Derivation and Application of Quantum Hamilton Equations of Motion

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Zusammenfassung

Die grundlegende Struktur der (klassischen) analytischen Mechanik ist gleichermaßen in der Theorie der mikroskopischen Systeme anzutreffen. So stellen die Schrödingergleichung, die stochastischen kinematischen Gleichungen von Edward Nelson und das quantenmechanische Hamiltonische Prinzip, welches von Michele Pavon abgeleitet wurde, drei äquivalente Theorien dar, welche jeweils die Dynamik eines Quantenteilchens eindeutig beschreiben. Jedoch bestehen diverse Schwierigkeiten bei der praktischen Umsetzung der stochastischen Methoden, sei es beim Lösen der stochastischen Bewegungsgleichungen von Nelson oder bei der Auswertung des Variationsprinzips von Pavon. Es ergibt sich folglich die Notwendigkeit der Wellenfunktion zur weiteren Analyse im stochastischen Modell, wodurch sich die praktische Umsetzbarkeit bisher meist auf Systeme beschränkt, bei denen eine analytische Lösung der Schrödingergleichung gefunden werden kann.
Durch die Interpretation des Variationsprinzips von Pavon als ein stochastisches optimales Steuerungsproblem gelingt es, quantenmechanische Hamiltonische Bewegungsgleichungen (für Ort und Geschwindigkeit beziehungsweise Impuls) herzuleiten, welche äquivalent zur Schrödingergleichung sind und unabhängig von dieser gelöst werden können. Die vorliegende Arbeit stellt die Grundlage und Vorgehensweise bereit, quantenmechanische Systeme ohne Kenntnis der Wellenfunktion mit Methoden der stochastischen Mechanik zu beschreiben. Insbesondere ist die Schrödingergleichung, genau wie die Hamilton-Jabobi Gleichung in der klassischen Theorie, *eine* mögliche Methode zur Beschreibung eines quantenmechanischen Systems, jedoch nicht die einzige.

Bei den sich ergebenden Hamiltonischen Bewegungsgleichungen handelt es sich um gekoppelte vorwärts-rückwärts stochastische Differentialgleichungen, die mit Hilfe eines iterativen Algorithmus numerisch gelöst werden. Dieser wird explizit erklärt und auf zwei verschiedene stationäre Probleme angewandt. Hierbei zeigt sich sowohl beim eindimensionalen harmonischen Oszillator, für den eine exakte Lösung bekannt ist, als auch bei der eindimensionalen Doppelmulde, die Güte des numerischen Algorithmus. Weiterhin werden die im Falle der Doppelmulde auftauchenden Tunnelprozesse genauer analysiert, wodurch der Zusammenhang von Energieaufspaltung und Tunnelzeit (*mean first passage time*) deutlich wird.

Abstract

The description of non-relativistic quantum systems is generally based upon the same fundamental structure as found in the theory of (classical) analytical mechanics. Thus, the Schrödinger equation, the stochastic kinematic equations of Edward Nelson and the quantum Hamilton principle, as introduced by Michele Pavon, are equivalent methods for a unique description of the motion of a quantum particle. However, in practical applications of these stochastic methods, substantial difficulties may arise. In general, neither the kinematic equations of Nelson, nor Pavon's variational can be evaluated in a straightforward way. In these approaches, the Schrödinger equation has to be faced from the beginning, meaning that applications are restricted to systems with a known analytical wave function.

However, if the variational problem of Pavon is interpreted as a stochastic optimal control problem, the quantum Hamilton equations of motion - that addressing the particle's position and velocity, or the particle's momentum - can be derived and solved uniquely, yielding an approach that is in fact independent of the Schrödinger equation. The thesis at hand introduces and demonstrates the description of quantum systems in terms of the above mentioned stochastic model, and does not require knowledge on the wave function to yield a proper solution to quantum-mechanical problems. Similar to the Hamilton-Jacobi equation in classical physics, the Schrödinger equation is thus one, but not the only, method to describe quantum systems.

The resulting Hamilton equations of motion are coupled forward-backward stochastic differential equations, which can be solved using an iterative algorithm. That algorithm is explained explicitly and is applied to two stationary cases. The accuracy of the algorithm is demonstrated using the example of a one-dimensional harmonic oscillator, where the exact wave function is known, as well as using a one-dimensional double-well potential. Furthermore, tunneling processes, as observed in case of the double-well potential, are thoroughly analyzed, yielding a strict relation between energy splitting and tunneling time (mean first passage time).

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CHAPTER 1

The need of an alternative approach to address quantum mechanics

Our modern society is highly dominated by high-end technology that in turn is largely based upon the understanding of microscopic systems. Just to name but a few, modern computers, smartphones, or also lasers found in any CD, DVD or blue-ray player benefit from, or even rely on, a quantum-mechanical understanding of small-scale processes. Especially the contributions of Max Planck [1901], Albert Einstein [1905], Werner Heisenberg [1925], Max Born and Pascual Jordan [Born and Jordan, 1925; Born et al., 1925], and Erwin Schrödinger [1926a,b,c,d, 1927a,b] (see also [Schrödinger, 1982]) revolutionized our understanding of such systems, and have provided the basis of modern quantum mechanics. Now being able to not only describe the macroscopic world, but also nature on its atomic scale, a multitude of phenomena that were not understood until then now turned out to be manageable, yielding new insights and stimuli for further research along this line. Modern technology has rapidly evolved from that. Despite its success in connecting the microscopic world to different experimental findings, quantum mechanics was controversially discussed in its beginning, with Einstein being perhaps the most famous opponent of this new theory. Nowadays, quantum mechanics is a well established part of modern physics, and is of indispensable value to elucidate phenomena on length scales beyond macroscopic effects. Still, the detailed interpretation of its outcomes can be as interesting as sophisticated.

In classical mechanics, there is a straightforward and intuitive interpretation of the required mathematical formalism as compared to physical reality. The state space equals the phase space, i.e. the state space is a set of points with elements directly given by the position and momentum of the particle(s). Measured quantities are functions which associate real numbers (the measured data) where elements from the phase space and the measured data are directly linked to physical properties of the system.
Furthermore, for the description of the dynamics of the system, different theories are

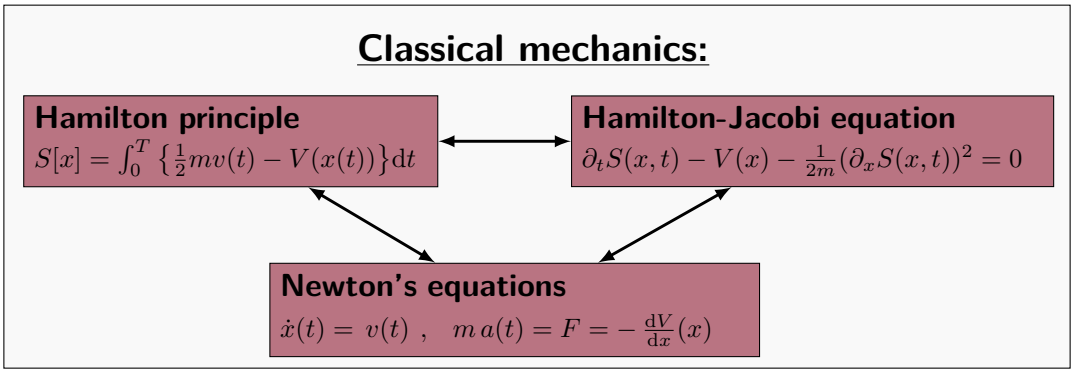

Figure 1.1.: *Schematic representation of the three equivalent theories, which describe the motion of a classical particle uniquely but independently from each other.*

available. Starting from the dynamic equations of Newton, Hamilton established a variational problem, i.e. Hamilton's principle, identifying classical paths as stationary points of the action functional. Moreover, the action function itself fulfills a non-linear, partial differential equation (PDE), called the Hamilton-Jacobi equation. All three approaches are equivalent to each other and describe the dynamic of the system uniquely. This general structure of analytical mechanics is visualized in **Figure 1.1**.

In 1925, based on the approach of Heisenberg [1925], the so-called matrix mechanics was introduced by Born, Jordan, and Heisenberg [Born and Jordan, 1925; Born et al., 1925]. This treatment was the first closed theory to describe quantum systems. Somewhat later, Schrödinger [1926a,c,d, 1927a,b] established his famous equation by making use of the analogy to the Hamilton-Jacobi formalism in classical mechanics. It turned out that this theory is equivalent to the matrix mechanics introduced by Heisenberg [Schrödinger, 1926b]. The Hilbert space, related to the solutions of the Schrödinger equation, leads to the identification of self-adjoint operators as a representation of physical observables [von Neumann, 1996], which is the standard way of thinking about modern physics. In detail, this means that the state space (Hilbert space) representation is essentially abstract, and interpretations are less straightforward as in the phase space of classical mechanics. In particular, elements of the Hilbert space (vectors and operators) are not directly linked to physical reality [Friebe et al., 2015]. Measured values of an observable are given by (real) eigenvalues of the related operators; however, as they represent a macroscopic pointer position at the time of the measurement, there is no direct link to the physical properties of the quantum system [Friebe et al., 2015]. Hence, it is impossible to make any statements about the system before performing the actual measurement, noting that the measurement itself will change the state of the system. In fact, repetitive measurements do not necessarily provide the same value for one and the same observable. Any approach is restricted to expectation values that in turn are

determined under a certain measurement probability that is correlated with the wave function of the original system. To make a long story short, it is hence apparent that the physical interpretation of the mathematical formalism of quantum mechanics is not as natural as in classical mechanics.

The most common and broadly accepted interpretation of quantum mechanics dates back to the work of Niels Bohr and Weiner Heisenberg in 1925 to 1927, and has been consolidated as the Copenhagen interpretation of quantum mechanics. The following points are of central importance:

1. The wave function, which is the solution to the Schrödinger equation, represents the state of a system and combines all known information about the system.

2. Heisenberg's uncertainty principle: Certain properties, e.g. the position and the momentum of the particle, cannot be simultaneously measured with highest precession. The more precisely the position of the particle is determined, the less precisely the momentum can be obtained.

3. In any measurement, the quantum system interacts with the laboratory device. Performing the measurement, the wave function collapses or is irreversibly reduced to an eigenstate of the observable that is detected. The result of such a measurement is a classical one and should be described in the ordinary language of classical physics.

4. The correspondence principle: For large quantum numbers (high quantum states), the properties of the system are in close agreement with those of the classical description [Born, 1920].

5. The description given by the wave function is probabilistic: the square of the absolute value of the wave function gives the probability density, i.e. the probability that a measurement on a quantum system yields a given result [Born, 1926].

Even though the Copenhagen interpretation of quantum mechanics has been well established, its correctness has always been a matter of debate, including also scepsis and criticism by Schrödinger and Einstein [Heisenberg, 1956]. Suggestions to the meaning of the wave function are still made; see, for instance, Aharonov et al. [1993] or Gau [2011].

Forty years after Schrödingers contributions, Edward Nelson [1966] published a work in which he derived the Schrödinger equation by assuming that the dynamics of a quantum particle can be represented in terms of time-reversible Brownian motion. Worth noting, the Born interpretation of the wave function [Born, 1926] is intrinsic to

this derivation. Identifying the diffusion coefficient as Planck's constant divided by two times the mass of the particle, and assuming the expectation value of the acceleration to be given by the force divided by the mass, he ended up with the Madelung equations [Nelson, 1966, 1985], which are, for the ground state of the system, equivalent to the Schrödinger equation [Madelung, 1927]. This theory "*attempts to provide a realistic, objective description of physical events in classical terms*" [Nelson, 1985], and overcomes difficulties in the ordinary theory of quantum mechanics. For instance, the duration of a tunneling process can be naturally defined, while the standard formulation of quantum mechanics would require the duration of the process to be accessed as the expectation value of a "time operator". Though, there is no time operator in quantum mechanics! In fact, a lot of efforts have been made to characterize tunneling times both experimentally [Martinis et al., 1988; Steinberg et al., 1993; Eckle et al., 2008] and theoretically [MacColl, 1932; Hartman, 1962; Büttiker and Landauer, 1982; Büttiker, 1983; Landauer, 1989; Landauer and Martin, 1994; Steinberg, 1995].

Soon after, variational principles where introduced and the kinematic laws and the Schrödinger equation could also be derived from this approach [Yasue, 1980, 1981a,b; Guerra and Morato, 1983; Guerra and Marra, 1984]. Finally, Michele Pavon [1995b] introduced the so-called quantum Hamilton principle in an analogous way to classical analytical mechanics, including also the kinematic equations as constraints to the search of the optimal path, which extremizes the action functional. Consequently, the same fundamental structure as in classical mechanics can be found for quantum systems. Similar to the Hamilton-Jacobi equation, the Schrödinger equation is a complete, but not the only, description of quantum systems.
The quantum-mechanical wave function and the drift coefficients are directly related to each other, as has been utilized to elucidate the dynamics of quantum systems in more detail. Applications include, but are not limited to, the double slit [McClendon and Rabitz, 1983; Nitta and Kudo, 2008], correlated quantum gases [Paul, 2012] and tunneling processes [Yasue, 1978; Chen and Wang, 1990; Imafuku et al., 1995, 1997; Aoki et al., 2000; Hara and Ohba, 2003].

Up to date, the analysis of (non-relativistic) quantum systems is based upon an analytical treatment of, or an numerical approach to, the Schrödinger equation. Even for approaches utilizing stochastic mechanics, the wave function must be known so as to address the kinematic equations postulated by Edward Nelson [1966]: Nelson's theory requires knowledge of two distinct velocities that in turn are defined by the real and imaginary part of the gradient of the logarithm of the wave function. Applications of stochastic mechanics are restricted to a small number of potentials of which the Schrödinger equation can be solved analytically. Even though the two velocities are

characterized by two coupled non-linear partial differential equations, which in turn are equivalent to the Madelung equations, solving these PDEs cannot be performed in a straightforward way. Consequently, finding a method to determine the velocities is reasonable and would expand the applicability of Nelson mechanics, as well as it would supply a complete description of a quantum system in parallel, and independent of, the Schrödinger equation.

In the study at hand, the quantum Hamilton principle of Pavon will be interpreted as a stochastic optimal control problem resulting in stochastic quantum Hamilton equations of motion. This set of equations can be solved - at least numerically - without any knowledge of the wave function, i.e., they constitute an independent and also more intuitive way to treat quantum systems.

> *Stochastic mechanics has a natural derivation from the variational principle [...]. Had the Schrödinger equation been derived in this way before the invention of matrix mechanics, the history of the conceptual foundations of modern physics would have been different.*
>
> – Edward Nelson [1985]

The thesis at hand is organized as follows: In the next chapter, fundamental aspects on stochastic processes and stochastic differential equations will be presented, followed by a in-detail description of the theory of Nelson mechanics in the third chapter. In chapter four, comprising the major part of this thesis, the derivation of the stochastic Hamilton equations of motion will be presented. Stationary systems will be addressed first, followed by an approach to the more general case of time-dependent problems. For the stationary case, a numerical algorithm will be introduced and applied to two exemplary cases. Prospects to further applications and developments will be discussed at the end of this chapter. Finally, the last chapter summarizes the central results obtained, and concludes with an assessment on the significance of the theory derived.

CHAPTER 2

Stochastic analysis

The central objective of the concepts and methods presented herein is to achieve an appropriate description of quantum dynamics using the theory of conservative Brownian motion [Nelson, 1966], i.e., the use of stochastic processes. The following chapter summarizes fundamental concepts required for stochastic analysis. For the sake of clarity, an overview of the most relevant definitions is also presented in section A.1 (appendix).

Definition 2.1 *A stochastic process $(X(t))_{t\in I}$ is a family of $\mathbb{R}^d$ (or complex-valued) random variables with an index set I [Arnold, 1973].*

Remark 2.2 *It is common[1] to write X_t instead of $X(t)$.*

The stochastic process $(X(t))_{t\in I}$ describes a time-dependent, random-based event. Its associated index set I is commonly interpreted as a set of different times, with the distinction of discrete times, $I \subseteq \mathbb{N}$, from continuous ones, $I \subseteq \mathbb{R}_+$. For any fixed $t \in I$, $X(t,\cdot)$ is a random variable, i.e., $X\colon \Omega \to \mathbb{R}^d$ is a measurable function from the sample space Ω into $\mathbb{R}^d$, while $X(\cdot,\omega)$ is a $\mathbb{R}^d$-valued function for all fixed $\omega \in \Omega$, and is called *realization* (*trajectory*, *path*) of the process [Arnold, 1973]. In fact, a stochastic process is always defined on a probability space $(\Omega, \mathcal{F}, P)$, which in turn is defined within the axiomatic system of Kolmogoroff [1933]. The sample space Ω includes all possible outcomes of the random experiment. The σ-algebra $\mathcal{F}$ is the event space and includes all events $A \in \mathcal{F}$ to which a probability is assigned. The probability measure $P\colon \mathcal{F} \to [0,1]$ assigns a probability to each event $A \in \mathcal{F}$. Furthermore, $P(\Omega) = 1$, and, given that A, B are disjoint, $P(A \cup B) = P(A) + P(B)$. A σ-algebra $\mathcal{F} \in \mathcal{P}(\Omega)$[2] is defined as follows [Meintrup and Schäffler, 2005].

Definition 2.3 (σ-algebra) *A set system $\mathcal{F} \in \mathcal{P}(\Omega)$, i.e. a set of subsets of Ω, will be called σ-algebra, if the following conditions are fulfilled:*

[1] In particular, the notation X_t will be used in the context of discrete processes.
[2] $\mathcal{P}(\Omega)$ is the power set of Ω

(i) *The basic set Ω is included, i.e. $\Omega \in \mathcal{F}$.*

(ii) *$\mathcal{F}$ is closed under complementation: If $A \in \mathcal{F}$, then $A^c := \Omega \setminus A \in \mathcal{F}$.*

(iii) *$\mathcal{F}$ is closed under countable unions: If $A_i \in \mathcal{F}$, $i \in \mathbb{N}$, then $\bigcup_{i=1}^{\infty} A_i \in \mathcal{F}$.*

The so-called Wiener process $(W_t)_{t\geq 0}$ on $(\Omega, \mathcal{F}, P)$ is an important example of stochastic processes, and is defined as follows:

Definition 2.4 *A stochastic process $(W(t))_{t\geq 0}$ will be called Wiener process (or Brownian motion), if the following conditions hold [Meintrup and Schäffler, 2005]:*

(W1) *$W(0) = 0$ almost sure.*

(W2) *$(W(t))_{t\geq 0}$ consists of independent increments.*

(W3) *The increments $W(t) - W(s)$, $0 \leq s < t$, are distributed as $N(0, t-s)$, i.e., a normal distribution with an expectation value equal to zero and variance[3] given by $(t-s)$.*

(W4) *$(W(t))_{t\geq 0}$ is a continuous process, i.e., almost all paths of the process are continuous.*

The existence of such processes can be proven; see e.g. Meintrup and Schäffler [2005]. The first three conditions can be verified using Kolmogorov's existence theorem [Meintrup and Schäffler, 2005]. Certainly, in no case a process defined by (W1)-(W3) contains only continuous paths [Meintrup and Schäffler, 2005]. Nonetheless, by making use of Kolmogorov's continuity theorem, [Øksendal, 2000], one can show that there is a continuous version of the process, and in the following, the assumption will be made that $(W_t)_{t\geq 0}$ is such a continuous version of the process.
Moreover, $(W(t))=\left(W^{(1)}(t), \ldots, W^{(d)}(t)\right)$ will be called d-dimensional Brownian motion, if the one-dimensional processes $\left(W^{(j)}(t)\right)_{t\geq 0}$, $1 \leq j \leq d$, are independent from each other [Øksendal, 2000].

Another important class of stochastic processes are the so-called Markov processes, i.e., processes in which the present, the past and future states are statistically independent of each other.

Definition 2.5 (Markov process) *Suppose $\mathcal{B}^d$ is the Borel σ-algebra, i.e. the smallest σ-algebra generated by open sets of $\mathbb{R}^d$. Let $\mathcal{F}_s$ be a σ-algebra which is generated*

[3] The variance is, actually, $\sigma^2(t-s)$, however, w.l.o.g. $\sigma = 1$, since the latter can indeed be achieved by (re)scaling the time axis.

by the process $(X(t))_{t\geq 0}$ *up to time* s*. Then, the process is called (weak, elementary) Markov process, if for* $0 \leq s \leq t$ *and all* $B \in \mathcal{B}^d$ *the condition*

$$P\{X(t) \in B \mid \mathcal{F}_s\} = P\{X(t) \in B \mid X_s\} \tag{2.1}$$

is fulfilled (with probability one) [Arnold, 1973].

This condition is called Markov property. There are many equivalent formulations of this feature; see, for instance, Arnold [1973] or Theorem A.4 in the appendix (section A.1).

In the following, it will be assumed that all processes considered herein are one-dimensional ones; however, the presented concepts can be trivially extended to the higher-dimensional case (addressed in section 2.2). Stochastic processes are often described by stochastic differential equations (SDEs), which in turn are motivated by an ordinary differential equation (ODE), i.e. writing

$$\frac{\mathrm{d}X}{\mathrm{d}t} = b(t, X(t)) + \sigma(t, X(t)) \cdot \xi(t) \quad . \tag{2.2}$$

Here, b, σ are given functions. $(\xi(t))_{t\leq 0}$ is called white noise process and has the following properties [Øksendal, 2000]:

(i) $t_1 \neq t_2 \;\Rightarrow\; \xi(t_1)$ and $\xi(t_2)$ are independent from each other.

(ii) $(\xi(t))_{t\geq 0}$ is stationary, i.e. the (joint) distribution of $\{\xi(t_1+t), \ldots, \xi(t_k+t)\}$ does not depend on t.

(iii) $\mathrm{E}[\xi(t)] = 0$ for all t.

Since reasonable processes fulfilling (i)-(iii) cannot be found [Øksendal, 2000], equation (2.2) is rewritten in such a way that the process $\xi(t)$ is replaced by a more suitable one. Let $0 = t_0 < t_1 < \cdots < t_n = T$ be a partition of the time interval $[0, T]$ and $\Delta t_i := t_{i+1} - t_i$, then the discretization of equation (2.2) reads

$$X_{t_{i+1}} - X_{t_i} = b(t_i, X_{t_i})\,\Delta t_i + \sigma(t_i, X_{t_i})\,\xi_{t_i}\,\Delta t_i \quad . \tag{2.3}$$

Replacing $\xi_{t_i}\,\Delta t_i$ by $\Delta W_i = W_{t_{i+1}} - W_{t_i}$, it follows that $(W(t))_{t\in[0,T]}$ has stationary increments with zero expectation value. In addition, processes with continuous paths turn out to be described by Brownian motion only [Øksendal, 2000]. Consequently,

$$X_{t_i} = X_0 + \sum_{k=0}^{i-1} b(t_k, X_{t_k})\,\Delta t_k + \sum_{k=0}^{i-1} \sigma(t_k, X_{t_k})\,\Delta W_k \quad . \tag{2.4}$$

If the limit $\Delta t_k \to 0$ is existent, then applications of the usual integration rules will yield

$$X(t) = X_0 + \int_0^t b(s, X(s))\,\mathrm{d}s + \text{“}\int_0^t \sigma(s, X(s))\,\mathrm{d}W(s)\text{”} \quad . \tag{2.5}$$

The first term is given by a ("normal") Riemann or Lebesgue integral, while the second term will be addressed in the following by defining

$$I[f] := \int_0^t f(s,\omega)\,\mathrm{d}W(s,\omega) \tag{2.6}$$

for a wide class of functions $f\colon [0,\infty) \times \Omega \to \mathbb{R}$.

2.1. Itô integrals

Definition 2.6 *Let the set $\mathcal{V} = \mathcal{V}(T)$ be the class of functions $f\colon [0,\infty) \times \Omega \to \mathbb{R}$ such that the following conditions hold for all $T > 0$ [Øksendal, 2000]:*

(i) $(t,\omega) \to f(t,\omega)$ *is $\mathcal{B} \times \mathcal{F}$-measurable, where $\mathcal{B}$ is the Borel σ-algebra on $[0,\infty)$.*

(ii) $f(t,\omega)$ *is $\mathcal{F}_t$-adapted.*

(iii) $\mathrm{E}\left[\int_0^T f(t,\omega)^2 \mathrm{d}t\right] < \infty$.

