\frac{2q\cos(\omega(t-t_a))-2a}{\sin(\omega(t-t_a))}+\frac{2q\cos(\omega(t-t_a))-2a}{\sin(\omega(t-t_a))}\cdot\frac{\partial}{\partial q}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\right]\\
&=-\frac{\omega}{2}\left[\frac{2\cos(\omega(t-t_a))}{\sin(\omega(t-t_a))}+\frac{2q\cos(\omega(t-t_a))-2a}{\sin(\omega(t-t_a))}\cdot\frac{\partial}{\partial q}\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)\right]\\
&\cdot\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)
\end{aligned}
$$

$$= -\frac{\omega}{2}\left[\frac{2\cos(\omega(t-t_a))}{\sin(\omega(t-t_a))} - \frac{2q\cos(\omega(t-t_a)) - 2a}{\sin(\omega(t-t_a))} \cdot \frac{q\omega\cos(\omega(t-t_a)) - a\omega}{\sin(\omega(t-t_a))}\right]$$
$$\cdot \sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}} \exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right)$$
$$= \left[-\frac{\omega\cos(\omega(t-t_a))}{\sin(\omega(t-t_a))} + \frac{q^2\omega^2\cos^2(\omega(t-t_a)) + a^2\omega^2 - 2aq\omega^2\cos(\omega(t-t_a))}{\sin^2(\omega(t-t_a))}\right]$$
$$\cdot \sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}} \exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right) . \tag{D.7}$$

Combining (D.5) and (D.7), we find

$$\frac{1}{2}\frac{\partial^2 K_\omega(a,q;t_a,t)}{\partial q^2} + \frac{\omega^2 q^2}{2} K_\omega(a,q;t_a,t)$$
$$= \left[-\frac{\omega\cos(\omega(t-t_a))}{2\sin(\omega(t-t_a))} + \frac{q^2\omega^2\cos^2(\omega(t-t_a)) + a^2\omega^2 - 2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))} + \frac{\omega^2 q^2}{2}\right]$$
$$\cdot \sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}} \exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right)$$
$$= \left[-\frac{\omega\cos(\omega(t-t_a))}{2\sin(\omega(t-t_a))} + \frac{q^2\omega^2\cos^2(\omega(t-t_a)) + q^2\omega^2\sin^2(\omega(t-t_a)) + a^2\omega^2 - 2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))}\right]$$
$$\cdot \sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}} \exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right)$$
$$= \left[-\frac{\omega\cos(\omega(t-t_a))}{2\sin(\omega(t-t_a))}\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}} + \frac{\omega^2(a^2+q^2) - 2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))}\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\right]$$
$$\cdot \exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right)$$
$$= \left[-\frac{\omega\cos(\omega(t-t_a))}{2\sin(\omega(t-t_a))}\sqrt{\frac{\omega^2}{4\pi^2\sin^2(\omega(t-t_a))}}\sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega}} + \frac{\omega^2(a^2+q^2) - 2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))}\right.$$
$$\left.\cdot\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\right] \cdot \exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right)$$
$$= \left[-\frac{\omega^2\cos(\omega(t-t_a))}{4\pi\sin^2(\omega(t-t_a))}\sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega}} + \frac{\omega^2(a^2+q^2) - 2aq\omega^2\cos(\omega(t-t_a))}{2\sin^2(\omega(t-t_a))}\right.$$
$$\left.\cdot\sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\right] \cdot \exp\left(-\frac{\omega}{2}\frac{(a^2+q^2)\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right) = \frac{\partial K_\omega(a,q;t_a,t)}{\partial t} . \tag{D.8}$$

Appendix E

Computation of the integral limit (3.71)

Recall result 3.1:

$$K_\omega(a,b;t_a,t_b) = \sqrt{\frac{\omega}{2\pi\sin(\omega(t_b-t_a))}}\exp\left(-\frac{\omega}{2}\frac{(a^2+b^2)\cos(\omega(t_b-t_a))-2ab}{\sin(\omega(t_b-t_a))}\right) \tag{E.1}$$

for $\omega(t_b-t_a)\in(0,\pi)$. We shall first compute a closed form of the integral

$$\begin{aligned}&\int_{\mathbb{R}} K_\omega(a,q;t_a,t)dq\\ &= \sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}}\exp\left(-\frac{\omega}{2}\frac{a^2\cos(\omega(t-t_a))}{\sin(\omega(t-t_a))}\right)\int_{\mathbb{R}}\exp\left(-\frac{\omega}{2}\frac{q^2\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)dq\ .\end{aligned} \tag{E.2}$$