The Itô integral $I[f]$ of a function $f \in \mathcal{V}$ will be defined as follows. The Itô integral will be introduced for a simple class of functions ϕ that are step-functions (also called elementary functions). Based upon that, it will be shown that every function $f \in \mathcal{V}$ can be approximated by step functions, such that $I[f]$ equals the limit of $I[\phi]$ as $\phi \to f$.

Definition 2.7 *A function $\phi \in \mathcal{V}(T)$ will be called elementary function, if there exists a decomposition $0 = t_0 < t_1 < \cdots < t_N = T$ along with $\mathcal{F}_{t_j}$-measurable random variables ϕ_j, $j = 0,\ldots,N$, with $\mathrm{E}(\phi_j^2) < \infty$ such that*

$$\phi(t,\omega) = \sum_{j=0}^{N-1} \mathbb{1}_{[t_j,t_{j+1})}(t)\,\phi_j(\omega) \;, \quad \phi(T,\omega) = \phi_N(\omega) \quad . \tag{2.7}$$

Definition 2.8 (Itô integral for elementary functions) *For an elementary function $\phi \in \mathcal{V}$ the Ito integral reads*

$$I[\phi] = \int_0^T \phi(t,\omega)\,\mathrm{d}W(t,\omega) = \sum_{j=0}^{N-1} \phi_j\,\left(W(t_{j+1}) - W(t_j)\right) \quad . \tag{2.8}$$

Following these considerations, it will be be shown that elementary functions are closed functions in $\mathcal{V}$.

Theorem 2.9 *For every function $f \in \mathcal{V}$ exists a sequence $(\phi_n)_{n\in\mathbb{N}} \subset \mathcal{V}$ such that*

$$\lim_{n\to\infty} \mathrm{E}\left[\int_0^T (f(t) - \phi_n(t))^2 \mathrm{d}t\right] = 0 \tag{2.9}$$

almost surely.

The proof of Theorem 2.9 can, for instance, be found in the textbook by Arnold [1973]. Thus, the stochastic integral $I[f]$ for an arbitrary function $f \in \mathcal{V}$ is defined as follows.

Definition 2.10 (Itô integral) *Let $f \in \mathcal{V}$ and let $(\phi_n)_{n\in\mathbb{N}} \in \mathcal{V}$ be a sequence of elementary functions such that theorem 2.9 holds. Then,*

$$\int_0^T f(t,\omega)\,\mathrm{d}W(t) = \operatorname*{ms\text{-}lim}_{n\to\infty} \int_0^T \phi_n(t,\omega)\,\mathrm{d}W(t) \tag{2.10}$$

is called Itô integral, where ms-lim *(see also appendix A.1) denotes the convergence in mean square.*

Furthermore, the Itô integral has to the following properties.

Theorem 2.11 *Let $f, g \in \mathcal{V}$. Then*

(i) $\alpha, \beta \in \mathbb{R}$

$$\Rightarrow \quad \int_0^T \Big(\alpha\, f(t,\omega) + \beta\, g(t,\omega)\Big)\,\mathrm{d}W(t) = \alpha \int_0^T f(t,\omega)\,\mathrm{d}W(t) \;+\; \beta \int_0^T g(t,\omega)\,\mathrm{d}W(t) \tag{2.11}$$

(ii) $a, b \in [0,T]$, $a < b$

$$\Rightarrow \quad \int_0^T \mathbb{1}_{[a,b]}\,\mathrm{d}W(t) = W(b) - W(a) \tag{2.12}$$

(iii) $0 < U < T$. *Then for almost all ω*

$$\int_0^T f(t,\omega)\,\mathrm{d}W(t) = \int_0^U f(t,\omega)\,\mathrm{d}W(t) \;+\; \int_U^T f(t,\omega)\,\mathrm{d}W(t) \tag{2.13}$$

holds.

(iv) $\mathrm{E}\left[\int_0^T f(t,\omega)\,\mathrm{d}W(t)\right] = 0$

(v) $\mathrm{E}\left[\int_0^T f(t,\omega)\,\mathrm{d}W(t)\right]^2 = \mathrm{E}\left[\int_0^T f(t,\omega)^2\,\mathrm{d}t\right] = \int_0^T \mathrm{E}\left(f(t,\omega)^2\right)\mathrm{d}t$

(vi) $\int_0^T f(t,\omega)\,\mathrm{d}W(t)$ *is $\mathcal{F}_T$-measurable.*

(vii) $\forall c > 0,\ L > 0$:

$$P\left\{\left|\int_0^T f(t,\omega)\,\mathrm{d}W(t)\right| > c\right\} \leq P\left\{\left|\int_0^T f(t,\omega)^2\,\mathrm{d}t\right| > c\right\} + \frac{L}{c^2} \tag{2.14}$$

(viii) The Itô integral has with probability one continuous realizations.

Remark 2.12 *It is possible to expand the definition of the Itô integral to a more general class of processes. Let the properties given by Definition 2.6 (i), (ii) be valid, and let* $P\left\{\int_0^T f^2(t,\omega)\mathrm{d}t < \infty\right\}$ *be true, then (i), (iii), (iv) and (viii) of Theorem 2.11 are fulfilled as well.*

The definition using elementary functions is very convenient since the value of the integral is independent of the choice of the sequence (ϕ_n). Moreover, the Itô integral leads to a martingale, which is an important computational advantage [Øksendal, 2000]. However, there are different ways to define the stochastic integral, e.g. by the use of Stratonovich integral. It is noted that the different definitions of the stochastic integral can in fact yield different results [Arnold, 1973; Øksendal, 2000].
Finally, the wanted integral from equation (2.6) can be easily determined using the following corollary [Arnold, 1973]:

Corollary 2.13 *Let* $f(t,\omega) \in \mathcal{V}$ *with probability one be a continuous function with respect to* t*, and* $0 = t_0 < t_1 < \cdots < t_N = t$*,* $\delta_N = \max_k(t_{k+1} - t_k)$*, then*

$$\int_0^t f(s,\omega)\mathrm{d}W(s) = \underset{\delta_N \to 0}{\text{P-lim}} \sum_{k=0}^{N-1} f(t_k,\omega)\ (W(t_{k+1}) - W(t_k)) \quad . \tag{2.15}$$

Here, P-lim *denotes the convergence in probability.*

2.2. Existence and uniqueness for solutions of SDE's

Now, addressing to all possible solutions $X(t,\omega)$ of equation (2.2), the Itô interpretation of equation (2.2) is that X_t satisfies the stochastic integral equation

$$X(t) = X_0 + \int_0^t b(s, X(s))\,\mathrm{d}s + \int_0^t \sigma(s, X(s))\,\mathrm{d}W(s) \quad , \tag{2.16}$$

or, in differential form

$$\mathrm{d}X(t) = b(t, X(t))\,\mathrm{d}t + \sigma(t, X(t))\,\mathrm{d}W(t)\ , \quad X(t=0) = X_0 \quad , \tag{2.17}$$

which is called stochastic differential equation. Note that equation (2.17) is only a formal notation, meaning that the process fulfills the integral equation. Finally, the

existence and uniqueness of such equations can be questioned, as well as fundamental features of their solutions should be clarified, as done below.

Theorem 2.14 (Existence and uniqueness theorem for SDEs)
Let $T > 0$ and $b(\cdot,\cdot)\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$, $\sigma(\cdot,\cdot)\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^{d\times m}$ be measurable functions satisfying

$$|b(t,x) + \sigma(t,x)| \leq C(1+|x|) \ , \quad x \in \mathbb{R}^d, \ t \in [0,T] \tag{2.18}$$

for a constant value of C, and let

$$|b(t,x) - b(t,y)| + |\sigma(t,x) - \sigma(t,y)| \leq D|x-y| \ , \quad x,y \in \mathbb{R}^d, \ t \in [0,T] \tag{2.19}$$

be valid for a constant D. Moreover, let X_0 be a $\mathcal{F}_0$-measurable random variable and $(W(t))_{t\in[0,T]}$ be an m-dimensional Wiener process.
Then, the stochastic differential equation

$$\mathrm{d}X(t) = b(t,X(t))\,\mathrm{d}t + \sigma(t,X(t))\,\mathrm{d}W(t) \ , \quad X(t=0) = X_0 \tag{2.20}$$

has a unique solution $(X(t))_{t\in[0,T]}$ with the following properties:

1. *$(X(t))_{t\in[0,T]}$ has with probability one continuous realizations, i.e. for fixed ω the function $X(t,\omega)$ is continuous with respect to t.*
2. *$X(t)$ is adapted to the filtration $\mathcal{F}_t$.*
3. *$\mathrm{E}\left[\int_0^T |X(t)|^2 \mathrm{d}t\right] < \infty$.*

The theorem and its proof can be found in many textbooks of stochastic differential equations, see for instance, Arnold [1973] or Øksendal [2000]. Note that the derivation of the Itô integral was presented for one-dimensional processes, while the theorem of existence and uniqueness also applies to the multidimensional case. It is further noted that *uniqueness* has to be understood as follows. Let $(X(t))_{t\in[0,T]}$ and $(Y(t))_{t\in[0,T]}$ be solutions to equation (2.20), then this SDE has a unique solution if and only if $P\{X(t) = Y(t) \ , \ \forall t \in [0,T]\} = 1$.

Another important property is given by the following theorem, the validity of which is proven in ref. [Arnold, 1973].

Theorem 2.15 *If the conditions of Theorem 2.14 are fulfilled, then the solution $X(t)$ of equation (2.20) is a Markov process for $t \in [0,T]$, and the transition probability reads*

$$P\{t,A;\, s,x\} := P\{X(t) \in A | X(s) = x\} = P\{X_{s,x}(t) \in A\} \quad . \tag{2.21}$$

Here, $X_{s,x}(t)$ is the solution of the SDE (equation (2.20)) with the initial point $X(t=s)=x$, that is, $X_{s,x}(t)$ is the solution of

$$X_{s,x}(t) = x + \int_s^t b(u, X(u))\,\mathrm{d}u + \int_s^t \sigma(u, X(u))\,\mathrm{d}W(u) \quad . \tag{2.22}$$

If a density $p(t, y; s, x)$ to the probability $P(t, A;\ s, x)$ exists, then the density will fulfill a forward as well as a backward Fokker-Planck equation [Arnold, 1973].

Theorem 2.16 *Let $(X_t)_{t\in[0,T]}$ be a d-dimensional Markovian process characterized by equation (2.20), and having the transition probability density $p(t, y; s, x)$. If the partial derivatives $\partial_t p$, $\partial_y p$ and $\partial_{yy} p$ exist, then the density $p(t, y; s, x)$ is a fundamental solution to the forward Kolmogorov or Fokker-Planck equation ($t > s$, fixed s and x),*

$$\begin{aligned} 0 = &\frac{\partial}{\partial t}\, p(t, y; s, x) + \sum_{i=1}^{d} \frac{\partial}{\partial y_i}\Big(b_i(t, y)\, p(t, y; s, x)\Big) \\ &- \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} \frac{\partial^2}{\partial y_i\, \partial y_j}\Big[\Big(\sigma(t, y)\, \sigma^*(t, y)\Big)_{ij}\, p(t, y; s, x)\Big] = 0 \quad , \end{aligned} \tag{2.23}$$

with $\sigma^*(t, y)$ being the transposed matrix of $\sigma(t, y)$. Analogously, if the partial derivatives $\partial_s p$, $\partial_x p$ and $\partial_{xx} p$ are existent, the density $p(t, y; s, x)$ will fulfill the backward Kolmogorov or Fokker-Planck equation ($s < t$, fixed t and y),

$$\begin{aligned} 0 = &\frac{\partial}{\partial s}\, p(t, y; s, x) + \sum_{i=1}^{d} b_i(s, x)\, \frac{\partial}{\partial x_i}\, p(t, y; s, x) \\ &+ \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} \Big(\sigma(s, x)\, \sigma^*(s, x)\Big)_{ij}\, \frac{\partial^2}{\partial x_i\, \partial x_j}\, p(t, y;\ s, x) \quad . \end{aligned} \tag{2.24}$$

2.3. Example – Brownian motion

For the purpose of illustrating the presented mathematical concepts, and as a link to the physical background of this thesis, Brownian motion will be discussed in this section. Brownian motion was observed and documented for the first time by the Scottish botanist R. Brown, who became aware of the natural motion of pollen particles immersed in a solvent. It took about 80 years until Einstein and Smoluchowski came up with a theoretical description of this phenomenon, and this breakthrough still gives the basis for theoretical considerations [Paul and Baschnagel, 2013].

The concept of Brownian motion is sketched in **Figure 2.1** and can be treated in the framework of theoretical physics as follows. Collisions with the fluid, i.e. the smaller

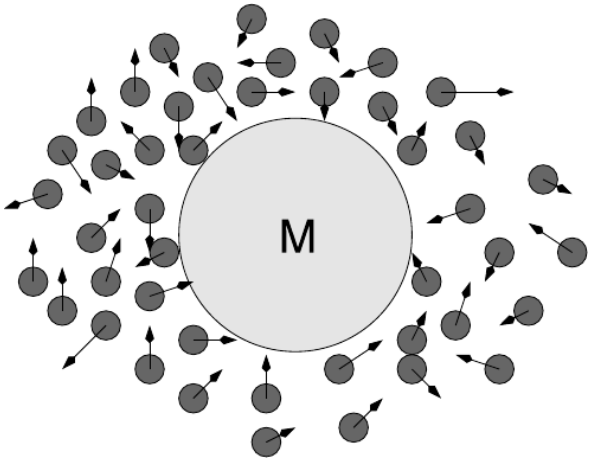

Figure 2.1.: *Scheme of a Brownian particle with mass M in a fluid of much smaller and lighter particles, taken from [Paul and Baschnagel, 2013].*

particles, cause a random force and a viscous drag to the Brownian particle. The viscous drag force is given by

$$\boldsymbol{f}_{\text{drag}} = -\gamma M \boldsymbol{v} \quad , \tag{2.25}$$

where γ is the kinetic viscosity of the medium, M is the mass and $\boldsymbol{v}$ is the velocity of the Brownian particle. As for the random force, it is assumed that all encounters are uncorrelated. Based upon the mass difference, fluid particles move much faster than the Brownian particle, and encounters are approximated as instantaneous events along with random velocity changes of the Brownian particle. Thus, velocity changes are well-represented by a Wiener process of strength σ, and the position and the velocity of the particle can be characterized using two coupled SDEs,

$$\mathrm{d}\boldsymbol{X}(t) = \boldsymbol{v}\,\mathrm{d}t \quad , \tag{2.26}$$

$$M\,\mathrm{d}\boldsymbol{v}(t) = -\gamma M \boldsymbol{v}(t)\,\mathrm{d}t + \sigma\,\mathrm{d}\boldsymbol{W}(t) \quad . \tag{2.27}$$

Note that the position of the Brownian particle is described by a deterministic equation. Moreover, it is possible to add an external force $\boldsymbol{F}$ to the particle, which will occur in the drift term of the velocity. Here, free Brownian motion will be assumed, such that $\boldsymbol{F} = 0$ holds. The above equations are equivalent to the Fokker-Planck equation

$$\frac{\partial p(t,\boldsymbol{x},\boldsymbol{v})}{\partial t} = [-\nabla_{\boldsymbol{x}} + \gamma\nabla_{\boldsymbol{v}}] \cdot \Big(\boldsymbol{v}\, p(t,\boldsymbol{x},\boldsymbol{v})\Big) + \frac{1}{2}\left(\frac{\sigma}{M}\right)^2 \Delta_{\boldsymbol{x}} p(t,\boldsymbol{x},\boldsymbol{v}) \quad , \tag{2.28}$$

which was used in 1940 by H. Kramers to describe the kinetics of chemical reactions [Paul and Baschnagel, 2013]. For the sake of simplicity, only the one-dimensional case

will be studied. The velocity process

$$\mathrm{d}v(t) = -\gamma v\,\mathrm{d}t + \frac{\sigma}{M}\,\mathrm{d}W(t) \quad , \; v(t=0) = v_0 \quad , \tag{2.29}$$

which is also called Orstein-Uhlenbeck process, is a linear SDE. The solution of that process reads (see Appendix theorem A.7)

$$v(t) = v_0\,\mathrm{e}^{-\gamma t} + \frac{\sigma}{M}\int_0^t \mathrm{e}^{-\gamma\,(t-s)}\,\mathrm{d}W(s) \quad . \tag{2.30}$$

Moreover, the probability density of the velocities fulfills the Fokker-Planck equation [Paul and Baschnagel, 2013]

$$\frac{\partial p(t,v)}{\partial t} = \gamma\,\frac{\partial}{\partial v}\Big(v\,p(t,v)\Big) + \frac{1}{2}\left(\frac{\sigma}{M}\right)^2\frac{\partial^2 p(t,v)}{\partial v^2} \quad . \tag{2.31}$$

Taking the average of equation (2.30), one gets

$$\mathrm{E}[v(t)] = \mathrm{E}[v_0]\,\mathrm{e}^{-\gamma t} \quad . \tag{2.32}$$

Furthermore, one can easily check that the second momentum is given by [Paul and Baschnagel, 2013]

$$\mathrm{E}\left[v^2(t)\right] = \frac{\sigma^2}{2\gamma M^2} + \left(\mathrm{E}\left[v_0^2\right] - \frac{\sigma^2}{2\gamma M^2}\right)\mathrm{e}^{-2\gamma t} \quad . \tag{2.33}$$

Since

$$\lim_{t\to\infty}\mathrm{E}\left[v^2(t)\right] = \frac{\sigma^2}{2\gamma M^2} =: \mathrm{E}\left[v^2(\infty)\right] \quad , \tag{2.34}$$

the stationary value of the mean square of the velocity is reached for $t \to \infty$ and has to be equal to the mean thermal velocity of the Brownian motion [Paul and Baschnagel, 2013], i.e.,

$$\frac{M}{2}\mathrm{E}\left[v^2(\infty)\right] = \frac{k_B T}{2} \quad \Rightarrow \quad \sigma^2 = 2\gamma m k_B T \quad , \tag{2.35}$$

where k_B is the Boltzmann constant and T is the absolute temperature of the fluid, i.e., of the environment of the Brownian particle. As a consequence, equation (2.30) accounts for the thermal equilibrium of the particle, if and only if the two parameters γ, σ are interrelated by equation (2.35).
The motional process can be determined by integration of equation (2.30), yielding

$$X(t) = x_0 + \frac{v_0}{\gamma}\left(1 - \mathrm{e}^{-\gamma t}\right) + \frac{\sigma}{M}\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{e}^{-\gamma\,(t'-s)}\,\mathrm{d}W(s) \quad . \tag{2.36}$$

For $\gamma \to \infty$ taken such that $D := \frac{\sigma^2}{2\gamma M^2}$ stays constant, the distribution of the motion process converges to that one of a Gaussian process, i.e., [Arnold, 1973]

$$X^{(0)}(t) = x_0 + \sqrt{2D}\, W_t \quad . \tag{2.37}$$

Hence, in the theory of Ornstein-Uhlenbeck, the Brownian particle has a continuous velocity (though no continuous acceleration), whose existence is lost in the transition $X(t) \to X^{(0)}(t)$ [Arnold, 1973].

2.4. Itô formula

Last but not least, the important theorem of Itô will be introduced, as it is very helpful to evaluate Itô integrals. In fact, the basic definition of Itô integrals it not very useful to calculate the value of a given integral [Øksendal, 2000]. This situation is reminiscent of deterministic Riemann integrals, for which the use of the fundamental theorem of calculus, plus the chain rule, is commonly preferred. However, in the stochastic case, there is no differentiation theory, but only integration theory. Still, it turns out that it is possible to establish an Itô integral counterpart of the chain rule, called Itô formula (see, for instance, ref. [Øksendal, 2000]).

Theorem 2.17 (Itô formula) *Let $f\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}$ be a continuous function with the continuous partial derivatives*

$$f_t(t,x) = \frac{\partial}{\partial t} f(t,x) \ , \ f_{x_i}(t,x) = \frac{\partial}{\partial x_i} f(t,x) \ , \ f_{x_i,x_j}(t,x) = \frac{\partial^2}{\partial x_i x_j} f(t,x) \quad , \tag{2.38}$$

$i,j = 1,\dots,d$. Let $(X(t))_{t\in[0,T]}$ be the d-dimensional process given by equation (2.20). Then, the process

$$Y(t) = f(t, X(t)) \ , \quad Y_0 = f(0, X_0) \tag{2.39}$$

is also a stochastic differential with respect to the same Wiener process $(W_t)_{t\in[0,T]}$, and

$$\begin{aligned} \mathrm{d}Y(t) = &\left[b(t,X(t))\, f_x(t,X(t)) + \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} f_{x_i,x_j}(t,X(t)) \Big(\sigma(t,X(t))\,\sigma^*(t,X(t))\Big)_{ij} \right] \mathrm{d}t \\ &+ f_x(t,X(t))\,\sigma(t,X(t))\,\mathrm{d}W(t) \end{aligned} \tag{2.40}$$

holds.

This theorem can be expanded for vector-valued processes, where every component $Y_k(t)$ fulfills theorem 2.17.

For one-dimensional problems, the presented formula becomes simpler, that is,

$$\mathrm{d}Y(t) = \left[f_t(t, X(t)) \; + \; f_x(t, X(t))\, b(t, X(t)) \; + \; \frac{1}{2}\sigma^2(t, X(t))\, f_{xx}(t, X(t)) \right] \mathrm{d}t$$
$$+ \; \sigma(t, X(t))\, f_x(t, X(t))\, \mathrm{d}W(t) \quad . \tag{2.41}$$

Example 2.18 *As an example, the Itô formula will be used to determine the value of*

$$\int_0^t W(s)\, \mathrm{d}W(s) \quad . \tag{2.42}$$

Similar to the deterministic case, one can assume that the term $\frac{1}{2}W^2(t)$ *appears in the solution to equation (2.42). Therefore, the Itô formula is applied to the function* $f(x) = \frac{1}{2}x^2$*, i.e., the process* $Y(t) = f(W(t))$ *is given by*

$$\frac{1}{2}W^2(t) = Y(t) = \underbrace{f(W_0)}_{=0} + \int_0^t \frac{1}{2}\mathrm{d}s \; + \; \int_0^t W(s)\, \mathrm{d}W(s) \quad , \tag{2.43}$$

where $b(t, x) = 0$ *and* $\sigma(t, x) \equiv 1$*. Consequently, the wanted integral reads*

$$\int_0^t W(s)\, \mathrm{d}W(s) = \frac{1}{2}\left(W^2(t) - t \right) \quad . \tag{2.44}$$

CHAPTER 3

Stochastic mechanics

In 1966, Edward Nelson [1966] introduced a new interpretation of quantum systems. He assumed the interaction of the particle with the environment to be not negligible, which is in contrast to the standard formalism of quantum mechanics (and classical mechanics), where the system is always treated to be an isolated one. The particles are described as classical ones following Newton's dynamical law augmented by a random term that describes the interaction with the environment. However, such a behavior cannot be observed in a macroscopic system. In order to fulfill the correspondence principle, the diffusion coefficient has to be indirectly proportional to the mass of the particle. Nelson [1966] then derived the Schrödinger equation by starting from the kinematic properties of conservative (time-reversible) diffusion processes and assumed the expectation value of the acceleration to be given by the force divided by the mass of the particle. He showed that for each solution of the Schrödinger equation there is a stochastic process which is similar to the relation between the solution of the Hamilton-Jacobi equations and the Newtonian equations of motion in the classical theory.

Sometimes, Nelson mechanics is presented as a stochastic variant of de Broglie's and Bohm's pilot-wave theory [Bohm, 1952a,b; de Broglie, 1970; Bohm and Hiley, 1982] (and references therein), but there is a crucial conceptual difference between them [Bacciagaluppi, 2005]. In the pilot-wave theory it is assumed that there is a physically real wave, satisfying the Schrödinger equation together with a particle that follows a well-defined trajectory [Bohm and Hiley, 1982]. The momentum of this particle is related to the wave function. As a consequence, the wave function is an intrinsic assumption to this theory. In contrast to this, Nelson only assumed that the particle follows a (time-reversible) diffusion process in the configuration space. Based upon that, he derived the Schrödinger equation, i.e. the wave function is not a part of the ontology of the theory [Bacciagaluppi, 2005].

3.1. The principle of stochastic mechanics and its equivalence to the Schrödinger equation

The work presented herein aims to describe non-relativistic particles in an empty space, i.e., no friction can be attributed to the space, and the motion of the particle cannot be described on the basis of the Langevin equation. Therefore, it is assumed that the particle follows the d-dimensional stochastic (Markov) process $(\mathbf{X}(t))_{t\geq 0}$ characterized by the SDE

$$\mathrm{d}\mathbf{X}(t) = \mathbf{b}(\mathbf{X}(t), t)\,\mathrm{d}t + \sqrt{2\,\nu}\,\mathrm{d}\mathbf{W}_f(t) \quad , \; \mathbf{X}(t=0) = \mathbf{x}_0 \in \mathbb{R}^d \quad , \tag{3.1}$$

where $(\mathbf{W}_f(t))_{t\geq 0}$ is a d-dimensional (forward in time) Wiener process, defined in Definition 2.4, and $\mathbf{W}_f(t)$ is independent of all $\mathbf{X}(s)$ with $s \leq t$. The (constant) diffusion coefficient ν will be defined later. Note that this is only a formal notation for the Itô-integral equation,

$$\mathbf{X}(t) = \mathbf{x}_0 + \int_0^t \mathbf{b}(\mathbf{X}(s), s)\,\mathrm{d}s + \sqrt{2\,\nu}\int_0^t \mathrm{d}\mathbf{W}_f(s) \quad . \tag{3.2}$$

In most cases, $\mathbf{X}(t)$ describes the location of an object at time t, which is reasonable since all the results of a measurement can be interpreted as time-dependent macroscopic positions of various objects (pointer, marks on photographic plates, etc.) [Nelson, 1988]. As discussed in the previous chapter, the paths of a stochastic process are, in general, nowhere differentiable. To describe the dynamics of a system, a substitute of the time-derivative is needed. Therefore, the mean-forward in time derivative is defined as [Nelson, 1966]

$$D\mathbf{X}(t) := \lim_{\Delta t \to 0} \mathrm{E}\left[\frac{\mathbf{X}(t+\Delta t) - \mathbf{X}(t)}{\Delta t}\middle| \mathbf{X}(t)\right] \quad . \tag{3.3}$$

Analogously, the mean-backward in time derivative reads [Nelson, 1966]

$$D^*\mathbf{X}(t) := \lim_{\Delta t \to 0} \mathrm{E}\left[\frac{\mathbf{X}(t) - \mathbf{X}(t-\Delta t)}{\Delta t}\middle| \mathbf{X}(t)\right] \quad . \tag{3.4}$$

Indeed, if $\mathbf{X}(t)$ is (in mean) differentiable, then $D\,\mathbf{X}(t) = D^*\,\mathbf{X}(t)$.

Example 3.1 (Ornstein-Uhlenbeck process) *As analyzed in the last chapter, the Langevin equations for describing the dynamics of a diffusive particle in an external force are given by*

$$\mathrm{d}\boldsymbol{X}(t) = \boldsymbol{v}\,\mathrm{d}t \quad , \tag{3.5}$$

$$M\,\mathrm{d}\boldsymbol{v}(t) = \Big[-\gamma M \boldsymbol{v}(t) + \mathbf{F}(\mathbf{X}(t))\Big]\mathrm{d}t + \sigma\,\mathrm{d}\boldsymbol{W}_f(t) \quad . \tag{3.6}$$

Therefore, the mean derivatives of the velocity are

$$D\,\mathbf{v}(t) = -\gamma\mathbf{v}(t) + M^{-1}\,\mathbf{F}(\mathbf{X}(t)) \quad , \tag{3.7}$$

$$D^*\,\mathbf{v}(t) = \gamma\mathbf{v}(t) + M^{-1}\,\mathbf{F}(\mathbf{X}(t)) \quad , \tag{3.8}$$

resulting in

$$\tfrac{1}{2}DD^*\,\mathbf{X}(t) + \tfrac{1}{2}D^*D\,\mathbf{X}(t) = M^{-1}\,\mathbf{F}(\mathbf{X}(t)) \quad . \tag{3.9}$$

This relation can be interpreted as the dynamic law for the Ornstein-Uhlenbeck theory.

As seen from the above example, it is worthwhile to define the second mean derivative of a stochastic process as

$$\mathbf{a}(t) = \tfrac{1}{2}DD^*\,\mathbf{X}(t) + \tfrac{1}{2}D^*D\,\mathbf{X}(t) \quad , \tag{3.10}$$

which may be called mean acceleration. The theory discussed here requires that the drift term is given by a measurable function. Then, the mean-forward derivative is given by exactly this function, since

$$\begin{aligned} D\mathbf{X}(t) &= \lim_{\Delta t\to 0} \mathrm{E}\left[\tfrac{1}{\Delta t}\int_t^{t+\Delta t}\mathbf{b}(\mathbf{X}(s),s)\,\mathrm{d}s + \tfrac{\sqrt{2\nu}}{\Delta t}\int_t^{t+\Delta t}\mathrm{d}\mathbf{W}_f(s)\,\middle|\,\mathbf{X}(t)\right] \\ &= \lim_{\Delta t\to 0} \mathrm{E}\left[\tfrac{1}{\Delta t}\int_t^{t+\Delta t}\mathbf{b}(\mathbf{X}(s),s)\,\mathrm{d}s\,\middle|\,\mathbf{X}(t)\right] \\ &= \mathrm{E}\left[\lim_{\Delta t\to 0}\tfrac{1}{\Delta t}\int_t^{t+\Delta t}\mathbf{b}(\mathbf{X}(s),s)\,\mathrm{d}s\,\middle|\,\mathbf{X}(t)\right] \\ &= \mathrm{E}\left[\mathbf{b}(\mathbf{X}(t),t)|\,\mathbf{X}(t)\right] = \mathbf{b}(\mathbf{X}(t),t) \quad . \end{aligned} \tag{3.11}$$

In general, the SDE in equation (3.1) is asymmetric in time, i.e., if the diffusion process started at $\mathbf{x}_0$ and goes forward in time towards a new point $\mathbf{X}(t)$, and moved then backwards in time with the same duration as before, it would not be mandatory that the process reaches the same point again. A backward stochastic differential equation (BSDE)

$$\mathrm{d}\mathbf{X}(t) = \mathbf{b}^*(\mathbf{X}(t),t)\,\mathrm{d}t + \sqrt{2\,\nu}\,\mathrm{d}\mathbf{W}_b(t) \;\;,\;\; \mathbf{X}(t=T) = \mathbf{x}_T(\omega) \tag{3.12}$$

is introduced, which also describes the process $(\mathbf{X}(t))_{t\geq 0}$ at time t. $(\mathbf{W}_b(t))_{t\geq 0}$ is a d-dimensional backward in time Wiener process (as opposed to $(\mathbf{W}_f(t))_{t\geq 0}$). $(\mathbf{W}_b(t))_{t\geq 0}$ has the same properties as $(\mathbf{W}_f(t))_{t\geq 0}$, except of the fact that $\mathbf{W}_b(t)$ is independent of of all $\mathbf{X}(s)$ with $s \geq t$. Note that the starting point of the backward equation has to be the endpoint of the forward solution and depends thus on randomness, denoted by

the dependence on ω. The time horizon is given by T, which must be a sufficiently large parameter. Furthermore, equation (3.12) is once more just a formal notation for the following stochastic integral equation:

$$\mathbf{X}(t) = \mathbf{x}_T - \int_t^T \mathbf{b}^*(\mathbf{X}(s), s)\,\mathrm{d}s - \sqrt{2\,\nu}\int_t^T \mathrm{d}\mathbf{W}_b(s) \tag{3.13}$$

Conditions for the existence and uniqueness to the solution of such a backward SDE are formulated in the same way as for forward SDEs, and, for instance, are presented and proven by Peng [1993].

Analogously to the mean-forward derivative, one can show that the mean-backward derivative is given by the drift term of the backward equation, i.e. $D^*\mathbf{X}(t) = \mathbf{b}^*(\mathbf{X}(t), t)$. Indeed, the two Wiener processes are equivalent, but not equal [Nelson, 1988], and one can determine the following relation:

Corollary 3.2 *Suppose the process* $\mathbf{X}(t)$ *to be the solution of equations (3.1) and (3.12), then*

$$\mathbf{W}_b(t_1) - \mathbf{W}_b(t_0) = \frac{1}{\sqrt{2\,\nu}}\int_{t_0}^{t_1}\Big(\mathbf{b}(\mathbf{X}(t), t) - \mathbf{b}^*(\mathbf{X}(t), t)\Big)\mathrm{d}t + \mathbf{W}_f(t_1) - \mathbf{W}_f(t_0) \tag{3.14}$$

is fulfilled for all $t_1 \geq t_0 \geq 0$ *[Nelson, 1988].*

A more detailed analysis of these processes is in order, and will be presented in a way analogous to the original work by Nelson [1966]. For additional insights beyond the aspects summarized below, see references [Nelson, 1985, 1988, 2001]. Note that $(\mathbf{x}(t), t)$ will be replaced by its shorter form $(\mathbf{x}, t)$ for ease of notation.

The probability density $p(\mathbf{x}, t)$ of the process $(\mathbf{X}(t))_{t\geq 0}$ satisfies the forward Fokker-Planck equation,

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = -\nabla\cdot\Big(\mathbf{b}(\mathbf{x}, t)\,p(\mathbf{x}, t)\Big) + \nu\Delta p(\mathbf{x}, t) \quad , \tag{3.15}$$

and the backward Fokker-Planck equation,

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = -\nabla\cdot\Big(\mathbf{b}^*(\mathbf{x}, t)\,p(\mathbf{x}, t)\Big) - \nu\Delta p(\mathbf{x}, t) \quad . \tag{3.16}$$

Let the *current velocity* $\mathbf{v}(\mathbf{x}, t)$ be defined by

$$\mathbf{v}(\mathbf{x}, t) := \tfrac{1}{2}\Big(\mathbf{b}(\mathbf{x}, t) - \mathbf{b}^*(\mathbf{x}, t)\Big) \quad , \tag{3.17}$$

then the average of the two Fokker-Planck equations yields the equation of continuity,

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = -\nabla \cdot \Big(\mathbf{v}(\mathbf{x},t)\, p(\mathbf{x},t)\Big) \quad . \tag{3.18}$$

Theorem 3.3 *Suppose that* $\mathbf{X}(t)$ *and* $\mathbf{Y}(t)$ *are stochastic processes of the discussed type with respect to the same families of* σ*-algebras and that* $D\mathbf{X}(t)$*,* $D^*\mathbf{X}(t)$*,* $D\mathbf{Y}(t)$*,* $D^*\mathbf{X}(t)$ *are square integrable, continuous functions of* t*. Then,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{E}\left[\mathbf{X}(t)\,\mathbf{Y}(t)\right] = \mathrm{E}\left[D\mathbf{X}(t)\cdot\mathbf{Y}(t)\right] + \mathrm{E}\left[\mathbf{X}(t)\cdot D^*\mathbf{Y}(t)\right] \tag{3.19}$$

holds [Nelson, 2001].

Using an Itô formula, one can show that the mean-forward and mean-backward derivative of a function depending on the process $\mathbf{X}(t)$ are given by [Nelson, 1966, 2001]

$$Df(\mathbf{X}(t),t)) = \left(\frac{\partial}{\partial t} + \mathbf{b}\cdot\nabla + \nu\Delta\right) f(\mathbf{X}(t),t)) \tag{3.20}$$

$$D^*f(\mathbf{X}(t),t)) = \left(\frac{\partial}{\partial t} + \mathbf{b}^*\cdot\nabla - \nu\Delta\right) f(\mathbf{X}(t),t)) \quad . \tag{3.21}$$

If the smooth functions f and g have a compact support in time[1], then Theorem 3.3 shows that

$$\int_{-\infty}^{\infty} \mathrm{E}\Big[Df(\mathbf{X}(t),t))\cdot g(\mathbf{X}(t),t))\Big]\mathrm{d}t = -\int_{-\infty}^{\infty} \mathrm{E}\Big[f(\mathbf{X}(t),t))\cdot D^*g(\mathbf{X}(t),t))\Big]\mathrm{d}t \quad , \tag{3.22}$$

or, equivalently [Nelson, 2001],

$$\begin{aligned}&\int_{-\infty}^{\infty}\int_{\mathbb{R}^d}\left(\frac{\partial}{\partial t} + \mathbf{b}\cdot\nabla + \nu\Delta\right) f(\mathbf{x},t)\cdot g(\mathbf{x},t)\, p(\mathbf{x},t)\mathrm{d}\mathbf{x}\,\mathrm{d}t \\ &= -\int_{-\infty}^{\infty}\int_{\mathbb{R}^d} f(\mathbf{x},t)\cdot\left(\frac{\partial}{\partial t} + \mathbf{b}^*\cdot\nabla - \nu\Delta\right) g(\mathbf{x},t)\cdot p(\mathbf{x},t)\mathrm{d}\mathbf{x}\,\mathrm{d}t \quad .\end{aligned} \tag{3.23}$$

For A being a partial differential operator, let $A^\dagger$ be its (Lagrange) adjoint with respect to the Lebesque measure on $\mathbb{R}^d$, and let A^* be the adjoint operator of A. Then,

$$\int_{-\infty}^{\infty}\int_{\mathbb{R}^d}\Big(Af(\mathbf{x},t)\Big)\, g(\mathbf{x},t)\, p(\mathbf{x},t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

[1] A smooth function with a compact support is a special continuous function that assumes only the value 0 outside of the support.

equals both

$$\int_{-\infty}^{\infty}\int_{\mathbb{R}^d} f(\mathbf{x},t)\, A^{\dagger}\Big(g(\mathbf{x},t)\, p(\mathbf{x},t)\Big)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

and

$$\int_{-\infty}^{\infty}\int_{\mathbb{R}^d} f(\mathbf{x},t)\,\Big(A^{*}g(\mathbf{x},t)\Big)\, p(\mathbf{x},t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t \quad ,$$

resulting in $A^{*} = p^{-1}A\,p$ [Nelson, 2001]. Consider

$$A^{\dagger} = \left(\frac{\partial}{\partial t} + \mathbf{b}\cdot\nabla + \nu\Delta\right)^{\dagger} = -\frac{\partial}{\partial t} - \mathbf{b}\cdot\nabla - \nabla\cdot + \nu\,\Delta \quad ,$$

then

$$\begin{aligned} -p^{-1}(\mathbf{x},t)\frac{\partial p(\mathbf{x},t)}{\partial t} &= \frac{\nabla\cdot(\mathbf{b}(\mathbf{x},\mathbf{t})\,p(\mathbf{x},t))}{p(\mathbf{x},t)} - \nu\frac{\Delta p(\mathbf{x},t)}{p(\mathbf{x},t)} \\ &= \nabla\cdot\mathbf{b}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t)\cdot\frac{\nabla p(\mathbf{x},t)}{p(\mathbf{x},t)} - \nu\frac{\Delta p(\mathbf{x},t)}{p(\mathbf{x},t)} \end{aligned} \tag{3.24}$$

holds, where the above mentioned relation (equation (3.23)) and the forward Fokker-Planck equation are used [Nelson, 2001]. Inserting this relation in equation (3.23), one gets

$$-\frac{\partial}{\partial t} - \mathbf{b}^{*}(\mathbf{x},t)\cdot\nabla + \nu\Delta = -\frac{\partial}{\partial t} - \mathbf{b}(\mathbf{x},t)\cdot\nabla + 2\nu\frac{\nabla p(\mathbf{x},t)}{p(\mathbf{x},t)}\cdot\nabla + \nu\Delta \quad . \tag{3.25}$$

Defining

$$\mathbf{u}(\mathbf{x},t) := \tfrac{1}{2}\Big(\mathbf{b}(\mathbf{x},t) - \mathbf{b}^{*}(\mathbf{x},t)\Big) \quad , \tag{3.26}$$

one finally concludes that

$$\mathbf{u}(\mathbf{x},t) = \nu\,\frac{\nabla p(\mathbf{x},t)}{p(\mathbf{x},t)} \quad . \tag{3.27}$$

Since $\mathbf{u}(\mathbf{x},t)$ is the velocity acquired by the Brownian particle in equilibrium with an external force to balance the osmotic force, $\mathbf{u}$ is called *osmotic velocity* [Nelson, 1966]. Using the continuity equation (3.18), the partial time derivative of the osmotic velocity reads

$$\begin{aligned} \nu\,\frac{\partial}{\partial t}\Big[\ln\nabla p(\mathbf{x},t)\Big] &\overset{3.18}{=} \nu\,\nabla\left(\frac{\dot{p}(\mathbf{x},t)}{p(\mathbf{x},t)}\right) \\ &\overset{(3.18)}{=} -\nu\,\nabla\left(\frac{p(\mathbf{x},t)\,\nabla\cdot\mathbf{v}(\mathbf{x},t) + \mathbf{v}(\mathbf{x},t)\cdot\nabla p(\mathbf{x},t)}{p(\mathbf{x},t)}\right) \\ \Rightarrow \quad \frac{\partial\mathbf{u}(\mathbf{x},t)}{\partial t} &\overset{3.18}{=} -\nu\nabla\Big(\nabla\cdot\mathbf{v}(\mathbf{x},t)\Big) - \nabla\Big(\mathbf{v}(\mathbf{x},t)\cdot\mathbf{u}(\mathbf{x},t)\Big) \quad . \end{aligned} \tag{3.28}$$

Using equation (3.20) and (3.21), the mean acceleration, defined in equation (3.10), is given by

$$\begin{aligned}\mathbf{a}(\mathbf{x},t) &= \tfrac{1}{2}D\mathbf{b}^*(\mathbf{x},t) \,+\, \tfrac{1}{2}D^*\mathbf{b}(\mathbf{x},t) \\ &= \frac{1}{2}\left[\frac{\partial \mathbf{b}^*(\mathbf{x},t)}{\partial t} \,+\, (\mathbf{b}(\mathbf{x},t)\cdot\nabla)\mathbf{b}^*(\mathbf{x},t) \,+\, \nu\,\Delta\mathbf{b}^*(\mathbf{x},t)\right] \\ &\quad + \frac{1}{2}\left[\frac{\partial \mathbf{b}(\mathbf{x},t)}{\partial t} \,+\, (\mathbf{b}^*(\mathbf{x},t)\cdot\nabla)\mathbf{b}(\mathbf{x},t) \,-\, \nu\,\Delta\mathbf{b}(\mathbf{x},t)\right] \\ &= \frac{\partial \mathbf{v}(\mathbf{x},t)}{\partial t} \,-\, \nu\Delta\mathbf{u}(\mathbf{x},t) \,+\, \Big(\mathbf{v}(\mathbf{x},t)\cdot\nabla\Big)\mathbf{v}(\mathbf{x},t) \,-\, \Big(\mathbf{u}(\mathbf{x},t)\cdot\nabla\Big)\mathbf{u}(\mathbf{x},t) \quad .\end{aligned} \tag{3.29}$$

Since macroscopic particles follow a deterministic Newton equation, the diffusion coefficient has to be inversely proportional to the mass m of the particle, and Nelson [1966] concluded that

$$\nu = \frac{\hbar}{2m} \quad . \tag{3.30}$$

The constant $\hbar = {}^{h}/_{2\pi}$ is the reduced Planck's constant and denotes a quantum of action. Furthermore, suppose the particle being influenced by an external force, then the dynamical assumption, $\mathbf{F} = m\,\mathbf{a}$, is made, where the mean acceleration $\mathbf{a}$ is given by equation (3.10). This situation agrees with the assumption made in the Ornstein-Uhlenbeck theory of Brownian motion with friction. Since the mean acceleration equals the classical acceleration, given of course that $\mathbf{x}(t)$ is two times continuously differentiable, the above treatment can be understood as a stochastic extension to Newton's law for classical particles.

Consider also the case that the external force is derived from a potential, i.e. $\mathbf{F}(\mathbf{x},t) = -\nabla V(\mathbf{x},t)$. Then the particle follows a Markov process in the coordinate space characterized by the forward and backward SDE's

$$\begin{cases} \mathrm{d}\mathbf{X}(t) & = [\mathbf{v}(\mathbf{X}(t),t) \,+\, \mathbf{u}(\mathbf{X}(t),t)]\,\mathrm{d}t \,+\, \sqrt{\frac{\hbar}{m}}\,\mathrm{d}\mathbf{W}_f(t) \\ \mathbf{X}(t=0) & = \mathbf{x}_0 \in \mathbb{R}^d \end{cases} , \tag{3.31}$$

$$\begin{cases} \mathrm{d}\mathbf{X}(t) & = [\mathbf{v}(\mathbf{X}(t),t) \,-\, \mathbf{u}(\mathbf{X}(t),t)]\,\mathrm{d}t \,+\, \sqrt{\frac{\hbar}{m}}\,\mathrm{d}\mathbf{W}_b(t) \\ \mathbf{X}(t=T) & = \mathbf{x}_T(\omega) \end{cases} . \tag{3.32}$$

The velocities are given by non-linear partial differential equations (PDEs), namely

$$\begin{aligned}\frac{\partial \mathbf{v}(\mathbf{x},t)}{\partial t} &= \frac{\mathbf{F}(\mathbf{x},t)}{m} + \frac{\hbar}{2m}\Delta\mathbf{u}(\mathbf{x},t) - \Big(\mathbf{v}(\mathbf{x},t)\cdot\nabla\Big)\mathbf{v}(\mathbf{x},t) + \Big(\mathbf{u}(\mathbf{x},t)\cdot\nabla\Big)\mathbf{u}(\mathbf{x},t) \\ &= -\frac{\nabla V(\mathbf{x},t)}{m} + \frac{\hbar}{2m}\Delta\mathbf{u}(\mathbf{x},t) - \Big(\mathbf{v}(\mathbf{x},t)\cdot\nabla\Big)\mathbf{v}(\mathbf{x},t) \\ &\quad + \Big(\mathbf{u}(\mathbf{x},t)\cdot\nabla\Big)\mathbf{u}(\mathbf{x},t) \quad , \qquad (3.33)\end{aligned}$$

$$\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = -\frac{\hbar}{2m}\nabla\Big(\nabla\cdot\mathbf{v}(\mathbf{x},t)\Big) - \nabla\Big(\mathbf{v}(\mathbf{x},t)\cdot\mathbf{u}(\mathbf{x},t)\Big) \quad . \qquad (3.34)$$

If the current and osmotic velocity are known from the beginning, and the Cauchy problem for these coupled non-linear PDEs can be solved for all $\mathbf{x}$, then the process will be completely known [Nelson, 1966].