For convenience, we assume that $t-t_a$ is sufficiently small to ensure that $\cos(\omega(t-t_a))>0$ (this is fine since we shall take the limit $t\downarrow t_a$ in the end anyways). The first step is to rewrite the numerator of the exponent in the integrand. We have

$$q^2\cos(\omega(t-t_a))-2aq = \left(\sqrt{\cos(\omega(t-t_a))}q-\frac{a}{\sqrt{\cos(\omega(t-t_a))}}\right)^2-\frac{a^2}{\cos(\omega(t-t_a))}\ , \tag{E.3}$$

hence

$$\begin{aligned}&\int_{\mathbb{R}}\exp\left(-\frac{\omega}{2}\frac{q^2\cos(\omega(t-t_a))-2aq}{\sin(\omega(t-t_a))}\right)dq\\ &=\int_{\mathbb{R}}\exp\left(-\frac{\omega}{2}\frac{\left(\sqrt{\cos(\omega(t-t_a))}q-\frac{a}{\sqrt{\cos(\omega(t-t_a))}}\right)^2-\frac{a^2}{\cos(\omega(t-t_a))}}{\sin(\omega(t-t_a))}\right)dq\end{aligned}$$

$$= \exp\left(\frac{\omega a^2}{2\sin(\omega(t-t_a))\cos(\omega(t-t_a))}\right)$$
$$\int_{\mathbb{R}} \exp\left(-\left[\sqrt{\frac{\omega}{2\sin(\omega(t-t_a))}}\left(\sqrt{\cos(\omega(t-t_a))}q - \frac{a}{\sqrt{\cos(\omega(t-t_a))}}\right)\right]^2\right) dq$$
$$= \exp\left(\frac{\omega a^2}{2\sin(\omega(t-t_a))\cos(\omega(t-t_a))}\right)$$
$$\int_{\mathbb{R}} \exp\left(-\left[\sqrt{\frac{\omega\cos(\omega(t-t_a))}{2\sin(\omega(t-t_a))}}q - a\sqrt{\frac{\omega}{2\sin(\omega(t-t_a))\cos(\omega(t-t_a))}}\right]^2\right) dq \,. \tag{E.4}$$

A change of variable

$$u = \sqrt{\frac{\omega\cos(\omega(t-t_a))}{2\sin(\omega(t-t_a))}}q \tag{E.5}$$

gives

$$\int_{\mathbb{R}} \exp\left(-\left[\sqrt{\frac{\omega\cos(\omega(t-t_a))}{2\sin(\omega(t-t_a))}}q - a\sqrt{\frac{\omega}{2\sin(\omega(t-t_a))\cos(\omega(t-t_a))}}\right]^2\right) dq$$
$$= \sqrt{\frac{2\sin(\omega(t-t_a))}{\omega\cos(\omega(t-t_a))}}\int_{\mathbb{R}} \exp\left(-\left[u - a\sqrt{\frac{\omega}{2\sin(\omega(t-t_a))\cos(\omega(t-t_a))}}\right]^2\right) du \tag{E.6}$$
$$\overset{(2.10)}{=} \sqrt{\frac{2\sin(\omega(t-t_a))}{\omega\cos(\omega(t-t_a))}}\sqrt{\pi} = \sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega\cos(\omega(t-t_a))}} \,.$$

Plugging this into (E.4) gives

$$\int_{\mathbb{R}} \exp\left(-\frac{\omega}{2}\frac{q^2\cos(\omega(t-t_a)) - 2aq}{\sin(\omega(t-t_a))}\right) dq = \sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega\cos(\omega(t-t_a))}} \exp\left(\frac{\omega a^2}{2\sin(\omega(t-t_a))\cos(\omega(t-t_a))}\right) , \tag{E.7}$$