As seen before, the osmotic velocity is a gradient, meaning that

$$\mathbf{u}(\mathbf{x},t) = \tfrac{\hbar}{m}\nabla R(\mathbf{x},t) \quad . \qquad (3.35)$$

Let the current velocity also be given by the gradient of a scalar function, i.e.

$$\mathbf{v}(\mathbf{x},t) = \tfrac{1}{m}\nabla S(\mathbf{x},t) \quad . \qquad (3.36)$$

Then, equation (3.33) and (3.34) convert into

$$\nabla\left(\frac{\partial S}{\partial t}\right) = \nabla\left(-V - \frac{1}{2m}(\nabla S)\cdot(\nabla S) + \frac{\hbar^2}{2m}(\nabla R)\cdot(\nabla R) + \frac{\hbar^2}{2m}\Delta R\right) \qquad (3.37)$$

$$\nabla\left(\frac{\partial R}{\partial t}\right) = \nabla\left(-\frac{1}{2m}\Delta S - \frac{\hbar}{m}(\nabla R)\cdot(\nabla S)\right) \qquad (3.38)$$

by making use of $\nabla(\mathbf{a}^2) = 2(\nabla\cdot\mathbf{a})\,\mathbf{a}$, which is fulfilled for all rotation-free vectors, $\nabla\times\mathbf{a} = 0$. For the sake of clarity, the position $\mathbf{x}$ and time t have been omitted in the above equations, even though the functions discussed depend on them. Introducing

$$\Psi(\mathbf{x},t) = \mathrm{e}^{R(\mathbf{x},t)+\frac{i}{\hbar}S(\mathbf{x},t)} \quad , \qquad (3.39)$$

equation (3.37) and equation (3.38) are transformed into a linear PDE that in fact equals the Schrödinger equation [Nelson, 1966, 2001], since

$$\mathrm{i}\hbar\left(\frac{\partial R}{\partial t} + \frac{\mathrm{i}}{\hbar}\frac{\partial S}{\partial t}\right) = V - \frac{\hbar^2}{2m}\left(\Delta R + \frac{i}{\hbar}\Delta S\right) - \frac{\hbar^2}{2m}\left[\left(\nabla R + \frac{i}{\hbar}\nabla S\right)^2\right] \qquad (3.40)$$

$$\Leftrightarrow \quad \mathrm{i}\hbar\frac{\partial\Psi(\mathbf{x},t)}{\partial t} = -\left[\frac{\hbar^2}{2m}\Delta + V(\mathbf{x},t)\right]\Psi(\mathbf{x},t) \quad . \qquad (3.41)$$

Note that this equivalence is only fulfilled for a node-free wave function Ψ; otherwise, R as well as $\mathbf{u}$ will diverge at the nodes of the wave function. The PDEs for the two scalar functions R and S,

$$\frac{\partial S}{\partial t} = -V - \frac{1}{2m}(\nabla S)\cdot(\nabla S) + \frac{\hbar^2}{2m}(\nabla R)\cdot(\nabla R) + \frac{\hbar^2}{2m}\Delta R \tag{3.42}$$

$$\frac{\partial R}{\partial t} = -\frac{1}{2m}\Delta S - \frac{\hbar}{m}(\nabla R)\cdot(\nabla S) \quad , \tag{3.43}$$

are Madelung equations [Madelung, 1927]. Equation (3.42) is also very similar to the Hamilton-Jacobi equation in classical mechanics and corresponds to the hydrodynamic equation of vortex-free flow with an external force field [Madelung, 1927]. To be more specific, it is the quantum-mechanical counterpart to the classical Hamilton-Jacobi equation. The additional term depends on the strength of the stochastic forces and goes to zero for $\nu \to 0$ [Paul and Baschnagel, 2013]. Equation (3.43) matches a hydrodynamic continuity equation [Madelung, 1927] and is another form of equation (3.18).

In summary, for each solution of the Schrödinger equation there is a Markov process characterized by two velocities. The probability density of the process – fulfilling both the forward and backward Fokker-Planck equation – equals the quantum-mechanical density given by the square of the absolute value of $\Psi(\mathbf{x}, t)$. For all quantum-mechanical observables defined by self-adjoined operators on the Hilbert space, an associated stochastic process can be defined. Nonetheless, the reverse statement does not hold in general [Paul and Baschnagel, 2013].

The expectation value of a quantum-mechanical observable $\mathbf{O}(\mathbf{x}, t)$ is given by

$$\begin{aligned}\langle\Psi|\mathbf{O}(\mathbf{x},t)|\Psi\rangle &= \int_{\mathbb{R}^d} \mathbf{O}(\mathbf{x},t)\,|\Psi(\mathbf{x},t)|^2\,\mathrm{d}\mathbf{x} = \int_{\mathbb{R}^d} \mathbf{O}(\mathbf{x},t)\,p(\mathbf{x},t)\,\mathrm{d}\mathbf{x} \\ &= \mathrm{E}[\mathbf{O}(\mathbf{X}(t),t)] \quad ,\end{aligned} \tag{3.44}$$

which is the definition of the expectation value of a stochastic variable, too. For operators like the momentum operator $\hat{\mathbf{p}} = -\mathrm{i}\hbar\nabla$, and also functions of them, the situation is somewhat different. Still, one can easily check that the expectation value

of the momentum operator equals the expectation value of the current velocity, i.e.

$$\begin{aligned}\frac{1}{m}\langle\Psi|\,\hat{\mathbf{p}}\,|\Psi\rangle &= \frac{1}{m}\int_{\mathbb{R}^d}\Psi^*(\mathbf{x},t)\,(-\mathrm{i}\hbar\,\nabla)\Psi(\mathbf{x},t)\,\mathrm{d}^3\mathbf{x}\\ &= \int_{\mathbb{R}^d}\Psi^*(\mathbf{x},t)\,\left(-\frac{\mathrm{i}\hbar}{m}\,\nabla R(\mathbf{x},t)\,+\,\frac{1}{m}\,\nabla S(\mathbf{x},t)\right)\Psi(\mathbf{x},t)\;\mathrm{d}^3\mathbf{x}\\ &= -\,\mathrm{i}\,\mathrm{E}[\mathbf{u}]+\mathrm{E}[\mathbf{v}]=\;\mathrm{E}[\mathbf{v}]\quad ,\end{aligned}\tag{3.45}$$

since

$$\mathrm{E}[\mathbf{u}]=\;\frac{\hbar}{2m}\int_{\mathbb{R}^d}\frac{\nabla p(\mathbf{x},t)}{p(\mathbf{x},t)}\,p(\mathbf{x},t)\,\mathrm{d}^3\mathbf{x}=\;\frac{\hbar}{2m}\int_{\mathbb{R}^d}\nabla p(\mathbf{x},t)\,\mathrm{d}^3\mathbf{x}=0\quad .\tag{3.46}$$

However, the osmotic velocity is of physical significance, noting that the second moment contributes to the kinetic energy of the particle [Nelson, 1988]. The total energy, in turn, is given by

$$E_{\mathrm{tot}}=\;\frac{m}{2}\mathbf{v}^2(\mathbf{x},t)\,+\,\frac{m}{2}\mathbf{u}^2(\mathbf{x},t)\,+\,V(\mathbf{x},t)\quad ,\tag{3.47}$$

and the conservation of energy can be expressed in term of [Paul and Baschnagel, 2013]

$$\left(\frac{\partial}{\partial t}\,+\,\mathbf{v}(\mathbf{x},t)\cdot\nabla\right)E_{\mathrm{tot}}=\,0\quad .\tag{3.48}$$

The stochastic, path-oriented picture of quantum systems allows the definition of those observables that are not accessible in the standard description of quantum systems. For example, tunneling processes can be described in a natural way in stochastic mechanics, as will be presented in the next section.

Remark 3.4 *Indeed, one can easily check that the solutions of equation (3.31) and (3.32) are given by the same process. Suppose* $(\mathbf{X}(t))_{t\geq[0,T]}$ *being the solution of the forward equation (3.31), i.e.*

$$\mathbf{X}(t)=\,\mathbf{x}_0\,+\int_0^t\left[\mathbf{v}(\mathbf{X}(s),s)\,+\,\mathbf{u}(\mathbf{X}(s),s)\right]\mathrm{d}s\,+\,\sqrt{\frac{\hbar}{m}}\int_0^t\mathrm{d}\mathbf{W}_f(s)\quad ,\tag{3.49}$$

and $(\mathbf{Y}(t))_{t\geq[0,T]}$ *being the solution of the backward equation (3.32), i.e.*

$$\mathbf{Y}(t)=\,\mathbf{x}_T(\omega)\,-\int_t^T\left[\mathbf{v}(\mathbf{X}(s),s)\,-\,\mathbf{u}(\mathbf{X}(s),s)\right]\mathrm{d}s\,-\,\sqrt{\frac{\hbar}{m}}\int_t^T\mathrm{d}\mathbf{W}_b(s)\quad ,\tag{3.50}$$

where $\mathbf{x}_T(\omega)=\mathbf{X}(t=T)$ *is the end point of the forward process. Then, the backward*

process reads

$$\begin{aligned}\mathbf{Y}(t) = \mathbf{x}_0 &+ \int_0^T [\mathbf{v}(\mathbf{X}(s),s) + \mathbf{u}(\mathbf{X}(s),s)]\,\mathrm{d}s + \sqrt{\frac{\hbar}{m}}\int_0^T \mathrm{d}\mathbf{W}_f(s) \\ &- \int_t^T [\mathbf{v}(\mathbf{X}(s),s) - \mathbf{u}(\mathbf{X}(s),s)]\,\mathrm{d}s - \sqrt{\frac{\hbar}{m}}\int_t^T \mathrm{d}\mathbf{W}_b(s) \\ = \mathbf{x}_0 &+ \int_0^t [\mathbf{v}(\mathbf{X}(s),s) + \mathbf{u}(\mathbf{X}(s),s)]\,\mathrm{d}s + \sqrt{\frac{\hbar}{m}}\int_0^T \mathrm{d}\mathbf{W}_f(s) \\ &+ 2\int_t^T \mathbf{u}(\mathbf{X}(s),s)\mathrm{d}s - \sqrt{\frac{\hbar}{m}}\int_t^T \mathrm{d}\mathbf{W}_b(s) \quad .\end{aligned}$$

Using Corollary 3.2 the backward Wiener process can be expressed in terms of the forward Wiener process, yielding

$$\mathbf{W}_b(T) - \mathbf{W}_b(t) = 2\sqrt{\frac{m}{\hbar}}\int_t^T \mathbf{u}(\mathbf{X}(s),s)\,\mathrm{d}s + \mathbf{W}_f(T) - \mathbf{W}_f(t) \quad ,$$

and

$$\begin{aligned}\mathbf{Y}(t) = \mathbf{x}_0 &+ \int_0^t [\mathbf{v}(\mathbf{X}(s),s) + \mathbf{u}(\mathbf{X}(s),s)]\,\mathrm{d}s + \sqrt{\frac{\hbar}{m}}\int_0^T \mathrm{d}\mathbf{W}_f(s) \\ &+ 2\int_t^T \mathbf{u}(\mathbf{X}(s),s)\,\mathrm{d}s - 2\int_t^T \mathbf{u}(\mathbf{X}(s),s)\,\mathrm{d}s - \sqrt{\frac{\hbar}{m}}\int_t^T \mathrm{d}\mathbf{W}_f(s) \\ = \mathbf{x}_0 &+ \int_0^t [\mathbf{v}(\mathbf{X}(s),s) + \mathbf{u}(\mathbf{X}(s),s)]\,\mathrm{d}s + \sqrt{\frac{\hbar}{m}}\int_0^t \mathrm{d}\mathbf{W}_f(s) = \mathbf{X}(t) \quad .\end{aligned}$$

3.2. Tunneling processes in Nelson mechanics

Out of the fundamental effects known from quantum mechanics, tunneling processes are among the most fascinating ones, and serve together with the wave-particle dualism as a prime example illustrating differences between classical and quantum systems. While a classical particle may not pass through a potential barrier V_0 higher than its energy E, the same does not hold for quantum systems. Still, the duration of such processes is a matter of debate, noting that there is no time operator in Hilbert-space theory. In stochastic mechanics, on the opposite, the duration of a process is well defined, thus overcoming shortcomings in the standard approach.

In the following, tunneling will be used to demonstrate the benefit of using stochastic mechanics applied to quantum systems. To address tunneling processes, a one-dimensional double-well potential will be considered[2], see **Figure 3.1**. Due to the symmetry of the

[2]See also Appendix A.7

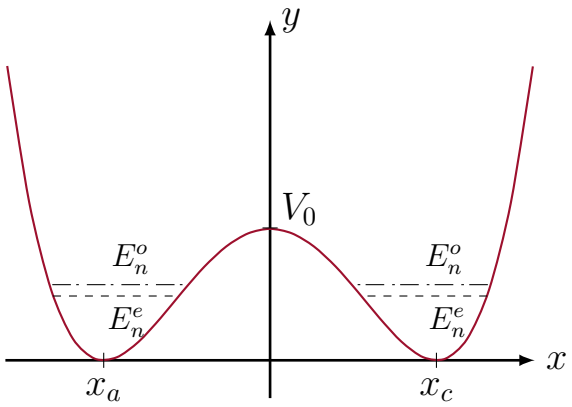

Figure 3.1.: *Sketch of a one-dimensional double-well potential with energy eigenvalues belonging to an even and odd solution to the Schrödinger equation, respectively [Paul and Baschnagel, 2013].*

potential, the wave function of a particle located in this potential has to be either even or odd. Let E_n^e be the energy of the even wave function and let $E_n^o = E_n^e + \Delta E_n$ be the energy of the odd wave function. Since all odd solutions have an additional zero crossing at $x = 0$, an energy splitting $\Delta E_n > 0$ occurs [Paul and Baschnagel, 2013]. The wave functions $\Psi_e(x)$ and $\Psi_o(x)$ of the associated energy values are solutions of the one-dimensional Schrödinger equation,

$$\mathrm{i}\hbar\,\partial_t \Psi(x,t) = \left[-\frac{\hbar^2}{2m}\,\partial_{xx} + V(x)\right]\,\Psi(x,t) \quad . \tag{3.51}$$

The wave functions are stationary and there is no net probability current from one well to the other in these states [Paul and Baschnagel, 2013]. Thus, the relation between tunneling frequency and energy splitting will be derived using the approximation presented in the textbook by Paul and Baschnagel [2013].

The wave function of a particle localized in the right or left well of the double-well potential are denoted by $\Psi_R(x)$ and $\Psi_L(x)$, respectively, with the assumption of $\Psi_R(0) = 0$ and $\Psi'_R(0) = 0$, since $V_0 \gg E$. The even and the odd wave function can be constructed by superposition of $\Psi_L(x)$ and $\Psi_R(x)$, that is,

$$\Psi_e(x) = \frac{1}{\sqrt{2}}\left[\Psi_L(x) + \Psi_R(x)\right] \quad , \quad \Psi_o(x) = \frac{1}{\sqrt{2}}\left[\Psi_R(x) - \Psi_R(x)\right] \quad . \tag{3.52}$$

Considering that the particle is localized on the right-hand side of the wall ($x > 0$) at time $t = 0$, i.e., $\Psi(x,0) = \Psi_R(x)$, the evolution of the wave function is expressed as

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\,\mathrm{e}^{-\frac{\mathrm{i}E_n^e t}{\hbar}}\left[\Psi_e(x) + \mathrm{e}^{-\frac{\mathrm{i}\Delta E_n t}{\hbar}}\,\Psi_o(x)\right] \quad . \tag{3.53}$$

For $\mathrm{e}^{-\frac{\mathrm{i}\Delta E_n t}{\hbar}} = -1$, the particle will be on the left-handed side of the barrier, so that the tunneling period,

$$\tau_n = \frac{\pi\hbar}{\Delta E_n} \quad , \tag{3.54}$$

is characterized by the energy difference between the even and the odd state. It is noted that the eigenvalues of the Schrödinger equation can often only be determined approximately, e.g. by making use of the WKB-approximation (see for example the textbook by Landau and Lifschitz [1979] or the Appendix, section A.6). This situation is opposed to conservative diffusion processes, whose duration can be determined directly. The average time needed by a particle to go from a position x to another position x_c located on the opposite side of the barrier, is characteristic of the tunneling period, and referred to as the mean first passage time. This aspect will be discussed in the following for a stationary one-dimensional Fokker-Planck equation.

Suppose the motion of the particle being described by

$$\mathrm{d}X(t) = b(X(t))\,\mathrm{d}t + \sigma(X(t))\,\mathrm{d}W_f(t) \quad , \tag{3.55}$$

where the conditional probability density for the transition from $(x, 0)$ to (x', t) is given by the stationary[3] forward Fokker-Planck equation (equation (2.23)),

$$p(x', t; x, 0) = -\frac{\partial}{\partial x'}\left[b(x')\,p(x', t; x, 0)\right] + \frac{1}{2}\frac{\partial^2}{\partial x'^2}\left[\sigma^2(x')\,p(x', t; x, 0)\right] \quad . \tag{3.56}$$

To determine the mean first passage time, knowledge of the distribution of first passage times is required. Given that the particle starts at $x \in (-\infty, x_c)$ at $t = 0$, the probability that the particle is still in the same interval for times $t > 0$ is [Paul and Baschnagel, 2013]

$$G(x, t) = \int_{-\infty}^{x_C} p(x', t; x, 0)\,\mathrm{d}x' = \int_{-\infty}^{x_C} p(x', 0; x, -t)\,\mathrm{d}x' \quad . \tag{3.57}$$

At the right-hand side of this equation it is used that the actual time may be shifted by an arbitrary Δt, chosen here as $\Delta t = -t$. The function $G(x, t)$ characterizes also the probability that the first passage time τ_{x_c} of the particle going from x to x_c is larger than t, i.e. [Paul and Baschnagel, 2013]

$$G(x, t) = P(\tau_{x_c} \geq t) = \int_t^\infty p_{\mathrm{fpt}}(\tau_{x_c})\,\mathrm{d}\tau_{x_c} \quad , \tag{3.58}$$

where $p_{\mathrm{fpt}}(\tau_{x_c})$ is the desired density of the first passage times. Equation (3.56) and (3.57) show that $p_{\mathrm{fpt}}(\tau_{x_c})$ depends on the initial state of the Brownian particle. Therefore,

[3] The drift and diffusion coefficient are *not* explicitly time-dependent.

also the backward Fokker-Planck equation (equation (2.24)),

$$\frac{\partial}{\partial t}p(x',t';x,t) = -b(x)\,\frac{\partial}{\partial x}p(x',t';x,t) - \frac{1}{2}\,\sigma^2(x)\,\frac{\partial^2}{\partial x^2}p(x',t';x,t) \quad , \tag{3.59}$$

needs to be considered. The studied first passage time problem $p(x',t';x,t)$ is also related to the following boundary conditions [Paul and Baschnagel, 2013]:

1. Absorbing boundary at $x = x_c$: $\quad p(x',t';x_c,0) = 0.$

2. Reflecting boundary for $x \to -\infty$: $\quad \frac{\partial}{\partial x}p(x',t';x,0) \overset{x\to-\infty}{\longrightarrow} 0.$

Determining the partial time derivative of $G(x,t)$ and inserting equation (3.56) into (3.57) yields

$$\begin{aligned}
\frac{\partial G(x,t)}{\partial t} &= \frac{\partial}{\partial t}\left[\int_{-\infty}^{x_c} p(x',0;x,-t)\,\mathrm{d}x'\right] = \int_{-\infty}^{x_c}\frac{\partial}{\partial t}\,p(x',0;x,-t)\,\mathrm{d}x' \\
&= \int_{-\infty}^{x_c}\left[b(x)\,\frac{\partial}{\partial x}p(x',0;x,-t) + \frac{1}{2}\,\sigma^2(x)\,\frac{\partial^2}{\partial x^2}p(x',0;x,-t)\right]\mathrm{d}x' \\
&= \left[b(x)\,\frac{\partial}{\partial x} + \frac{1}{2}\,\sigma^2(x)\,\frac{\partial^2}{\partial x^2}\right]\int_{-\infty}^{x_c} p(x',0;x,-t)\,\mathrm{d}x' \\
&= \left[b(x)\,\frac{\partial}{\partial x} + \frac{1}{2}\,\sigma^2(x)\,\frac{\partial^2}{\partial x^2}\right] G(x,t) \quad .
\end{aligned} \tag{3.60}$$

Furthermore, $G(x,t)$ is subject to the following boundary conditions [Paul and Baschnagel, 2013]:

$$G(x,0) = \begin{cases} 1\,, & x \le x_c \\ 0\,, & x > x_c \end{cases} \quad , \quad G(x_c,t) = 0 \quad , \quad \lim_{x\to-\infty}\frac{\partial G(x,t)}{\partial x} = 0 \quad . \tag{3.61}$$

Since $G(x,t)$ is the complement of the cumulative probability distribution of first passage times, the expectation value of an arbitrary function $f(\tau_{x_c})$ is given by

$$\mathrm{E}\left[f(\tau_{x_c})\right] = -\int_0^\infty f(t)\,\frac{\partial G(x,t)}{\partial t}\,\mathrm{d}t \quad . \tag{3.62}$$

Consequently, the mean first passage time from x to x_c reads

$$\tau_{\mathrm{mfpt}}(x;x_c) = \mathrm{E}[\tau_{x_c}] = -\int_0^\infty t\,\frac{\partial G(x,t)}{\partial t}\,\mathrm{d}t = \int_0^\infty G(x,t)\,\mathrm{d}t \quad , \tag{3.63}$$

where the last term is determined using integration by parts. In addition, an ordinary differential equation can be derived for the mean first passage time. For this purpose,

equation (3.60) is integrated over time from zero to infinity, which yields

$$\int_0^\infty \frac{\partial G(x,t)}{\partial t}\,\mathrm{d}t = -1 = b(x)\,\frac{\mathrm{d}\tau_{\mathrm{mfpt}}(x)}{\mathrm{d}x} + \frac{\sigma^2(x)}{2}\,\frac{\mathrm{d}^2\tau_{\mathrm{mfpt}}(x)}{\mathrm{d}x^2} \tag{3.64}$$

for all $x \leq x_c$, noting that the boundary conditions

$$\tau_{\mathrm{mfpt}}(x_c) = 0 \quad , \quad \lim_{x\to\infty} \frac{\mathrm{d}\tau_{\mathrm{mfpt}}(x)}{\mathrm{d}x} = 0 \tag{3.65}$$

have to be fulfilled. The first derivative of the general solution of this equation is given by [Paul and Baschnagel, 2013]

$$\begin{aligned}\tau'_{\mathrm{mfpt}}(x) = \bar{\tau}_0 \exp\left[-\int_{-\infty}^{x} \frac{2\,b(x')}{\sigma^2(x')}\,\mathrm{d}x'\right] \\ - 2\exp\left[-\int_{-\infty}^{x} \frac{2\,b(x')}{\sigma^2(x')}\,\mathrm{d}x'\right] \cdot \int_{-\infty}^{x} \frac{1}{\sigma^2(x')} \exp\left[\int_{-\infty}^{x'} \frac{2\,b(x'')}{\sigma^2(x'')}\,\mathrm{d}x''\right]\mathrm{d}x' \quad .\end{aligned} \tag{3.66}$$

Since $\tau'_{\mathrm{mfpt}}(x)$ has to vanish for $x \to -\infty$, only the particular solution remains [Paul and Baschnagel, 2013]. Using $\tau_{\mathrm{mfpt}}(x_c) = 0$ and the abbreviation

$$\phi(x) = \exp\left[\int_{-\infty}^{x} \frac{2\,b(x')}{\sigma^2(x')}\,\mathrm{d}x'\right] \quad , \tag{3.67}$$

the mean first passage time finally reads

$$\tau_{\mathrm{mfpt}}(x) = 2\int_x^{x_c} \phi^{-1}(x) \int_{-\infty}^{x'} \frac{\phi(x'')}{\sigma^2(x'')}\,\mathrm{d}x''\,\mathrm{d}x' \quad . \tag{3.68}$$

Going back to a quantum particle, one has

$$b(x) = \frac{\hbar}{m}\partial_x \ln|\Psi_e(x)| \quad , \quad \sigma^2(x) = \frac{\hbar}{m} \quad , \tag{3.69}$$

and the mean first passage time in the n-th energy state is given by

$$\tau_{\mathrm{mfpt}}(x) = \frac{2m}{\hbar}\int_x^{x_c} \frac{1}{p_n(x')} \int_{-\infty}^{x'} p_n(x'')\,\mathrm{d}x''\mathrm{d}x' \quad , \tag{3.70}$$

where $p_n(x) = |\Psi_n(x)|^2$ denotes the stationary probability density in the n-th energy eigenstate. Thus, the diffusion process quantifies tunneling periods even for stationary systems, with a qualitatively similar behavior to the non-stationary case [Paul and Baschnagel, 2013]. Furthermore, it has been shown that the mean first passage time and the tunneling time (equation (3.54)) are equivalent for a rectangular barrier [Chen and Wang, 1990]. Finally, it is noted that any particle described by a conservative

diffusion process is a classical one, and thus cannot pass a potential barrier higher than the particle's energy. However, due to interactions of the particle with the environment, the particle's energy is not constant but experiences fluctuations around the mean value. Hence, the particle is driven over the barrier by the omnipresent quantum fluctuations [Paul and Baschnagel, 2013].

3.3. The development of variational principles

Nelson's theory of conservative diffusion processes represents the kinematic description of a quantum particle. However, in this context, the question arises whether the Schrödinger equation can also be derived from a stochastic variational principle, according to the original idea of Schrödinger [1926a]. It is well known that there is a close relation between classical mechanics and deterministic control theory, i.e. the Hamilton-Jacobi equation can be understood as a programming equation for an optimal control problem [Guerra and Morato, 1983]. Finding a generalization of Hamilton's principle to the quantum-mechanical case would not only be a methodical advantage, but, basically, also worthwhile for physical interpretations.

Being one of the first, Yasue [1980] described the original variational problem of Schrödinger in the light of stochastic mechanics. Starting from a stationary diffusion process $\mathbf{X}(t)$ described by

$$\mathrm{d}\mathbf{X}(t) = \mathbf{u}(\mathbf{X}(t))\,\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\mathrm{d}\mathbf{W}_f(t) \quad , \tag{3.71}$$

he assumed that the process $\mathbf{X}(t)$ (or $\mathbf{u}(\mathbf{X}(t))$) is controlled in such a way that the generalized Newton equation,

$$\frac{m}{2}\,(D\,D^* + D^*\,D)\,\mathbf{X}(t) = -\,\nabla_{\mathbf{x}}\,V(\mathbf{x})|_{\mathbf{x}=\mathbf{X}(t)} \quad , \tag{3.72}$$

is fulfilled. However, this means that for every potential $V(\mathbf{x})$ there exists one stochastic control problem given by equation (3.71), fulfilling the condition defined in equation (3.72) and yielding the solution $\mathbf{b}(\mathbf{x})$. Furthermore, Yasue [1980] showed that this condition is equivalent to the assumption that the cost function

$$\mathrm{E}\left[\overline{\lim_{T\to\infty}}\;T^{-1}\int_0^T\left\{\tfrac{m}{2}|D\mathbf{X}(t)|^2 + V(\mathbf{X}(t)) - E\right\}\mathrm{d}t\right] \tag{3.73}$$

becomes extremal for $\mathbf{b}(\mathbf{x})$, and that the solution is given by the osmotic velocity, such that $\mathbf{b}(\mathbf{x}) = \mathbf{u}(\mathbf{x})$. This stochastic variational problem can be interpreted as a generalization of the energy minimization in classical mechanics and is equivalent to the

stationary Schrödinger equation. In subsequent publications, the relation between, and also equivalence of, the original control problem of Nelson (equations (3.71) and (3.72)), the stationary Schrödinger equation and equation (3.73) has been discussed in more detail [Yasue, 1981a,b]. In particular, the benefits of describing quantum phenomena using this theory have been emphasized [Yasue, 1981b]. Among others, this includes tunneling effects that can be described in a more natural way.

Guerra and Morato [1983] extended the variational problem to the general (non-stationary) case. However, some difficulties arise since the programming equations are in general not time-reversible, which is claimed for quantum systems. This situation can be overcome by making use of a suitable choice of the stochastic action functional [Guerra and Morato, 1983]. Accounting for the Lagrangian function,

$$L(t, \mathbf{x}(t)) = \frac{m}{2}\left(\mathbf{v}^2(\mathbf{x}(t), t) - \mathbf{u}^2(\mathbf{x}(t), t)\right) - V(\mathbf{x}) \quad , \tag{3.74}$$

the stochastic action functional reads [Guerra and Morato, 1983]

$$J(t_0, T; p_0, \mathbf{u}, \mathbf{v}) = \int_{t_0}^{T} \mathrm{E}\left[L(\mathbf{X}(t), t)\right] \mathrm{d}t \quad . \tag{3.75}$$

It is noted that the action functional depends on the initial probability density of the particle's position. The process $\mathbf{X}(t)$ relies on finite-energy diffusion, i.e., equations (3.31) and (3.32) apply. The negative sign of the osmotic-velocity term is of physical significance, noting that $\frac{m}{2}\mathbf{u}^2$ reflects rather a potential than a kinetic contribution, which is in agreement with Schrödinger's variational problem [Guerra and Morato, 1983]. As a consequence, the Lagrangian field can be chosen in such a way that the required quantum-mechanical corrections to the Hamilton-Jacobi equation arise. Furthermore, the gradient form of the current velocity follows directly from the variational principle without further assumptions, as is also the case in the original work by Nelson [1966]. It is worth mentioning that in classical mechanics as well as in the common theory of stochastic optimal control, the variational problems are formulated optimally[4], which is not considered by Guerra and Morato [1983].

Finally, relations between quantum mechanics and classical analytical mechanics were revealed in a coherent way by introducing two variational principles, the saddle points of which yield the osmotic and current velocity [Pavon, 1995b]. Let U be the family of stochastic processes $(\mathbf{z}(t))_{t\in[t_0,T]}$ having a finite energy on $[t_0, T]$ (square integrable),

[4]The desired cost function becomes extremal for the optimal control, instead of stationary ($\delta J = 0$).

i.e., it satisfies [Pavon, 1995b]

$$\mathrm{E}\left[\int_{t_0}^{T} \mathbf{z}(t)\cdot\mathbf{z}(t)\,\mathrm{d}t\right] < \infty \quad . \tag{3.76}$$

The first variational principle is the so-called saddle point action principle, i.e., searching for $\hat{\mathbf{u}}, \hat{\mathbf{v}}$ under the condition

$$J_R(\hat{\mathbf{X}}, \hat{\mathbf{u}}, \hat{\mathbf{v}}) = \min_{\mathbf{v}\in U}\max_{\mathbf{u}\in U} \mathrm{E}\left[\int_{t_0}^{T}\left\{\frac{m}{2}\mathbf{v}^2(t) - \frac{m}{2}\mathbf{u}^2(t) - V(\mathbf{X}(t))\right\}\mathrm{d}t + S_0(\mathbf{X}(t_0))\right] \quad . \tag{3.77}$$

This variational problem is essentially related to that one of Guerra and Morato [1983] and Schrödinger [1926a], but is now formulated optimally ("min-max"-problem) and contains the osmotic velocity as a second optimal control variable. The function $S_0(\mathbf{x})$ is characterized by the initial conditions to the Schrödinger equation. The deterministic part determines the current velocity by minimizing the action functional, while the term containing the background noise maximizes the action functional by the choice of the osmotic velocity. Finally, the saddle point equilibrium solution is given by the motion process $(\mathbf{X}(t))_{t\in[t_0,T]}$ described by equation (3.31) and (3.32). That means, in search of the optimal path, the kinematic equations serve as constraints and extremize the action functional. This situation is reminiscent of classical analytical mechanics. In addition, let X_μ be a family of finite energy diffusion processes. The solution $(\hat{\mathbf{X}}, \hat{\mathbf{u}}, \hat{\mathbf{v}})$ for the stochastic game (equation (3.77)) is given by a triple in $X_\mu \times U \times U$, satisfying the property

$$J_R(\mathbf{X}_1, \mathbf{u}_1, \hat{\mathbf{v}}) \leq J_R(\hat{\mathbf{X}}, \hat{\mathbf{u}}, \hat{\mathbf{v}}) \leq J_R(\mathbf{X}_2, \hat{\mathbf{u}}, \mathbf{v}_2) \tag{3.78}$$

for all $(\mathbf{X}_1, \mathbf{u}_1, \hat{\mathbf{v}})$ and $(\mathbf{X}_2, \hat{\mathbf{u}}, \mathbf{v}_2)$ in $X_\mu \times U \times U$ [Pavon, 1995b].

Suppose that the function $\Lambda(\mathbf{x}, \mathbf{u}, \mathbf{v})$ is a finite constant on $C \subset X_\mu$, where the constraints are fulfilled. Let $(\hat{\mathbf{X}}, \hat{\mathbf{u}}, \hat{\mathbf{v}})$ be the solution of the unconstrained problem $(\Lambda + J_R)(\mathbf{x}, \mathbf{u}, \mathbf{v})$. Then, $(\hat{\mathbf{X}}, \hat{\mathbf{u}}, \hat{\mathbf{v}})$ is also a solution to the original problem. To find the equilibrium solution, one has to find the Lagrangian functional $\Lambda(\mathbf{x}, \mathbf{u}, \mathbf{v})$. Pavon [1995b] showed that

$$\begin{aligned}\Lambda^{F,G}(\mathbf{X}, \mathbf{u}, \mathbf{v}) =& \mathrm{E}\Bigg[\int_{t_0}^{T}\left[\hbar\mathbf{u}\cdot\nabla F + \frac{\hbar}{2}\Delta F - \frac{\partial G}{\partial t} - \mathbf{v}\cdot\nabla G\right](\mathbf{X}(t), t)\mathrm{d}t \\ &+ G(\mathbf{X}(t), t) - G(\mathbf{X}(t_0), t_0)\Bigg] \quad ,\end{aligned} \tag{3.79}$$

where

$$\hat{\mathbf{v}} = \frac{1}{m}\nabla G(\mathbf{x}, t) \quad , \quad \hat{\mathbf{u}} = \frac{\hbar}{m}\nabla F(\mathbf{x}, t) \quad . \tag{3.80}$$

It turns out that the scalar functions $\hat{F} = R$ and $\hat{G} = S$, for which the Lagrangian functional becomes constant on X_μ, are given by equation (3.42), i.e.,

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V(\mathbf{x}) - \frac{\hbar}{2}\left[(\nabla R)^2 + \Delta R\right] = 0 \quad . \tag{3.81}$$

The second variational problem, the saddle point entropy production principle, is given by the following cost function

$$J_I(\mathbf{X}, \mathbf{u}, \mathbf{v}) = \mathrm{E}\left[\int_{t_0}^{T} m\mathbf{v}\cdot\mathbf{u}\,\mathrm{d}t + \hbar R_0(\mathbf{X}(t_0))\right] \quad . \tag{3.82}$$

As before, the function $R_0(\mathbf{x})$ is characterized by the initial conditions to the Schrödinger equation, and the current and osmotic velocity are given by the saddle point of this functional, i.e. $(\hat{\mathbf{X}}, \hat{\mathbf{u}}, \hat{\mathbf{v}}) \in X_\mu \times U \times U$ is the solution of [Pavon, 1995b]

$$J_I(\hat{\mathbf{X}}, \hat{\mathbf{u}}, \hat{\mathbf{v}}) = \max_{\mathbf{v}\in U}\min_{\mathbf{u}\in U} J_I(\mathbf{X}, \mathbf{u}, \mathbf{v}) \quad . \tag{3.83}$$

Based upon a similar approach, Pavon [1995b] derived the Lagrangian functional

$$\begin{aligned}\Xi^{F,G}(\mathbf{x}, \mathbf{u}, \mathbf{v}) = \mathrm{E}\Bigg[\int_{t_0}^{T}\left[-\frac{1}{\hbar}\mathbf{u}\cdot\nabla G - \frac{1}{2m}\Delta G - \frac{\partial F}{\partial t} - \mathbf{v}\cdot\nabla F\right](\mathbf{X}(t), t)\,\mathrm{d}t \\ + F(\mathbf{X}(t), t) - F(\mathbf{X}(t_0), t_0)\Bigg] \quad ,\end{aligned} \tag{3.84}$$

where the solution[5] is characterized by equation (3.43), i.e.,

$$\frac{\partial R}{\partial t} + \frac{1}{m}\nabla R\cdot\nabla S + \frac{1}{2m}\Delta S = 0 \quad , \tag{3.85}$$

and

$$\hat{\mathbf{v}} = \frac{1}{m}\nabla G(\mathbf{x}, t) \quad , \quad \hat{\mathbf{u}} = \frac{\hbar}{m}\nabla F(\mathbf{x}, t) \quad . \tag{3.86}$$

It is worth noting that both stochastic games have to be solved simultaneously in order to find a unique solution for the two velocities and the associated optimal path.

[5]The functions F and G for which the Lagrangian functional becomes finite and constant under the given constraints

Finally, Pavon [1995b] combined both stochastic games in one (complex-valued) variational problem, known as the quantum Hamilton principle, in which the saddle point action principle and the saddle point entropy production principle are accounted for as the real and imaginary part of the resulting equation. Thus,

$$J(\mathbf{X}, \mathbf{u}, \mathbf{v}) = \mathrm{E}\left[\int_{t_0}^{T} \left\{\frac{m}{2}\left(\mathbf{v} - \mathrm{i}\mathbf{u}\right)^2 - V(\mathbf{X}(t))\right\}\mathrm{d}t + \Phi_0(\mathbf{X}(t_0))\right] \quad , \tag{3.87}$$

where $\Psi(\mathbf{x}, t_0) = \exp\left\{\frac{i}{\hbar}\Phi_0(\mathbf{x})\right\}$. The quantum Hamilton principle can be understood as the generalization of the classical principle to the quantum world, noting that not only the Madelung equations, but also the wave function itself is determined by a variational problem [Pavon, 1995b].

Concluding this section, the presented variational principles ultimately show that quantum mechanics is based upon the same fundamental structure as classical mechanics, and, again, that the wave function can also be derived from a variational principle.

CHAPTER 4

From optimal control theory to the Schrödinger equation

Analogously to classical mechanics, the osmotic velocity $u(x,t)$ and the current velocity $v(x,t)$ are given by the solution to a stochastic optimal control problem [Yasue, 1980, 1981a,b; Guerra and Morato, 1983; Pavon, 1995b, 1996], which can be solved using methods often applied in finance. Finding the Nash equilibrium of a stochastic optimal control problem is the quantum-mechanical counterpart to Hamilton's principle of least action. Two major findings have been derived: (i) based upon this concept, the Madelung equations have been derived, which are equivalent to the Schrödinger equation [Madelung, 1927], and (ii), stochastic Hamilton equations of motion were introduced, which generalize the classical Hamilton equations with respect to the quantum world. These equations can be solved independently from the Schrödinger equation and characterize the dynamics of a quantum system uniquely. Thus, they give a suitable basis for advanced method development so as to derive a complete description of non-relativistic quantum systems in parallel to the standard way. Analyzing stochastic Hamilton equations of motion ultimately opens up new possibilities to study quantum systems. Systems without an exactly solvable Schrödinger equation, such as the double-well potential, could be studied, along with a new numerical approach to the wave function.

Before the mathematical methods are explained, this chapter deals with the derivation and numerical simulation of the stochastic Hamilton equations of motion by solving an optimal control problem. For the sake of clarity, stationary problems will be studied first and will also be discussed for specific physical systems. After that, all methods will be expanded to the general (non-stationary) case, which will be described in the last part of this chapter.

4.1. General statements about stochastic optimal control theory

The theory of stochastic optimal control systems is often applied to different scientific problems, e.g., control strategy for electro-rheological or magneto-rheological dampers [Ying et al., 2003]. Here, damping forces can be adjusted through external electric and magnetic fields, respectively. Another outstanding example in finance is the optimization of the investment policy of pension plans [Devolder et al., 2003]. As a consequence of the broad applicability and high significance, stochastic control problems are often analyzed in mathematics [Hamadène and Lepeltier, 1995; Hamadène, 1998; Baghery and Øksendal, 2007; Øksendal and Sulem, 2009; Grecksch, 2002; Øksendal and Sulem, 2014; Josa-Fombellida and Rincón-Zapatero, 2015].
In this section, the maximum principle for general stochastic games of forward-backward stochastic differential equations (FBSDEs) is explained. Øksendal and Sulem [2014] derived a general formulation for Levy processes including jumps. In the thesis at hand, jump processes are not required, and the mathematical treatment can be somewhat simplified. Notations used in the following are adapted from the work by Øksendal and Sulem.

Let $(\Omega, \mathcal{F}, \{\mathcal{F}\}_{t\geq 0}, P)$ be a filtered complete probability space, where P is a reference probability measure. All following stochastic processes are defined on this space. The controlled forward SDE

$$\mathrm{d}X(t) = b(t, X(t), u(t), \omega)\,\mathrm{d}t + \sigma(t, X(t), u(t), \omega)\,\mathrm{d}W(t)\ , \quad X(0) = x_0 \in \mathbb{R} \tag{4.1}$$

is considered for $t \in [0, T]$ ($T > 0$ is a fixed constant), where $(W(t))_{t\geq 0}$ is a (forward) Wiener process, and $(X(t))_{t\geq 0}$ and $(u(t))_{t\geq 0}$ define the state and control process, respectively. As before, the dependence of the respective functions on ω is used to denote a possible dependence on randomness, meaning that b and σ are stochastic processes. It will also be assumed that $\mathbb{F} = \{\mathcal{F}_t, t \leq 0\}$ is the P-augmentation of the natural filtration associated with the Wiener process $(W(t))_{t\geq 0}$. $u(t) = (u_1(t), u_2(t))$ characterizes the control of the two "players" $i = 1, 2$. Suppose there are two sub-filtrations $\mathcal{E}_t^{(i)} \subseteq \mathcal{F}_t\ , t \in [0, T]$ representing the information available to the player $i = 1, 2$ at time t. Let $\mathcal{A}_i$ be the set of admissible control processes for the player i, contained in the set of $\mathcal{E}_t^{(i)}$-predictable processes for $i = 1, 2$, with values $A_i \subset \mathbb{R}$ and $\mathbb{U} = A_1 \times A_2$ [Øksendal and Sulem, 2014]. It is supposed that the functions $b(t, x, u, \omega)$ and $\sigma(t, x, u, \omega)$ are known functions in such a way that equation (4.1) has a unique solution for each $x_0 \in \mathbb{R}$ and $u \in \mathbb{U}$ [Øksendal and Sulem, 2014]. Next, the associated

controlled backward SDEs (each for one player) are considered to be of the form

$$\begin{cases} \mathrm{d}Y_i(t) = & -g_i(t, X(t), Y_i(t), Z_i(t), u(t), \omega)\mathrm{d}t \; + \; Z_i(t)\mathrm{d}W(t) \quad , \; t \in [0, T] \\ Y_i(T) = & h_i(X(T), \omega) \; , \; i = 1, 2 \end{cases} \quad . \tag{4.2}$$

The functions $g_i(t, x, y, z, u, \omega)$ are known functions for all x, y, z in $\mathbb{R}$, u in $\mathbb{U}$, and $h_i(x, \omega)$ is $\mathcal{F}_T$-measurable for each x in $\mathbb{R}$, such that the BSDEs (equation (4.2)) have a unique solution[1] (Y_i, Z_i) for each $u \in \mathbb{U}$ [Øksendal and Sulem, 2014].
The so called performance function or cost function is defined as

$$J_i(u) := \mathrm{E}\left[\int_0^T f_i(t, X^u(t), u(t), \omega)\mathrm{d}t \; + \; \phi_i(X^u(T), \omega) \; + \; \Psi_i(Y_i^u(0))\right] \quad , \; i = 1, 2 \quad . \tag{4.3}$$

Here, the index u illustrates that the variable (e.g. $X^u(t)$) depends on the control $u = (u_1, u_2)$. The function $f_i(t, X^u(t), u(t))\colon [0, T] \times \mathbb{R} \times \mathbb{U} \to \mathbb{R}$, $\phi_i(x)\colon \mathbb{R} \to \mathbb{R}$ and $\Psi_i(x)\colon \mathbb{R} \to \mathbb{R}$ have to be given in such a way that the integrals and the expectation values are existent [Øksendal and Sulem, 2014]. The functions f_i may, for instance, be profit rates, while $\phi_i(x)$ and $\Psi_i(x)$ represent final and initial costs, respectively. In physics, the integrand of the action (cost) function is usually given by the Lagrangian function.

4.1.1. Non-zero sum case – Finding the Nash equilibrium

Consider that the two optimal controls are sought as the Nash equilibrium [Nash, 1951] of the stochastic game (equation (4.1 – 4.3)), where a Nash equilibrium is a pair $(\hat{u}_1, \hat{u}_2) \in \mathcal{A}_1 \times \mathcal{A}_2$ such that [Øksendal and Sulem, 2014]

$$J_1(u_1, \hat{u}_2) \leq J_1(\hat{u}_1, \hat{u}_2) \quad \text{for all } u_1 \in \mathcal{A}_1 \tag{4.4}$$

$$\text{and} \qquad J_2(\hat{u}_1, u_2) \leq J_2(\hat{u}_1, \hat{u}_2) \quad \text{for all } u_2 \in \mathcal{A}_2 \quad . \tag{4.5}$$

In short, this means that there is no reason for player one to deviate from the control or, so to say, to deviate from the strategy $\hat{u}_1$ as long as player two stays with strategy $\hat{u}_2$. Hence, one can say that a Nash equilibrium is (in some cases) a likely outcome of the game [Øksendal and Sulem, 2014].

To find the Nash equilibrium of the problem, it is useful to define the Hamilton functions

[1] Both $Y(t)$ and $Z(t)$ are defined by the backward SDE.

$$H_i(t, x, y, z, u_1, u_2, \lambda, p, q) \ , \ i = 1, 2,$$

$$\begin{aligned} H_i(t, x, y, z, u_1, u_2, \lambda_i, p_i, q_i) := f_i(t, x, y, z, u_1, u_2) \ + \ \lambda_i \, g_i(t, x, y, z, u_1, u_2) \\ + \ p_i \, b(t, x, u_1, u_2) \ + \ q_i \, \sigma(t, x, u_1, u_2) \quad , \end{aligned} \tag{4.6}$$

where $(\lambda_i(t), p_i(t), q_i(t))$ are so-called adjoint processes, noting that the maximum principle can be used to find the optimal controls [Øksendal and Sulem, 2014]. It should be taken into account that – even though the optimal controls as well as the adjoint processes are functions of the controlled processes $(X(t), Y_i(t), Z_i(t))$ – the variables in the Hamiltonian are considered as being independent from each other. In simple terms, the maximum principle says that the cost functions and the associated Hamilton functions have their Nash equilibrium at the same control $(\hat{u}_1, \hat{u}_2)$, i.e., the mathematical problem can be solved by finding the maximum of the related Hamilton function instead of identifying the function u that extremizes the cost functional. Necessary and sufficient conditions[2], as well as related mathematical proofs, can be found in the work of Øksendal and Sulem [2014].

For the sake of simplicity, the following shortened notation

$$\frac{\partial H_i}{\partial x}(t) = \left.\frac{\partial H_i}{\partial x}\right|_{x=X(t)} (t, x, Y_i(t), Z_i(t), u_1(t), u_2(t), \lambda_i(t), p_i(t), q_i(t)) \tag{4.7}$$

is used for the partial derivative (and, in a similar fashion, for also other variables). Note that the control equations (equation (4.1) and (4.2)) for the player i are characterized by three controlled variables, namely $X(t)$, $Y_i(t)$ and $Z_i(t)$. Hence, there is a related adjoint process $(\lambda_i(t), p_i(t), q_i(t))$ for each of the players i, and the following definition applies [Øksendal and Sulem, 2014]:

Definition 4.1 *The adjoint process $\lambda_i(t)$, which is the adjoint process associated to the backward controlled equation, is given by a forward SDE*

$$\begin{cases} \mathrm{d}\lambda_i(t) &= \frac{\partial H_i}{\partial y}(t) \, \mathrm{d}t \ + \ \frac{\partial H_i}{\partial z}(t) \, \mathrm{d}W(t) \\ &= \lambda_i(t) \left[\frac{\partial g_i}{\partial y}(t) \, \mathrm{d}t \ + \ \frac{\partial g_i}{\partial z}(t) \, \mathrm{d}W(t) \right] \quad , \ t \in [0, T] \ , \\ \lambda_i(0) &= \Psi_i' \left(Y_i(0) \right) \quad . \end{cases} \tag{4.8}$$

$p_i(t)$ and $q_i(t)$, which, are the associated adjoint processes for $X(t), Z_i(t)$, and are

[2]The conditions for the maximum principle can be additionally found in the appendix, cf. section A.2.

defined by a backward SDE,

$$\begin{cases} \mathrm{d}p_i(t) &= -\frac{\partial H_i}{\partial x}(t)\,\mathrm{d}t \,+\, q_i(t)\,\mathrm{d}W(t)\ ,\ t\in[0,T]\ , \\ p_i(T) &= \phi_i'\left(X(T)\right) \,+\, h_i'(X(T))\,\lambda_i(T) \quad , \end{cases} \tag{4.9}$$

where functions with a prime ($'$) are first derivatives.

Starting from the maximum of the Hamilton functions, one ends up with SDEs for the optimal controls $u_1(t)$ and $u_2(t)$ in terms of the adjoint and the state processes.