which together with (E.2) gives

$$\int_{\mathbb{R}} K_\omega(a,q;t_a,t) dq$$
$$= \sqrt{\frac{\omega}{2\pi\sin(\omega(t-t_a))}} \exp\left(-\frac{\omega}{2}\frac{a^2\cos(\omega(t-t_a))}{\sin(\omega(t-t_a))}\right)\sqrt{\frac{2\pi\sin(\omega(t-t_a))}{\omega\cos(\omega(t-t_a))}}$$
$$\exp\left(\frac{\omega a^2}{2\sin(\omega(t-t_a))\cos(\omega(t-t_a))}\right) = \frac{1}{\sqrt{\cos(\omega(t-t_a))}} \exp\left(\frac{\omega}{2}\frac{a^2\left[1-\cos^2(\omega(t-t_a))\right]}{\sin(\omega(t-t_a))\cos(\omega(t-t_a))}\right)$$
$$= \frac{1}{\sqrt{\cos(\omega(t-t_a))}} \exp\left(\frac{\omega}{2}\frac{a^2\sin^2(\omega(t-t_a))}{\sin(\omega(t-t_a))\cos(\omega(t-t_a))}\right)$$
$$= \frac{1}{\sqrt{\cos(\omega(t-t_a))}} \exp\left(\frac{\omega}{2}\frac{a^2\sin(\omega(t-t_a))}{\cos(\omega(t-t_a))}\right) \,. \tag{E.8}$$

Finally, taking the limit yields

$$\lim_{t \downarrow t_a} \int\limits_{\mathbb{R}} K_\omega(a,q;t_a,t)dq = \lim_{t \downarrow t_a} \frac{1}{\sqrt{\cos(\omega(t-t_a))}} \exp\left(\frac{\omega}{2}\frac{a^2\sin(\omega(t-t_a))}{\cos(\omega(t-t_a))}\right) = 1 \ . \tag{E.9}$$

Bibliography

[1] R. P. Feynman, "Space-Time Approach to Non-Relativistic Quantum Mechanics," *Rev. Mod. Phys.*, vol. 20, no. 2, pp. 367–387, Apr. 1948.

[2] L. M. Brown, Ed., *Feynman's thesis: A new approach to quantum theory.* Singapore: World Scientific, 2005.

[3] P. A. M. Dirac, "The Lagrangian in quantum mechanics," *Phys. Z. Sowjetunion*, vol. 3, no. 1, pp. 64–72, Nov. 1933.

[4] ——, "On the analogy between classical and quantum mechanics," *Rev. Mod. Phys.*, vol. 17, no. 2-3, pp. 195–199, Apr. 1945.

[5] S. Mazzucchi, "Introduction," in *Mathematical Feynman Path Integrals and their Applications*, Singapore: World Scientific, 2009, ch. 1, pp. 1–14.

[6] J. Glimm and A. Jaffe, "The Feynman-Kac Formula," in *Quantum Physics: A Functional Integral Point of View*, 2nd ed., New York, NY, USA: Springer, 1987, ch. 3, pp. 43–55.

[7] S. A. Albeverio, R. J. Høegh-Krohn, and S. Mazzucchi, *Mathematical Theory of Feynman Path Integrals: An Introduction*, 2nd ed. Berlin, Heidelberg, Germany: Springer, 2008.

[8] D. Fujiwara, *Rigorous Time Slicing Approach to Feynman Path Integrals.* Tokyo, Japan: Springer, 2017.

[9] S. Mazzucchi, "Alternative Approaches to Feynman Path Integration," in *Mathematical Feynman Path Integrals and their Applications*, Singapore: World Scientific, 2009, ch. 6, pp. 177–190.

[10] M. Kac, "Wiener and integration in function spaces," *Bull. Amer. Math. Soc.*, vol. 72, no. 1, pp. 52–68, Jan. 1966.

[11] ——, "On Distributions of Certain Wiener Functionals," *Trans. Amer. Math. Soc.*, vol. 65, no. 1, pp. 1–13, Jan. 1949.

[12] J. Dunkel, P. Talkner, and P. Hänggi, "Relativistic diffusion processes and random walk models," *Phys. Rev. D*, vol. 75, no. 4, p. 043 001, Feb. 2007.

[13] V. I. Arnol'd, *Mathematical Methods of Classical Mechanics*, 2nd ed., trans. by K. Vogtmann and A. Weinstein. New York, NY, USA: Springer, 1989.

[14] F. Williams, "Euclidean Path Integrals," in *Topics in Quantum Mechanics*, Boston, MA, USA: Birkhäuser, 2003, ch. 13, pp. 299–305.