4.1.2. Zero-sum case

The zero-sum case

$$J_1(u_1,u_2) \,+\, J_2(u_1,u_2) = 0 \tag{4.10}$$

is a special case of the previous discussed stochastic game, where the Nash equilibrium equals the saddle point of $J(u_1,u_2) := J_1(u_1,u_2)$ [Øksendal and Sulem, 2014]. The above equations simplify considerably, and without loss of generality (w.l.o.g.), the optimal controls $\hat{u}_1, \hat{u}_2$ are sought in such a way that

$$J(\hat{u}_1,\hat{u}_2) = \max_{u_1}\min_{u_2} J(u_1,u_2) \quad , \tag{4.11}$$

where

$$J(u_1,u_2) := \mathrm{E}\left[\int_0^T f(t,X^u(t),u_1(t),u_2(t),\omega)\mathrm{d}t \,+\, \phi(X^u(T),\omega) \,+\, \Psi(Y^u(0))\right] \quad . \tag{4.12}$$

Only one Hamiltonian, as well as only one set of adjoint processes, are needed [Øksendal and Sulem, 2014]. For $g_1 = g_2 =: g$, $h_1 = h_2 =: h$, $f := f_1 = -f_2$, $\Psi := \Psi_1 = -\Psi_2$ and $\phi := \phi_1 = -\phi_2$, the controlled processes $(Y(t), Z(t))$ are solutions of

$$\begin{cases} \mathrm{d}Y(t) = & -g(t,X(t),Y(t),Z(t),u(t),\omega)\mathrm{d}t \,+\, Z(t)\mathrm{d}W(t) \quad ,\ t\in[0,T] \\ Y(T) = & h(X(T),\omega) \end{cases} \tag{4.13}$$

and the associated Hamiltonian reads

$$\begin{aligned} H(t,x,y,z,u_1,u_2,\lambda,p,q) := & f(t,x,y,z,u_1,u_2) \,+\, \lambda\, g(t,x,y,z,u_1,u_2) \\ & +\, p\, b(t,x,u_1,u_2) \,+\, q\,\sigma(t,x,u_1,u_2) \quad . \end{aligned} \tag{4.14}$$

The adjoint processes are given by

$$\begin{cases} \mathrm{d}\lambda(t) &= \lambda(t)\left[\frac{\partial g}{\partial y}(t)\,\mathrm{d}t \,+\, \frac{\partial g}{\partial z}(t)\,\mathrm{d}W(t)\right] \quad , \; t \in [0,T] \; , \\ \lambda(0) &= \Psi'\left(Y(0)\right) \end{cases} \tag{4.15}$$

and

$$\begin{cases} \mathrm{d}p(t) &= -\frac{\partial H}{\partial x}(t)\,\mathrm{d}t \,+\, q(t)\,\mathrm{d}W(t) \; , \; t \in [0,T] \; , \\ p(T) &= \phi'\left(X(T)\right) \,+\, h'(X(T))\,\lambda(T) \quad . \end{cases} \tag{4.16}$$

Note that $(\lambda(t), p(t), q(t)) = (\lambda_1(t), p_1(t), q_1(t)) = -\left(\lambda_2(t), p_2(t), q_2(t)\right)$ and $H = H_1 = -\,H_2$. Consequently, there is only one controlled forward and one controlled backward equation for the saddle-point of a given cost function, which can be determined by making use of the maximum principle, i.e., identifying the saddle point of the associated Hamiltonian.

In the simplest case, one control is constant (w.l.o.g. $u_2 \equiv 0$) and the stochastic game simplifies to a stochastic optimal control problem, as, for instance, studied in ref. [Hamadène and Lepeltier, 1995; Hamadène, 1998; Øksendal and Sulem, 2009].

Furthermore, it is possible that the controlled equation for the stochastic optimal control problem (one control u) depends on a forward *as well as* backward Wiener process, i.e., [Bahlali and Gherbal, 2010]

$$\begin{cases} -\mathrm{d}\,y^u(t) = & b(t, y^u(t), z^u(t), u(t))\,\mathrm{d}t \,+\, \sigma((t, y^u(t), z^u(t), u(t))\,\mathrm{d}W_b(t) \\ & -z^u(t)\mathrm{d}W_f(t) \\ y^u(T) = & \xi \quad . \end{cases} \tag{4.17}$$

Such an equation is called backward doubly stochastic differential equation (BDSDE), where the deterministic part of this equation goes backward in time. $\xi \in \mathbb{R}$ is an arbitrary number and can depend on randomness. $(W_f(t))_{t\in[0,T]}$ is a forward in time Wiener process, while $(W_b(t))_{t\in[0,T]}$ goes backward in time. Based upon these considerations, one aims for the optimal control $\hat{u}(t)$ so as to maximize the cost function [Bahlali and Gherbal, 2010].

$$J(u) = \mathrm{E}\left[\int_0^T f(t, y^u(t), u(t), \omega)\mathrm{d}t \,+\, \Psi(y^u(0))\right] \quad . \tag{4.18}$$

Despite of the different mathematical structure of the control equation, the resulting stochastic optimal control problem is similar to that one discussed by Øksendal and

Sulem [2009]. Thus, the optimal control can be found using a maximum principle. Necessary and sufficient conditions for BDSDEs are analyzed and proven in ref. [Bahlali and Gherbal, 2010].

In the next section, stationary quantum systems will be analyzed in terms of a stochastic optimal control problem, where the osmotic velocity is given by exactly that optimal control that maximizes the related action functional.

Following these considerations, also non-stationary systems will be analyzed, noting that the current and the osmotic velocity are determined by the Nash equilibrium of the two distinct variational problems. In addition, it will be possible to reconsider the control equations in terms of a BDSDE so as to find the wanted optimal control, in turn extremizing the combined action functional introduced by Pavon [1995b].

4.2. Stationary quantum systems

In Nelson mechanics, the motion of a particle is described by a stochastic process $(X(t))_{t\in[0,T]}$ that is characterized by stochastic differential equations. For the sake of simplicity, only one dimensional problems will be presented; however, all equations can be extended to higher dimensions.

For stationary systems, the wave function $\Psi(x)$ is given by the solution of the stationary Schrödinger equation,

$$\left[-\frac{\hbar^2}{2\,m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\Psi(x) = E\,\Psi(x) \quad , \tag{4.19}$$

and the current velocity equals zero. Hence, the motion process $(X(t))_{t\in[0,T]}$ is described by the following forward and backward SDEs,

$$\begin{cases} \mathrm{d}X(t) & = u(X(t))\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\mathrm{d}W_f(t)\ , \quad t\in[0,T] \\ X(t=0) & = x_0 \in \mathbb{R} \end{cases} \quad , \tag{4.20}$$

$$\begin{cases} \mathrm{d}X(t) & = -u(X(t))\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\mathrm{d}W_b(t)\ , \quad t\in[0,T] \\ X(t=T) & = x_T(\omega) \end{cases} \tag{4.21}$$

Here, $x_T(\omega)$ is the endpoint of the forward SDE and, consequently, depends on randomness. On the other hand, x_0 is a fixed initial value, which can be chosen arbitrarily. As before, $W_f(t)$ is a forward (independent of all X(s) with $s < t$) and $W_b(t)$ is a backward (independent of all $X(s)$ with $s > t$) Wiener process. It should also be noted that in

the stationary case, the osmotic velocity is only a function of the motional process and, therefore, no explicit time-dependence arises.

As discussed in chapter 3, the current and the osmotic velocities are given as the saddle point solutions of the two variational principles derived by Pavon [1995b]. In the stationary case, however, only one of them requires a more sophisticated mathematical treatment. The osmotic velocity is given by the maximum of the following action functional, i.e., searching for $\hat{u}(X(t))$ with

$$J(\hat{u}) = \max_{u} \mathrm{E}\left[\int_0^T \left(-\frac{m}{2}\,u^2(X(t)) \;-\; V(X(t))\right)\mathrm{d}t \;+\; S_0(x_0)\right] \quad . \tag{4.22}$$

The occurring time horizon is finite ($T \in \mathbb{R}$ is fixed) even if the total duration might be as long as desired. Worth noting, in the stationary case, equation (4.22) should be replaced by

$$J(\hat{u}) = \max_{u} \lim_{T\to\infty} \frac{1}{T}\,\mathrm{E}\left[\int_0^T \left(-\frac{m}{2}\,u^2(X(t)) \;-\; V(X(t))\right)\mathrm{d}t \;+\; S_0(x_0)\right] \quad . \tag{4.23}$$

This situation would require a solution to an optimal control problem with infinite time horizon [Agram and Øksendal, 2014], which complicates the mathematical treatment and reduces applicability. Using finite time horizon, on the other hand, is advantageous for numerical implementation, and, as a compromise, a sufficiently large, arbitrarily adjustable but fixed period will be considered.

The initial costs $S_0(x_0)$ are related to the initial condition of the Schrödinger equation, i.e., $\Psi(x_0, t=0) = \exp\left\{R(x_0,0) + \frac{i}{\hbar}S(x_0,0)\right\}$. It is noted that in the stationary case the function $S(x,t) = S(t)$ is only a function of time, hence $S_0(x) := S(x, t=0) = S(0)$ is constant for all $x \in \mathbb{R}$, and one can choose $S(0) = 0$.

The controlled process is given by the motional process (characterized by equation (4.20) and (4.21)) and depends on the control u, which is a function of $(X(t))_{t\in[0,T]}$. Therefore, the osmotic velocity is the solution of a so-called optimal feedback control problem, which is, in the stationary case, the quantum-mechanical counterpart of the least-action principle in classical mechanics.

In contrast to the treatment by Pavon [1995b], who includes the SDEs for the motional process as constraints for the search of the optimal path in order to extremize the action functional, equation (4.22) is interpreted as an optimal control problem. This means that the optimal control $u(X(t))$ is determined, in turn maximizing the action

functional.

As mentioned previously, direct evaluation of the cost functional is sophisticated and it is advantageous to derive the optimal control from the maximum principle. Using the general equations derived by [Øksendal and Sulem, 2014], one has

$$H(x,u,\lambda,p,q) = -\frac{m}{2}u^2 - V(x) + \lambda\, u + p\, u + \sqrt{\frac{\hbar}{m}}\, q \quad , \tag{4.24}$$

with the adjoint processes being defined by the following forward as well as backward SDEs,

$$\mathrm{d}\lambda(t) = 0 \quad , \ \lambda(0) = 0 \quad , \tag{4.25}$$

$$\mathrm{d}p(t) = \left.\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right|_{x=X(t)} \mathrm{d}t + q(t)\,\mathrm{d}W_b(t) \quad , \ p(T) = \lambda(T) \quad . \tag{4.26}$$

Due to the absence of any initial and final costs, one of the adjoint processes equals zero, and, using the maximum principle, the osmotic velocity reads

$$m\, u(X(t)) = p(t) \quad . \tag{4.27}$$

Inserting equation (4.27) into equation (4.26), one finally ends up with

$$\mathrm{d}u(t) = \frac{1}{m}\left.\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right|_{x=X(t)} \mathrm{d}t + \frac{q(t)}{m}\,\mathrm{d}W_b(t) \quad . \tag{4.28}$$

Since the adjoint process $\lambda(t)$ vanishes, the backward SDE of the motional process provides no further information to the optimal control problem, and needs thus not to be considered.

Equation (4.20) and (4.28) constitute a system of coupled forward-backward stochastic differential equations (FBSDEs), which equal the stochastic Hamilton equations of motion in the stationary case:

$$\mathrm{d}X(t) = u(X(t))\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\mathrm{d}W_f(t) \ , \quad X(0) = x_0 \in \mathbb{R} \quad , \tag{4.29}$$

$$\mathrm{d}u(t) = \frac{1}{m}\left.\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right|_{x=X(t)} \mathrm{d}t + \frac{q(t)}{m}\,\mathrm{d}W_b(t) \ , \quad u(X(T)) = 0 \tag{4.30}$$

As such, these coupled equations describe the dynamics of a quantum particle uniquely and can be solved independently of the solution to the Schrödinger equation. Since

the osmotic velocity and the adjoint processes are functionals of the motional process, PDEs for them are derived by making use of Itô's formula [Ma et al., 1994], yielding

$$\begin{aligned} \mathrm{d}u(t) &= \left(u_t(t,x) \,+\, u_x(x,t)\,u(t,x) \,+\, \tfrac{\hbar}{2m} u_{xx}(x,t)\right)_{x=X(t)} \mathrm{d}t \\ &\quad + \left[\sqrt{\tfrac{\hbar}{m}}\, u_x(x,t)\right]_{x=X(t)} \mathrm{d}W_b(t) \\ &= \frac{1}{m}\,\frac{\mathrm{d}V(x)}{\mathrm{d}x}\bigg|_{x=X(t)} \mathrm{d}t + \frac{q(t)}{m}\,\mathrm{d}W_b(t) \\ \Rightarrow\; 0 &= u_t(t,x) \,+\, u_x(x,t)\,u(t,x) \,+\, \frac{\hbar}{2m} u_{xx}(x,t) - \frac{1}{m}\frac{\mathrm{d}V(x)}{\mathrm{d}x} \qquad (4.31) \\ q(x,t) &= \sqrt{\hbar\, m}\, u_x(x,t) \quad . \qquad (4.32) \end{aligned}$$

The above PDEs can be simplified to ODEs since the osmotic velocity is not explicitly time-dependent. The equation for the osmotic velocity equals the gradient of the time-*in*dependent Schrödinger equation and reads

$$0 = u(x)\,\frac{\mathrm{d}u(x)}{\mathrm{d}x} \,+\, \frac{\hbar}{2\,m}\frac{\mathrm{d}^2u(x)}{\mathrm{d}x^2} \,-\, \frac{1}{m}\frac{\mathrm{d}V(x)}{\mathrm{d}x} \quad , \qquad (4.33)$$

$$q(x) = \sqrt{\hbar\, m}\;\frac{\mathrm{d}u(x)}{\mathrm{d}x} \quad . \qquad (4.34)$$

Furthermore, the equation of the osmotic velocity is in accordance with the equation derived by Nelson [1966]. That means that the Schrödinger equation is *one* but not the only way to describe quantum systems uniquely, with thus an analogous situation to classical mechanics: For both classical and quantum systems there are three distinct, independent ways to quantity a particle's motion (see **Figure 4.1**).

Following these considerations, it is now possible to analyze systems the wave function of which cannot be determined analytically. Applications include, but are not limited to, the double well potential, the harmonic oscillator and particles in a Coulomb potential. The here presented approach addresses a numerical solution to the stationary Hamilton equations of motion, and it turns out that the wave function can be found in addition by solving the coupled FBSDEs, as is discussed later on.

Inserting the derived relations for the adjoint processes in the Hamilton function (equation (4.24)), one gets

$$H(x,u) = \frac{m}{2}u^2 - V(x) \,+\, \hbar\,\frac{\mathrm{d}u}{\mathrm{d}x} \quad . \qquad (4.35)$$

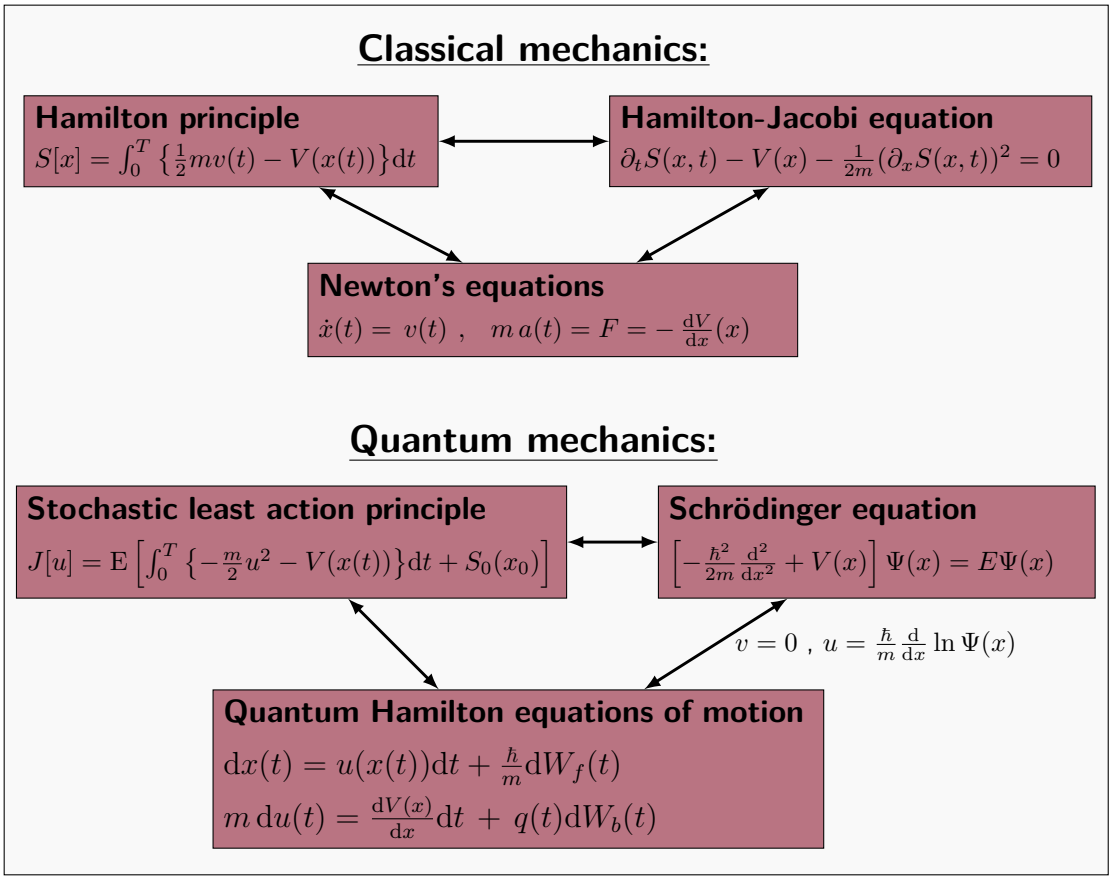

Figure 4.1.: *Schematic representation of the three equivalent theories describing the motion of a particle uniquely and independently from one another. Top: Case of classical particles. Bottom: Case of quantum particles.*

Worth mentioning, the Hamilton function has no longer the physical meaning of a Hamiltonian itself, which for the Nelson picture is given by $\frac{m}{2}u^2(x) + V(x)$. Instead, it is used in the way as in deterministic control theory, in which the mathematical Hamilton function coincides with the physical one.

Misawa [1986] succeeded in determining a Hamiltonian for stochastic mechanics from the Schrödinger equation, too. However, in his Hamilton function the last summand differs from that one in equation (4.35) by a factor $1/2$.

4.2.1. Excited states

In contrast to the variational principle of Yasue [1980], where the variational problem is formulated such that the difference between the total energy and a given energy (as a parameter) is extremized, the variational problem of Pavon [1995b] (equation (4.22)) is in fact independent of the energy. Therefore, the derived Hamilton equations of motion describe the ground state[3] of the system. Even if equation (4.22) is supplemented by

[3] The state with the smallest energy

the (constant) energy, i.e.

$$J(\hat{u}) = \max_{u} \lim_{T\to\infty} \frac{1}{T} \mathrm{E}\left[\int_0^T \left(-\frac{m}{2}\, u^2(X(t)) \;-\; V(X(t)) - E\right) \mathrm{d}t \;+\; S_0(x_0)\right] \quad , \tag{4.36}$$

the resulting Hamilton equations of motion of the modified problem are the same as for the original variational problem, noting that only the derivative of the integrand is needed in the backward SDE for the osmotic velocity. Consequently, also the modified variational problem provides a self-contained representation of the system's ground state.

Moreover, the equivalence between the Schrödinger equation and the equations for the velocities derived by Nelson [1966] (which equal the system's Madelung equations) are only fulfilled for a node-free wave function. It is possible to derive the excited states of a system from the ground state using the theory of supersymmetric Hamiltonians [Sukumar, 1985a,b; Grigorenko, 1991; Cooper et al., 1995; Markovich et al., 2012; Chou and Kouri, 2013]. Sukumar [1985a] showed that the Hamilton operator

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \tag{4.37}$$

with eigenfunctions $\Psi_n(x)$ and eigenvalues E_n, i.e. $\hat{H}_0\Psi_n(x) = E_n\,\Psi_n(x)$, $n = 0, 1, \ldots$, can be written as $\hat{H}_0 = \hat{A}_0^+\hat{A}_0^- \;+\; E_0$, with the operators $\hat{A}_0^\pm$ being defined by

$$\hat{A}_0^\pm := \frac{\hbar}{\sqrt{2m}}\left(\mp\frac{\mathrm{d}}{\mathrm{d}x} \;-\; \frac{1}{\Psi_0(x)}\frac{\mathrm{d}\Psi_0(x)}{\mathrm{d}x}\right) \quad , \tag{4.38}$$

where the operator $\hat{A}_0^+$ is the Hermitian adjoint of $\hat{A}_0^-$ [Sukumar, 1985a]. Except of E_0, the superpartner $\hat{H}_1 = \hat{A}_0^-\hat{A}_0^+ \;+\; E_0$ has the same energy spectrum as $\hat{H}_0$, where the ground state of $\hat{H}_1$ (and the associated ground state wave function $\varphi_0^1(x)$) is the first excited state of the original Hamilton operator $\hat{H}_0$. The first excited state wave function is given by [Sukumar, 1985a,b]

$$\Psi_1(x) = \frac{1}{\sqrt{E_1 - E_0}}\,\hat{A}_0^+\varphi_0^1(x) \quad . \tag{4.39}$$

Applying the operators $\hat{A}_0^\pm$ means switching between the eigenfunction spaces of the associated superpartners, i.e., between the eigenfunction space of $\hat{H}_0$ and $\hat{H}_1$ (cf. also **Figure 4.2**).

As shown by Grigorenko [1991], the same procedure can be applied to the stochastic description of quantum mechanics. The stationary Schrödinger equation of the ground

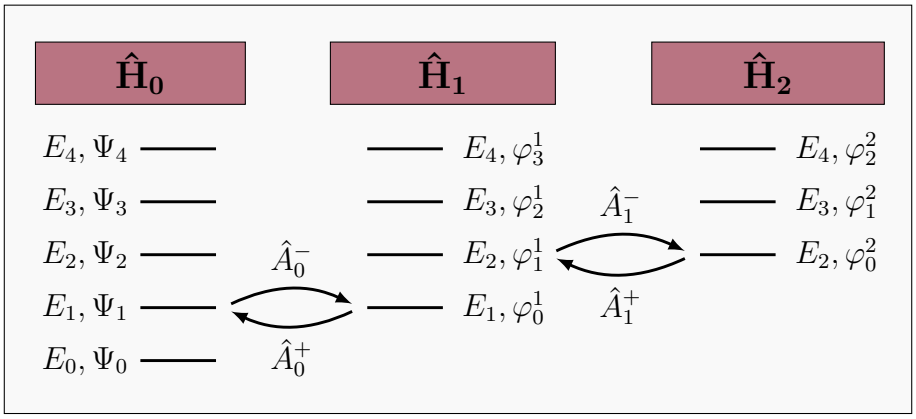

Figure 4.2.: *Operating principle for the operators $\hat{A}_i^{\pm}$, $i = 0, 1$.*

state $\Psi_0(x) = \mathrm{e}^{R_0(x)}$ leads to the equation

$$\left[-\frac{\hbar^2}{2m}R_0''(x) - \frac{\hbar^2}{2m}{R_0'}^2(x) + V(x) - E_0\right]\mathrm{e}^{R_0(x)} = 0 \quad . \tag{4.40}$$

Inserting the definition of the osmotic velocity, $u_0(x) = \frac{\hbar}{m}R_0'(x)$, one obtains

$$V(x) = E_0 + \frac{m}{2}u_0^2(x) + \frac{\hbar}{2}u_0'(x) \quad . \tag{4.41}$$

The operators $\hat{A}_0^{\pm}$ can be expressed using the osmotic velocity [Grigorenko, 1991],

$$\hat{A}_0^{\pm} = \sqrt{\frac{m}{2}}\left(-u_0(x) \mp \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right) \quad . \tag{4.42}$$

Hence, using the expression for the potential (equation (4.41)), the superpartner $\hat{H}_1$ reads

$$\begin{aligned}
\hat{H}_1 &= \hat{A}_0^-\hat{A}_0^+ + E_0 \\
&= E_0 + \left(-u_0(x) + \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)\left(-u_0(x) - \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right) \\
&= V(x) - \hbar u_0'(x) - \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \\
&=: V_1(x) - \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \quad .
\end{aligned} \tag{4.43}$$

Consequently, the first excited state can be found by identifying the ground state φ_0^1 of the modified potential $V_1(x)$ [Grigorenko, 1991]. In other words, that means that the optimal control problem for the modified potential $V_1(x)$ has to be solved in order to determine the exited state. Once the ground state $\varphi_0^1(x)$ is found, it can be transformed

into $\Psi_1(x)$ by making use of [Sukumar, 1985a,b]

$$\Psi_1(x) = \sqrt{\frac{m}{2(E_1 - E_0)}} \left(-u_0(x) - \frac{\hbar}{m} \frac{\mathrm{d}}{\mathrm{d}x} \right) \varphi_0^1(x) \quad . \tag{4.44}$$

If the Hamilton operator $\hat{H}_1 = \hat{A}_1^+ \hat{A}_1^- + E_1$ is factorized in the same way as $\hat{H}_0$, then the second state can be found in an analogous way, since $\hat{H}_2 = \hat{A}_1^- \hat{A}_1^+ + E_1$ (superpartner of $\hat{H}_1$). Finally, all excited states can be calculated iteratively by identifying the ground state of a sufficiently often modified potential. The n-th excited state wave function of the original Hamilton operator $\hat{H}_0$ is given by [Sukumar, 1985b; Markovich et al., 2012]

$$\begin{aligned} \Psi_n(x) &= \frac{\hat{A}_0^+ \, \hat{A}_1^+ \, \ldots \, \hat{A}_{n-1}^+ \varphi_0^n}{\sqrt{E_n - E_{n-1}} \sqrt{E_n - E_{n-2}} \cdots \sqrt{E_n - E_0}} \\ &= \prod_{i=0}^{n-1} \hat{A}_i^+ \left[E_n - E_i \right]^{-1/2} \varphi_0^n \quad , \end{aligned} \tag{4.45}$$

where φ_0^n is the ground state of the n-times modified potential. Further information on the excited states in the stochastic picture can be found in ref. [Patzold, 2018].