[15] C. Grosche and F. Steiner, "General Theory," in *Handbook of Feynman Path Integrals*, Berlin, Heidelberg, Germany: Springer, 1998, ch. 2, pp. 23–36.

[16] D. L. Cohn, *Measure Theory*, 2nd ed. New York, NY, USA: Birkhäuser, 2013.

[17] L. S. Schulman, *Techniques and Applications of Path Integration.* New York, NY, USA: Wiley, 1981.

[18] S. D. Chatterji, "The mathematical work of N. Wiener," *Curr. Sci.*, vol. 67, no. 12, pp. 930–936, Dec. 1994.

[19] P. Masani, Ed., *Norbert Wiener: Collected Works, Volume 1.* Cambridge, MA, USA: MIT Press, 1976.

[20] Z. Schuss, "The Probability Space of Brownian Motion," in *Theory and Applications of Stochastic Processes: An Analytical Approach*, New York, NY, USA: Springer, 2010, ch. 2, pp. 25–62.

[21] R. F. Bass, *Stochastic Processes*. New York, NY, USA: Cambridge Univ. Press, 2011.

[22] D. Stirzaker, *Stochastic Processes and Models*. London, UK: Oxford Univ. Press, 2005.

[23] K. Itô and H. P. J. McKean, "The standard Brownian motion," in *Diffusion Processes and their Sample Paths*, Berlin, Heidelberg, Germany: Springer, 1996, ch. 1, pp. 12–19.

[24] H. Kleinert, "Velocity Path Integral," in *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 5th ed., Hackensack, NJ, USA: World Scientific, 2009, ch. 2, pp. 189–190.

[25] L. C. Evans, "Heat Equation," in *Partial Differential Equations*, 2nd ed., Providence, RI, USA: American Mathematical Society, 2010, ch. 2.3, pp. 44–46.

[26] R. M. Mazo, "Historical Background," in *Brownian Motion: Fluctuations, Dynamics, and Applications*, New York, NY, USA: Oxford Univ. Press, 2002, ch. 1, p. 2.

[27] R. Fürth, Ed., *Investigations on the theory of the Brownian movement*, trans. by A. Cowper. New York, NY, USA: Dover, 1956.

[28] I. Karatzas and S. E. Shreve, *Brownian Motion and Stochastic Calculus*, 2nd ed. New York, NY, USA: Springer, 1998.

[29] T. Hida, *Brownian Motion*, trans. by T. Hida and T. P. Speed. New York, NY, USA: Springer, 1980.

[30] S. K. Mitter, "On the Analogy between Mathematical Problems of Non-Linear Filtering and Quantum Physics," *Ric. Autom.*, vol. 10, no. 2, pp. 163–216, Dec. 1979.

[31] B. Simon, "The Feynman-Kac Formula," in *Functional Integration and Quantum Physics*, New York, NY, USA: Academic Press, 1979, ch. 6, pp. 48–60.

[32] D. Yoshioka, "The Partition Function and the Free Energy," in *Statistical Physics: An Introduction*, Berlin, Heidelberg, Germany: Springer, 2007, ch. 3, pp. 35–39.

[33] L. D. Landau and E. M. Lifshitz, "The Gibbs Distribution," in *Statistical Physics*, 3rd ed., vol. 1, Oxford, UK: Butterworth-Heinemann, 1980, ch. III, pp. 79–110.

[34] E. Kreyszig, *Introductory Functional Analysis with Applications*. New York, NY, USA: Wiley, 1989.

[35] G. Roepstorff, "The Feynman-Kac Formula," in *Path Integral Approach to Quantum Physics*, Berlin, Heidelberg, Germany: Springer, 1994, ch. 2, pp. 39–108.

[36] R. Strichartz, *A Guide to Distribution Theory and Fourier Transforms*. Boca Raton, FL, USA: CRC Press, 1994.

[37] W. Gander, M. J. Gander, and F. Kwok, "Eigenvalue Problems," in *Scientific Computing - An Introduction using Maple and MATLAB*, 1st ed., Cham, Switzerland: Springer, 2014, ch. 7, pp. 387–486.

[38] C. Grosche and F. Steiner, "Perturbation theory," in *Handbook of Feynman Path Integrals*, Berlin, Heidelberg, Germany: Springer, 1998, ch. 4, pp. 123–140.

[39] S. Lang, *Complex Analysis*, 4th ed. New York, NY, USA: Springer, 1999.