Complete wave function

For stationary systems, the wave function associated with the n-th energy is given by

$$\Psi_n(x,t) = \Psi_n(x) \, \mathrm{e}^{-\frac{iE_n t}{\hbar}} \quad . \tag{4.46}$$

The derivation of $\Psi_n(x)$ from the optimal control problem is explained above; however, also the term for the constant phase shift can be derived from the Madelung equations. Since $\Psi_n(x,t) = \exp\{R_n(x) + \frac{i}{\hbar} S_n(t)\}$ in the stationary case, the equation for $S_n(t)$ reads

$$\frac{\mathrm{d}S_n(t)}{\mathrm{d}t} = \left[\frac{m}{2} u_n^2(x) + \frac{\hbar}{2} \frac{\mathrm{d}u_n(x)}{\mathrm{d}x} \right] - V(x) \quad . \tag{4.47}$$

Equation (4.41) can be transferred towards the n-th energy and, therefore, the right-hand part of equation (4.47) equals $-E_n$. Hence

$$\Psi_n(x,t) = \Psi_n(x) \, \mathrm{e}^{-\frac{i}{\hbar} S_n(t)} = \Psi_n(x) \, \mathrm{e}^{-\frac{i}{\hbar} E_n t} \quad . \tag{4.48}$$

4.3. Numerical solution to the stationary stochastic Hamilton equations of motion

In this section, methods to find a numerical solution of the stationary stochastic Hamilton equations of motion are described. A numerical approximation to the motional process $(X(t))_{t\in[0,T]}$ as well as for the osmotic velocity $u(X(t))$ can be found iteratively and starts with a rough guess on the osmotic velocity. In fact, the iteration method converges to the solution of the backward equation (almost) independently of the initial estimate $u^0(x)$, and therefore, the stating point can be chosen as the classical stationary ground state, i.e., choosing $u^0(x) \equiv 0$. The forward SDE can be solved numerically, the outcome of which is afterwards used to find a numerical solution to the backward equation. Consecutively, the resulting control estimate serves to solve the forward equation again, and this iterative procedure is repeated until sufficient convergence is achieved. The algorithm is thus subdivided into two major parts:

1. Solving the forward SDE
2. Solving the backward SDE

Furthermore, the equations are transformed into dimensionless ones. Therefore, characteristic lengths and times have to be chosen for the analyzed specific system, which is, however, not easily done in the general case.

4.3.1. Solving the forward equation

Before solving the forward equation, the time interval $[0, T]$ has to be discretized, $\Delta t_i := t_{i+1} - t_i$, $i = 0, \ldots, N-1$, where $t_0 = 0$ and $t_N = T$. Now, in the j-th iteration step, the time-continuous process $(X(t))_{t\in[0,T]}$ is addressed in terms of a discrete process, $\left(X_{t_i}^{\pi,j}\right)_{i=0,\ldots,N}$. The numerical calculation can, for instance, be performed by utilizing the Heun method for SDEs, which is a Runge-Kutta method of convergence order one[4] for additive noise [Kloeden, 2002].

Based upon the estimate of the osmotic velocity $u^{j-1}(x)$ determined in the previous

[4]Further information about the order of convergence can be found in the appendix, section A.4.

iteration step, the Heun method reads

$$\begin{aligned} X_0^{\pi,j} &= x_0 \quad , \; u^0(x) \equiv 0 \quad , \\ \tilde{X}_{t_{i+1}}^{\pi,j} &= X_{t_i}^{\pi,j} + \Delta t_i \, u^{j-1}\left(X_{t_i}^{\pi,j}\right) + \Delta W_i \quad , \\ X_{t_{i+1}}^{\pi,j} &= X_{t_i}^{\pi,j} + \frac{\Delta t_i}{2}\left[u^{j-1}\left(X_{t_i}^{\pi,j}\right) + u^{j-1}\left(\tilde{X}_{t_{i+1}}^{\pi,j}\right)\right] + \Delta W_i \end{aligned} \tag{4.49}$$

$$\tag{4.50}$$

for $i = 0, \ldots, N-1$, $j = 1, \ldots, N_{\text{iteration}}$, where $\Delta W_i := W(t_{i+1}) - W(t_i)$, $i = 0, \ldots, N-1$ are discrete increments of the Wiener process. Hence, they are normal distributed random numbers with mean value zero and variance Δt_i, and $\tilde{X}_{t_{i+1}}^{\pi,j}$ is a predictor for $X_{t_{i+1}}^{\pi,j}$ using an Euler step.

4.3.2. Solving the backward equation

As the next step, a solution to the BSDE given by equation (4.30) has to be found in order to determine a new estimate to the control u^j. This can be done in two ways: (i) evaluating the velocity's ODE (equation (4.33)), and (ii), solving the kinematic equation (eq. (4.30)) directly, which requires a method suitable for BDSEs.

Solving the ODE

Suppose that $u^{j-1}(x)$ being the estimate of the osmotic velocity determined in the previous iteration step, and suppose that the discrete process $\left(X_{t_i}^{\pi,j}\right)_{i=0,\ldots,N}$ determined by equation (4.49) being an approximation to the (forward) motional process. Then, a solution to the backward equation in the j-th iteration step $u^j(x)$ can be found by solving

$$\begin{aligned} 0 &= u^{j-1}(x)\,\frac{\mathrm{d}u^j(x)}{\mathrm{d}x} + \frac{1}{2}\frac{\mathrm{d}^2u^j(x)}{\mathrm{d}x^2} - \frac{\mathrm{d}V(x)}{\mathrm{d}x} \quad , \\ u^j(X_T^{\pi,j}) &= u^{j-1}(X_T^{\pi,j}) \quad , \quad \left.\frac{\mathrm{d}u^j(x)}{\mathrm{d}x}\right|_{x=X_T^{\pi,j}} = \left.\frac{\mathrm{d}u^{j-1}(x)}{\mathrm{d}x}\right|_{x=X_T^{\pi,j}} \end{aligned} \tag{4.51}$$

numerically. To solve the ODE uniquely, two boundary conditions are necessary. Therefore, at the final time T, the new estimator and its derivative are identified by accounting for the result of the preceding iteration step, i.e., the boundary conditions will be iterated, too. Thus, with a growing number of iteration steps, the iterative conditions become more precise, yielding $u^j(X_T) \approx u^{j-1}(X_T)$ for sufficiently large values j. The chosen boundary conditions are independent of possible final costs, which, in general, can occur in the cost function. In contrast to initial costs, which can be derived from the initial conditions of the Schrödinger equation, a physical meaning of

final costs does not exist in the general case. Hence, it is reasonable to use iterative conditions instead of $u^j(X_T^{\pi,j}) = 0$ obtained from the mathematical model, which is the classical stationary ground-state solution.

To get a numerical approximation to the solution of the backward equation, equation (4.51) is transformed into a first order ODE system and subsequently discretized backward in time using an implicit Euler method, which is solved on the points $\left(X_{t_i}^{\pi,j}\right)_{i=0,\dots,N}$. To increase the accuracy of the method, it is useful to determine more than one realization of the backward process. Therefore, suppose that $x_i^{m,j}$ is the m-th trajectory at time t_i of the discrete motion process $\left(X_{t_i}^{\pi,j}\right)_{i=0,\dots,N}$ for $m = 1, \dots, M$ and $i = 0, \dots, N$ in the j-th iteration step, and, suppose that $\Delta x_i^{m,j} := x_{i+1}^{m,j} - x_i^{m,j}$, $\theta_i^{m,j} := u^j(x_i^{m,j})$ and $\phi_i^{m,j} := u'^j(x_i^{m,j})$ with $m = 1, \dots, M$ and $i = 0, \dots, N$. Thus, one gets

$$\begin{aligned} \theta_N^{m,j} &= u^{j-1}(x_N^{m,j}) \ , \quad \phi_N^{m,j} = u'^{j-1}(x_N^{m,j}) \\ \begin{pmatrix} \theta_i^{m,j} \\ \phi_i^{m,j} \end{pmatrix} &= \begin{pmatrix} \theta_{i+1}^{m,j} \\ \phi_{i+1}^{m,j} \end{pmatrix} - \Delta x_i^{m,j} \cdot \begin{pmatrix} \phi_{i+1}^{m,j} \\ 2 \cdot \left[\frac{\mathrm{d}V(x)}{\mathrm{d}x}\Big|_{x=x_{i+1}^{m,j}} - u^j(x_{i+1}^{m,j})\, \phi_{i+1}^{m,j} \right] \end{pmatrix} \end{aligned} \tag{4.52}$$

for $m = 1, \dots, M$ and $i = N-1, \dots, 0$. Note again that the difference equations are solved backwards in time. The new estimate of the osmotic velocity is given by the arithmetic average over $\theta^{m,j}$ for $m = 1, \dots, M$. For this purpose, the x-domain is partitioned into L equidistant intervals, the resulting step size of which is

$$\delta = \frac{x_{\max} - x_{\min}}{L} \quad . \tag{4.53}$$

The parameters x_{min} and x_{max} are the borders of the range of values. Dependent on the specific problem, x_{min} and x_{max} have to be sufficiently large so as to ensure that the diffusion process (describing the motion itself) takes place within these borders. Then, one takes the average over all $\theta^j(x_i^{m,j})$, $m = 1, \dots, M$ and $i = 0, \dots, N$ of which arguments can be found in the same sub-interval, $D_l := [x_{min} + (l-1)\delta \, , \, x_{min} + l\delta]$, where $l = 1, \dots, L$. Consequently, the resulting step function $u^j(x)$ is the new estimate to the osmotic velocity, and is used as the drift term for the next iteration step. In addition, the adjoint process $q(t)$ can also be approximated by the difference equation system derived from equation (4.52), noting that the adjoint process equals the derivative of the osmotic velocity. Worth mentioning, $q(t)$ is the adjoint process to the diffusion coefficient, which, in general, is also a stochastic process. In this case, the constant diffusion coefficient is a feature of the physical system. Nonetheless, no knowledge of the adjoint process $q(t)$ is needed to determine the new estimate of the

osmotic velocity, and hence, the specific estimate of $q(t)$ is not explicitly calculated.

Still, the fixed range of x-values must be considered during all simulation steps. Empty sub-intervals might occur for intervals in which no values of the motional process are found. In such cases, it will be impossible to find a value for the new estimate of the osmotic velocity and the value stays the same as before. Furthermore, the diffusion of the motional process can be limited to an area smaller than the chosen x-domain during the whole simulation, resulting in an estimate of the velocity equal to the starting value u^0 outside this region.

For stationary problems, the ODE-based approach is a suitable alternative to solving the BSDE directly. Nevertheless, for the general case of non-stationary systems, a numerical approach to PDEs is necessary; see, for instance, refs. [Douglas et al., 1996; Zhang and Zheng, 2002; Milstein and Tretyakov, 2006; Ma et al., 2008]. The associated calculations are time-consuming, rendering a direct analysis of the BSDE the better choice. Beyond that, the latter *ansatz* is equivalent to solving the Schrödinger equation.

Direct evaluation of the BSDE

In the following, the direct evaluation of the coupled FBSDE system starting from equation (4.29-4.30) will be described. Following the same principles as done before, a x-domain is chosen via the parameters x_{min} and x_{max}, and is partitioned into L equidistant sub-intervals $D_l := [x_{\min} + (l-1)\,\delta\,,\, x_{\min} + l\,\delta]$ for $l = 1, \ldots,\ L$, where the width of the intervals δ is given by equation (4.53). In the same way, suppose that $u^{j-1}(x)$ is the estimate of the osmotic velocity determined in the preceding iteration step, and suppose that the discrete process $\left(X^{\pi,j}_{t_i}\right)_{i=0,\ldots,N}$ is an approximation to the motional process. ΔW_i, $i = 0 \ldots, N$, are discrete increments of the Wiener process. The backward equation is discretized using the Euler-Maruyama method, where the discrete process $\left(u^{\pi,j}_{t_i}\right)_{i=1,\ldots,N}$ of the j-th iterations step approximates the backward process, and is given by

$$
\begin{aligned}
u^{\pi,j}_{t_N} &= u^{j-1}(X^{\pi,j}_{t_N}) \quad ,\ q^{\pi,j}_{t_N} = 0 \quad , \\
u^{\pi,j}_{t_i} &= u^{\pi,j}_{t_{i+1}} \ - \ \Delta t_i \ \left.\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right|_{x=X^{\pi,j}_{t_i}} \ - \ q^{\pi,j}_{t_i}\,\Delta W_i \quad .
\end{aligned}
\tag{4.54}
$$

The outcome of the preceding iteration step provides the backward condition to avoid final costs of the action functional.

It may happen that equation (4.54) cannot be solved uniquely since both $u^{\pi,j}_{t_i}$ and

$q_{t_i}^{\pi,j}$ are unknown in the i-th time step [Bouchard and Touzi, 2004]. In the case of direct evaluation of the coupled FBSDE system, no additional information on the processes[5] is required for the numerical calculation, which is the common procedure in the mathematical community; see, for instance, refs. [Ma et al., 2002; Bouchard and Touzi, 2004; Zhang, 2004; Gobet et al., 2005; Lemor et al., 2006; Bender and Denk, 2007; Bender and Zhang, 2008; Bender and Steiner, 2012].

Because the solution scheme for the backward equation will be based on the numerical calculation of a conditional expectation, the conditional expectation and some properties of them are introduced next.

Conditional expectation

Let $(\Omega, \mathcal{F}, P)$ be a probability space. The conditional probability $P(A|B)$, i.e. the probability of the event $A \in \mathcal{F}$ given that $B \in \mathcal{F}$ has occurred, is given by

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \quad , \tag{4.55}$$

where $P(B) > 0$. Frequently, one aims for a prediction of the random variable $X : \Omega \to \mathbb{R}^d$, where $P(B) = 0$ almost sure (a.s.). The conditional expectation is then given as an extension to the previous conditional expectation [Arnold, 1973; Meintrup and Schäffler, 2005]. Especially, the studied condition is given by the set $B = \{X = x \in \mathbb{R}^d\}$, which is common in different fields of applications, e.g., stock price predictions based upon the current market situation.

Definition 4.2 (Conditional expectation) *Let $X \in L^1(\Omega, \mathcal{F}, P)$ be a real-valued random vector and $\mathcal{G}$ be a sub-σ-algebra of $\mathcal{F}$, i.e., $(\Omega, \mathcal{G}, P)$ is a coarsening of the original probability space, meaning in turn that X is not generally $\mathcal{G}$-measurable. Then, an integrable random variable $Y \in \mathbb{R}^d$ (a $\mathcal{G}$-measurable coarsening of X) is sought in such a way that it takes, on average, the same value as X, i.e., [Arnold, 1973]*

$$\int_C Y \mathrm{d}P = \int_C X \mathrm{d}P \quad \forall C \in \mathcal{G} \quad . \tag{4.56}$$

In accordance with the theorem of Radon-Nikodym[6], there exists exactly one, uniquely defined Y (a.s.), which is called conditional expectation of X given the condition $\mathcal{G}$. The common notation is [Arnold, 1973]

$$Y = \mathrm{E}\left[X \middle| \mathcal{G}\right] \quad . \tag{4.57}$$

[5] The ODEs for $u(x)$ and $q(x)$ are derived using the Ito formula

[6] The theorem is, for example, given in ref. [Schmidt, 2011; Behrends, 2013].

This definition is equivalent to the following one.

Definition 4.3 *Let $X \in L^1(\Omega, \mathcal{F}, P)$ be a real-valued random variable and $\mathcal{G}$ be a sub-σ-algebra of $\mathcal{F}$. Then, the random variable Y will be called conditional expectation of X given $\mathcal{G}$, provided that Y is $\mathcal{G}$-measurable, and [Meintrup and Schäffler, 2005]*

$$\mathrm{E}\,(X\,\mathbb{1}_C\,) = \mathrm{E}\,(Y\,\mathbb{1}_C\,) \quad \forall C \in \mathcal{G} \quad . \tag{4.58}$$

Theorem 4.4 *Let $X, Y \in L^1(\Omega, \mathcal{F}, P)$ and $\mathcal{G} \subset \mathcal{F}$, then the conditional expectation fulfills the following statements, which are to be understood in the "almost sure" sense [Arnold, 1973; Meintrup and Schäffler, 2005]:*

(i) $\mathcal{G} = \{\emptyset, \Omega\}$ *(trivial σ-algebra)* $\Rightarrow\ \mathrm{E}\,[X|\mathcal{G}] = \mathrm{E}(X)$.

(ii) X *is $\mathcal{G}$-measurable* $\Rightarrow\ \mathrm{E}[X|\mathcal{G}] = X$, *especially,* $\mathrm{E}[XY|\mathcal{G}] = X\,\mathrm{E}[Y|\mathcal{G}]$.

(iii) $\mathrm{E}\Big(\,\mathrm{E}[X|\mathcal{G}]\,\Big) = \mathrm{E}(X)$.

(iv) X *being independent of* $\mathcal{G}$ $\Rightarrow\ \mathrm{E}[X|\mathcal{G}] = \mathrm{E}(X)$.

(v) Linearity: $a, b \in \mathbb{R}$ *being constant:* $\mathrm{E}[aX + bY|\mathcal{G}] = a\,\mathrm{E}[X|\mathcal{G}] + b\,E[Y|\mathcal{G}]$.

(vi) Monotony: $X_1 < X_2 \ \rightarrow\ \mathrm{E}[X_1|\mathcal{G}] \leq \mathrm{E}[X_2|\mathcal{G}]$.

(vii) $\Big|\,\mathrm{E}[X|\mathcal{G}]\,\Big| \leq \mathrm{E}\Big[\,|X|\,\Big|\mathcal{G}\Big]$.

(viii) $\mathcal{G}_1 \subset \mathcal{G}_2 \ \Rightarrow\ \mathrm{E}\Big[\,\mathrm{E}[X|\mathcal{G}_2]\Big|\mathcal{G}_1\Big] = \mathrm{E}[X|\mathcal{G}_1]$,
$\mathcal{G}_2 \subset \mathcal{G}_1 \ \Rightarrow\ \mathrm{E}\Big[\,\mathrm{E}[X|\mathcal{G}_2]\Big|\mathcal{G}_1\Big] = \mathrm{E}[X|\mathcal{G}_2]$.

The conditional probability $P(A|\mathcal{G})$ of the event A given that the condition $\mathcal{G} \subset \mathcal{F}$ holds is a special conditional expectation defined by

$$P(A|\mathcal{G}) = \mathrm{E}[\mathbb{1}_A|\mathcal{G}] \quad , \tag{4.59}$$

and is a $\mathcal{G}$-measurable function on Ω [Arnold, 1973].
If $\mathcal{F} = \mathcal{G}(X)$ is the σ-algebra, which is generated by the random variable X, one writes [Arnold, 1973]

$$\mathrm{E}[Y|\mathcal{F}] = \mathrm{E}[Y|X] \quad . \tag{4.60}$$

Furthermore, for each $\mathcal{G}(X)$-measurable random variable Z there exists a measurable function h with $h(X) = Z$, i.e., the value of Z is already specified by the value of $X(\omega)$ [Arnold, 1973]. Hence, there exists a measurable function h on Ω with $\mathrm{E}[Y|X] = h(X)$, and one can write [Arnold, 1973]

$$h(x) = \mathrm{E}[\,Y|X = x] \quad , \tag{4.61}$$

which means, as an interpretation, that the value of the random variable Y is sought, considered that X takes the value $x \in \mathbb{R}^d$.

In addition, the conditional expectation can be understood in a different way, as is used later on in the numerical algorithm. If $X \in \mathbb{R}^d$ is a square-integrable random variable, yielding a stronger condition as the integrability condition before, the space of all square-integrable random variables, i.e.

$$\mathcal{L}^2 = \left\{ X \in \mathbb{R}^d \colon \mathrm{E}\left(X^2\right) < \infty \right\} \quad , \tag{4.62}$$

is a vector space [Kersting and Wakolbinger, 2014]. It holds that $(X+Y)^2 \leq 2X^2+2Y^2$, and hence, $(X+Y) \in \mathcal{L}^2$. Because $\mathrm{E}(XY) = 1/2\,\mathrm{E}\left((X+Y)^2 - X^2 - Y^2\right) < \infty$, the space $\mathcal{L}^2$ defines a Hilbert space by introducing the scalar-product

$$\langle X, Y \rangle := \mathrm{E}\left(XY\right) \quad , \forall X, Y \in \mathcal{L}^2 \quad , \tag{4.63}$$

with the resulting norm

$$||X|| := \sqrt{\langle X, X \rangle} = \sqrt{\mathrm{E}\left(X^2\right)} \quad , \forall X \in \mathcal{L}^2 \quad . \tag{4.64}$$

Based upon the theorem of Riesz and Fischer, the validity of which is proven in ref. [Schmidt, 2011], the space $\mathcal{L}^2$ is a complete one, and hence, projections into complete subspaces are well-defined. Defining the complete subset

$$\mathcal{L}^2(\mathcal{G}) := \left\{ X \in \mathcal{L}^2 \colon \; X \text{ is } \mathcal{G}\text{-measurable} \right\} \quad , \tag{4.65}$$

a projection Y from X into $\mathcal{L}^2(\mathcal{G})$ can be defined for all $X \in \mathcal{L}^2$ [Kersting and Wakolbinger, 2014]. Thus, for $X \in \mathcal{L}^2$ and $Y \in \mathcal{L}^2(\mathcal{G})$, the following statements are equivalent [Schmidt, 2011]:

1. $Y = \mathrm{E}[X|\mathcal{G}]$.
2. $\mathrm{E}\left((X-Y)^2\right) \leq \mathrm{E}\left((X-Z)^2\right) \quad , \forall Z \in \mathcal{L}^2(\mathcal{G})$.
3. $\mathrm{E}\Big(XZ\Big) = \mathrm{E}\Big(YZ\Big)$.

That means, the projection Y fulfills the characteristic properties of the conditional expectation. Based on (ii),

$$\mathrm{E}\left((X - \mathrm{E}[X|\mathcal{G}])^2\right) \leq \mathrm{E}\left((X-Z)^2\right) \tag{4.66}$$

holds for all $\mathcal{G}$-measurable, square-integrable random variables Z. Therefore, the conditional expectation minimizes the squared distance between the random variables

and X [Kersting and Wakolbinger, 2014].

Multiplying equation (4.54) by ΔW_i and taking the conditional expectation, one can derive an equation for the adjoint process $q_{t_i}^{\pi,j}$ in the i-th time step [Bender and Steiner, 2012], yielding

$$q_{t_i}^{\pi,j} = \frac{1}{\Delta t_i} \mathrm{E}\left[u_{t_{i+1}}^{\pi,j} \, \Delta W_i \middle| \, \mathcal{F}_{t_i}^{j} \right] \quad . \tag{4.67}$$

Here, $\mathcal{F}_{t_i}^{j}$ is the complete filtration generated by the discrete forward process up to time t_i in the j-th iteration step, i.e., $\mathcal{F}_{t_i}^{j}$ includes previous information on the motional process. The thus-achieved adjoint process is inserted into (4.54). Now, $u_{t_i}^{\pi,j}$ can be determined uniquely, for which the calculation of conditional expectations is indispensable in each time step.

Numerical approaches to coupled FBSDE systems are of high interest, especially in the field of finance regarding the conditional expectation [El Karoui et al., 1997]. Calculations exploiting Malliavin derivatives[7] (see refs. [Fournié et al., 1999, 2001; Bouchard et al., 2004; Bouchard and Touzi, 2004; Bouchard and Elie, 2008]) are computational expensive since Skohorod integrals need to be solved in each time step. Instead, one may make use of the fact that the conditional expectation can be considered as a projection into $\mathcal{L}^2(\mathcal{F}_{t_i}^{j})$, the latter being the Hilbert space of all square-integrable, $\mathcal{F}_{t_i}^{j}$-measurable random variables defined in equation (4.65). Algorithms based on this approach can be found in refs. [Gobet et al., 2005; Lemor et al., 2006; Bender and Denk, 2007; Bender and Steiner, 2012; Gobet and Turkedjiev, 2015].

Since the solution of the backward equation is a functional of the motion process, which in turn is a Markov process, only the last value of the motion process has to be considered in the conditional expectation described by equation (4.67) [Bouchard and Touzi, 2004]. Hence, the conditional expectation reads

$$q_{t_i}^{\pi,j} = \frac{1}{\Delta t_i} \mathrm{E}\left[u_{t_{i+1}}^{\pi,j} \, \Delta W_i \middle| \, \mathcal{F}_{t_i}^{j} \right] = \frac{1}{\Delta t_i} \mathrm{E}\left[u_{t_{i+1}}^{\pi,j} \, \Delta W_i \middle| \, X_{t_i}^{\pi,j} \right] \quad . \tag{4.68}$$

Now, one aims for the m-th realization $q_{t_i}^{m,j}$ of the random variable $q_{t_i}^{\pi,j}$ at time t_i in the j-th iteration step, where $q_{t_i}^{\pi,j}$ is a function of the forward process, i.e.

$$q_{t_i}^{m,j} = q_{t_i}^{\pi,j}(X_{t_i}^{\pi,j} = x_i^{m,j}) \ , \ m = 1, \ldots, M \ , \ i = 0, \ldots, N \ , \ , \ j = 1, \ldots, N_{\text{iteration}} \quad . \tag{4.69}$$

[7] Some information about Malliavin derivative can be found in the Appendix, section A.3.

Here, $x_i^{m,j}$ is m-th computed forward motional process at time t_i in the j-th iteration step. The m-th realization of the adjoint process in the j-th iteration step is given by

$$q_{t_i}^{m,j} = \frac{1}{\Delta t_i} \mathrm{E}\left[u_{t_{i+1}}^{\pi,j} \, \Delta W_i \middle| \, X_{t_i}^{\pi,j} = x_i^{m,j} \right] \quad , \; m = 1, \ldots, M \; , i = 0, \ldots, N-1 \quad . \tag{4.70}$$

A numerical approximation to the conditional expectation can be found by making use of the fact that $\mathrm{E}[Y|X]$ is the projection from Y into the space of all square-integrable functions that are measurable with respect to the σ-algebra generated by X. Hence, the numerical approach can be understood in terms of a least-square optimization, meaning that the function $f(X) = \mathrm{E}[Y|X]$ is characterized by

$$f(X) = \arg\min_{\nu} \mathrm{E}\left[|\nu(X) - Y|^2 \right] \quad , \tag{4.71}$$

where ν spans the full range of measurable functions, with $\mathrm{E}\left[|\nu(X)|^2\right] < \infty$ [Bender and Steiner, 2012]. In order to simplify the infinite-dimensional minimization problem, one can introduce an L-dimensional functional basis $\eta(x) = (\eta_1(x), \ldots, \eta_L(x))$ so that $f(x)$ can be approximated as

$$f(x) \approx \alpha \cdot \eta(x) \; , \; \text{with } \alpha \in \mathbb{R}^L \quad . \tag{4.72}$$

L needs to be sufficiently large so as to achieve a good approximation of $f(x)$. Thus,

$$\alpha = \arg\min_{\alpha \in \mathbb{R}^L} \mathrm{E}\left[\, |\eta(X)\alpha - Y|^2 \, \right] \quad . \tag{4.73}$$

Given that there are x^m, y^m, $m = 1, \ldots, M$ independent realizations of the processes X and Y, the expectation value in equation (4.73) can be replaced by the arithmetic average, yielding [Bender and Steiner, 2012]

$$\alpha = \arg\min_{\alpha \in \mathbb{R}^L} \frac{1}{M} \sum_{m=1}^{M} \left[\, |\eta(x^m)\alpha - y^m|^2 \, \right] \quad . \tag{4.74}$$

For the numerical implementation, a suitable functional basis has to be chosen and the factor α has to be determined in each time step. The so-called hypercube basis was first presented by Gobet et al. [2005] and gives a very useful basis to the approach of conditional expectations. In the one-dimensional case, this basis is given by indicator functions, i.e.

$$\eta(\cdot) = \left(\mathbb{1}_{D_l}(\cdot) \right)_{l=1,\ldots,L} \; , \; \text{with } \mathbb{1}_{D_l}(x) = \begin{cases} 1 \; , & x \in D_l \\ 0 \; , & \text{else} \end{cases} \quad , \tag{4.75}$$

where the intervals are defined above. Hence, $\eta(x)$, $x \in D_l$, is a L-dimensional vector, where all components are zero except of the l-th one.

Consequently, the m-th realization of the adjoint process $q_{t_i}^{\pi,j}$ at time t_i in the j-th iteration step is given by

$$q_{t_i}^{m,j} = \frac{1}{\Delta_i}\, \alpha_i^j\, \eta(x_i^{m,j}) \quad , \tag{4.76}$$

$$\text{with } \alpha_i^j = \frac{1}{M} \sum_{m=1}^{M} \eta(x_i^{m,j})\, u_{t_{i+1}}^{m,j}\, \Delta W_i \quad . \tag{4.77}$$

Finally, M realizations of the backward equation can be determined by the following scheme:

$$u_{t_N}^{m,j} = u^{j-1}(x_N^{m,j}) \quad , \; q_{t_N}^{m,j} = 0 \quad , \tag{4.78}$$

$$q_{t_i}^{m,j} = \frac{1}{\Delta_i}\, \alpha_i^j\, \eta(x_i^{m,j}) \; , \quad \alpha_i^j = \frac{1}{M} \sum_{m=1}^{M} \eta(x_i^{m,j})\, u_{t_{i+1}}^{m,j}\, \Delta W_i^m \quad , \tag{4.79}$$

$$u_{t_i}^{m,j} = u_{t_{i+1}}^{m,j} - \Delta_i \left.\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right|_{x=x_i^{m,j}} - q_{t_i}^{m,j}\, \Delta W_i^m \quad , \tag{4.80}$$

$$i = N-1, \ldots, \; 0 \quad , \quad m = 1, \ldots, \; M \quad , \quad j = 1, \ldots, N_{\text{iteration}} \quad .$$

The new estimate to the osmotic velocity is given by the arithmetic average of all values $u_{t_i}^{m,j}$ for which several values are found within one and the same interval.

Finally, it is noted that the number of realizations should be chosen with care. The number of realizations affects the convergence of the method and should be adjusted relative to the number of time steps and intervals [Bender and Steiner, 2012]. (As will be also addressed in section 4.4.1.) The number of pathways increases significantly with the number of time steps, thus leading to high computational effort for improper settings.

4.4. Examples – Stationary systems

In this section, the above introduced methods are applied to cases for which an numerical approximation can be found for both the osmotic velocity and the probability density. In particular, a one-dimensional harmonic oscillator and a one-dimensional double-well potential will be analyzed. In contrast to the double-well potential, where neither the wave function nor the osmotic velocity can be treated analytically, the Schrödinger equation for the harmonic oscillator can be solved exactly. Thus, the latter case also permits to compare analytical and numerical results.

4.4.1. One-dimensional harmonic oscillator

In the following, a one-dimensional harmonic oscillator described by the potential $V(x) = {}^{x^2}\!/_2$ will be studied. The harmonic potential is transformed into dimensionless variables using the characteristic length $\sqrt{{}^{\hbar}\!/_{m\omega}}$ and the characteristic time ω^{-1}. The exact solution of the time-independent Schrödinger equation,

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{x^2}{2}\right]\Psi(x) = E\,\Psi(x) \quad , \tag{4.81}$$

is a function of the associated energy eigenvalues $E_n = n + {}^1\!/_2$, $n \in \mathbb{N}_0$, and reads

$$\Psi_n(x) = \pi^{-1/4}\,(2^n\,n!)^{-1/2}\,\mathrm{e}^{-\frac{x^2}{2}}\,H_n(x) \quad . \tag{4.82}$$

$H_n(x)$ are the Hermite polynomials and are defined by

$$H_n(x) = (-1)^n\,\mathrm{e}^{x^2}\,\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left[\mathrm{e}^{-x^2}\right] = e^{x^2/2}\left(x - \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \mathrm{e}^{-\frac{x^2}{2}} \quad , \; n \in \mathbb{N}_0 \quad . \tag{4.83}$$

Note that $\mathbb{N}_0$ is the set of all natural numbers supplemented by zero.

The ground-state wave function ($n = 0$, $E_0 = {}^1\!/_2$) is given by $\Psi_0(x) = \pi^{-1/4}\,\mathrm{e}^{-\frac{x^2}{2}}$, which is a normal distribution centered at the minimum of the potential ($x = 0$), and with a variance $\sigma = {}^1\!/_{\sqrt{2}}$. The osmotic velocity is $u(x) = -x$, and the motional process can be determined solving

$$\mathrm{d}X(t) = u(X)\mathrm{d}t + \mathrm{d}W_f(t) \; , \quad X(0) = x_0 \in \mathbb{R} \quad . \tag{4.84}$$

A simulated representative trajectory and the mean path are displayed in **Figure 4.3**. The mean path was calculated as the average over 1000 individual trajectories. Relying on the procedure described above, the Heun method was utilized using equidistant time increments, $\Delta t_i = h = 0.001$ for all $i = 0, \ldots, N$. During the simulations, the

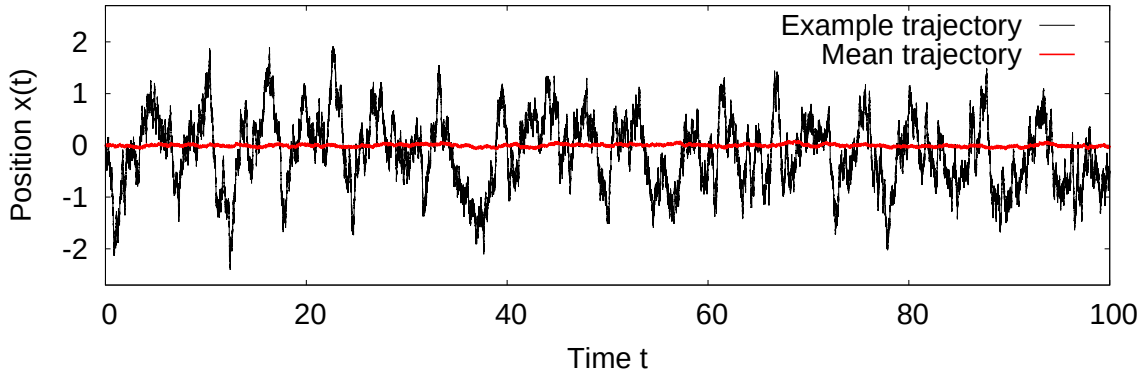

Figure 4.3.: *Single (black) and average (red) trajectory of a particle experiencing a one-dimensional harmonic oscillator potential. The mean trajectory is an average of* 1000 *paths, each of which consists of* 10^5 *time steps with time increment* $h = 0.001$.

starting point is chosen as $x_0 = 0$. (The choice of the initial condition is arbitrary and has no influence on the results) As seen in **Figure 4.3**, the mean path is nearly zero, and the difference between the single and the averaged trajectory is the smaller the more paths are generated, i.e. the algorithm converges to the wanted solution. In the classical stationary ground state ($x \equiv 0$), the particle rests at the minimum of the potential. Hence, the quantum-mechanical motion process fluctuates around the classical state with a certain probability density, the latter being equal to the square of the absolute value of the wave function. On average, the quantum-mechanical motional process coincides with the classical one. The probability density can be determined from the generated paths by calculating the normalized position histogram, cf. **Figure 4.4**. The so-obtained position histogram is normalized to an integral area equal to one. Obviously, the simulation result agrees well the analytically calculated, exact probability density.

Incorporating the methods introduced above, the osmotic velocity as well as the probability density will be determined numerically by analyzing the stationary Hamilton equations of motion,

$$\mathrm{d}X(t) = u(X(t))\mathrm{d}t + \mathrm{d}W_f(t) \ , \quad X(0) = x_0 \in \mathbb{R} \quad , \tag{4.85}$$

$$\mathrm{d}u(t) = X(t)\,\mathrm{d}t + q(t)\,\mathrm{d}W_b(t) \quad . \tag{4.86}$$

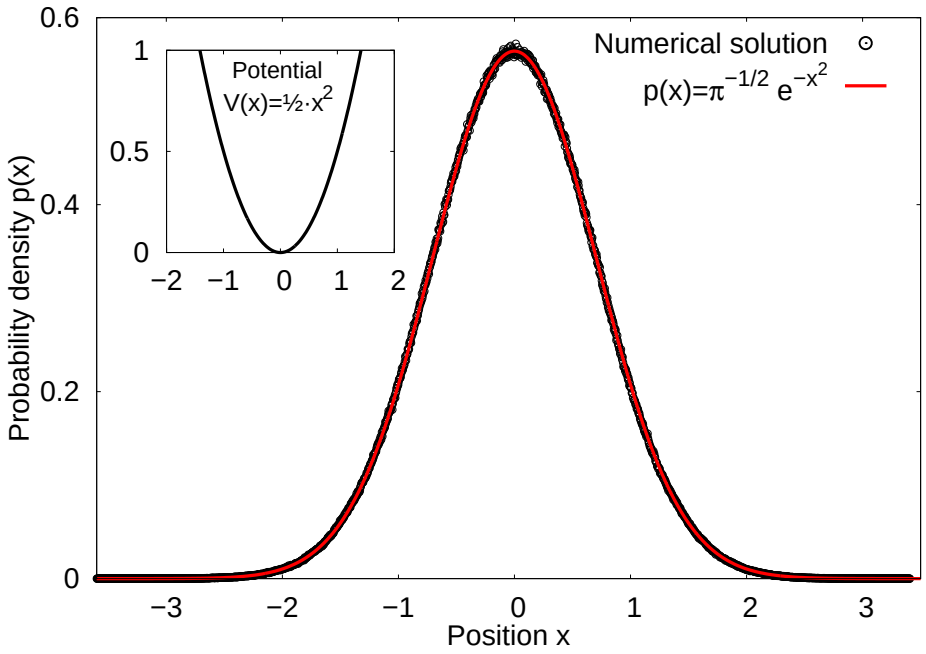

Figure 4.4.: *Simulated (black points) and exact (red curve) probability density for the one-dimensional harmonic oscillator. Additionally, in the upper left corner, the potential* $V(x) = x^2/2$ *is presented.*

Solving the ODE

At first the osmotic velocity is calculated by addressing the associated ODE in each single iteration step, the overall iteration scheme is repeated 100 times. Finally, all presented results are averaged over the individual simulations.

The results after different numbers of iterations and the exact solution of the osmotic velocity are shown in **Figure 4.5**. Computing not more that 10 iterations, the numerical result coincides with the exact one in a certain range. The more iterations are performed the larger is the range over which sufficient agreement between the simulated and analytical result is obtained. Since the initial estimate of the velocity equals the classical stationary ground state ($u^0 \equiv 0$), the simulation curve drops down to zero outside the range of convergence. Even though the standard deviation is considerably larger outside this domain, it decreases over the entire x-domain with an increasing number of repetitions. Both features are reflected in the inset of **Figure 4.5**, where all individual simulations are independent from each other

Using the osmotic velocity estimated after 1000 iteration steps, there are two opportunities to approximate the probability density. In option 1, 10 000 trajectories of the motional process[8], each with 20 000 time steps and time increment $h = 0.01$, are

[8] Alternatively, it is also possible to calculate a single, but very long path of the motional process.

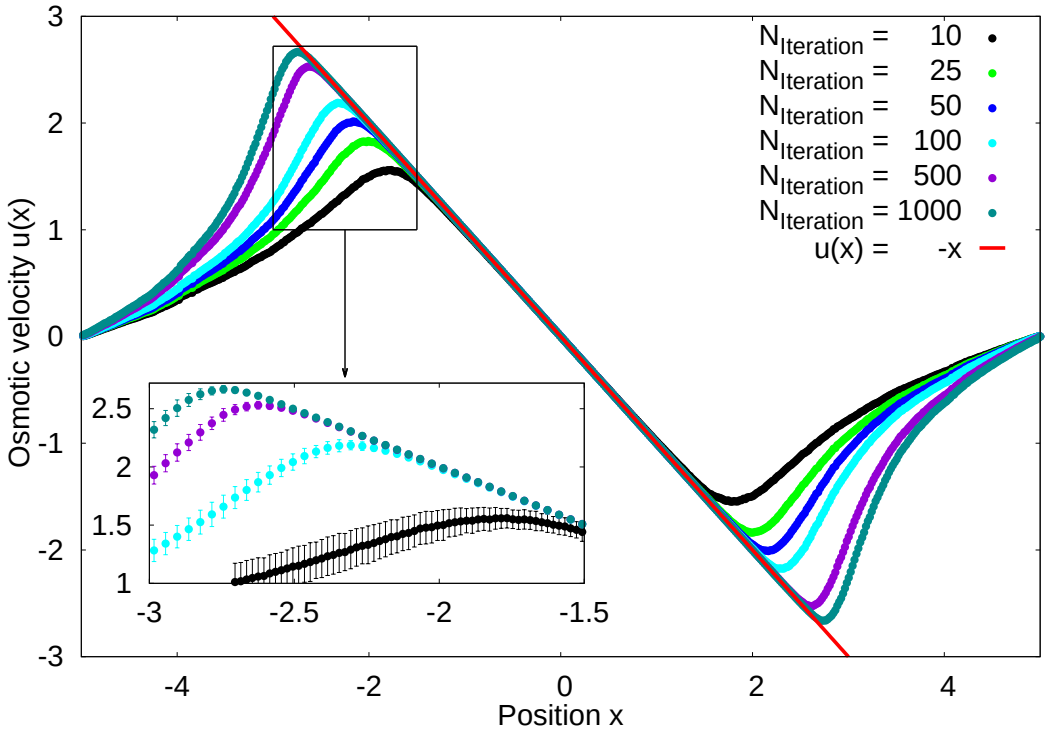

Figure 4.5.: *Numerical solution of the osmotic velocity (points) for the one-dimensional harmonic oscillator in the stationary case as a function of the number of iteration steps as compared to the exact solution (red line). The solution to the backward equation was determined by analyzing the associated ODE. The presented results are arithmetic averages of 100 independent simulations. In each iteration step, 1500 paths of the motion process with 3000 equidistant time steps ($h = 0.002$) are calculated. Inset: Zoomed section of the plot after 10, 100, 500 and 1000 iteration steps, where error bars reflect the standard deviation calculated from the spread of individual simulations.*

generated by numerically solving the forward SDE with the approximated velocity. In **Figure 4.6**, the probability density from this approach – given by the normalized position histogram – is compared to the exact solution calculated from the Schrödinger equation. The numerical result is in good agreement with the ground-state probability density. Relevant discrepancies occur only in a range outside of the 3σ-domain[9]. In the presented case, we have $\sigma = \sqrt{1/2} \approx 0.7071$ and hence, the 3σ-domain spans a range about $[-2.12\,,\,2.12]$. Furthermore, the numerical solution of $p(x)$ depends on new parameters such as the length of the generated paths, with in fact occurs as a parameter in the numerical approach to the forward equation.

In option 2, the probability density is determined by numerical integration using

[9]For normally distributed random numbers, 99.73% of all events are found inside the 3σ-interval.

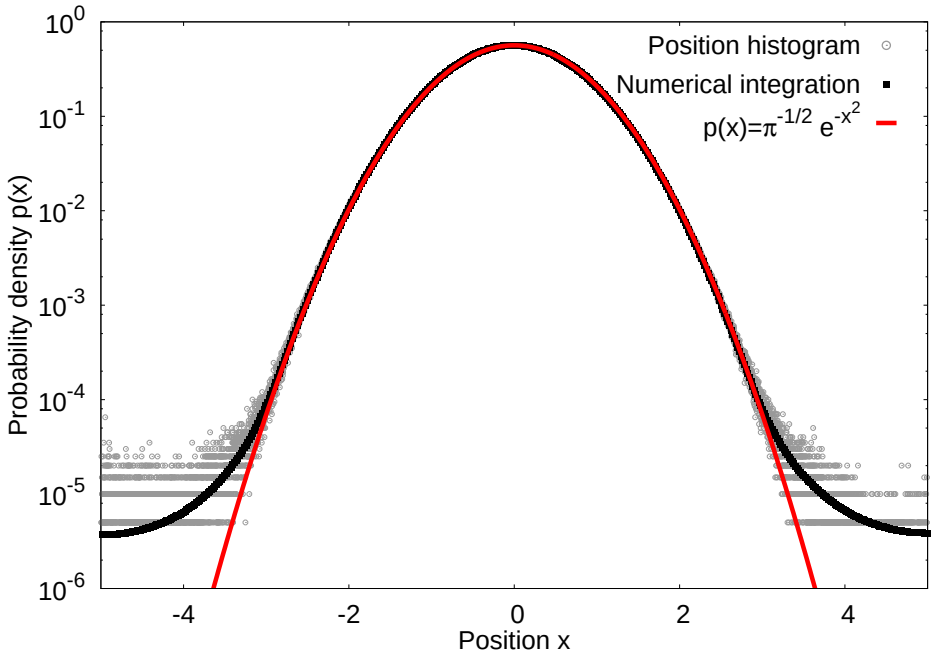

Figure 4.6.: *Probability density determined by either numerical integration (black points) or by elaborating a position histogram (gray points) are compared to the analytical result (red line) for the case of a stationary one-dimensional harmonic oscillator. Both cases rely on the osmotic velocity that is computed on the basis of 1000 iteration steps. The backward equation is solved by analyzing the associated ODE. The logarithmic representation emphasizes systematic deviations occurring at the regions at which the probability density is low.*

$$p(x) = |\Psi(x)|^2 = c_0 \exp\left\{2 \int_{-\infty}^{x} u(x')\mathrm{d}x'\right\} \quad . \tag{4.87}$$

Since $\int_{-\infty}^{\infty} p(x)\mathrm{d}x = 1$ the normalization constant c_0 is calculated as

$$c_0 = \left[\int_{-\infty}^{\infty} \exp\left\{2 \int_{-\infty}^{x} u(x')\mathrm{d}x'\right\}\mathrm{d}x\right]^{-1} \quad . \tag{4.88}$$

The so-obtained probability density (cf. again **Figure 4.6**) coincides with the exact solution within almost the entire range of validity found by the previous procedure. However, the quality (in terms of accuracy) of the normalized position histogram first of all depends on the statistical properties of the sampling, while a better convergence of the osmotic velocity does not necessarily improve the result of the probability density. In order to expand the range of coincidence between the analytical and the numerical result, more or (and) longer paths have to be generated, thus increasing the computational effort. The solution determined by *numerical integration* depends only on the quality of the osmotic velocity, and, in addition, the numerical integration is very simple. Thus, numerical integration as done in option 2 is preferred over option 1.

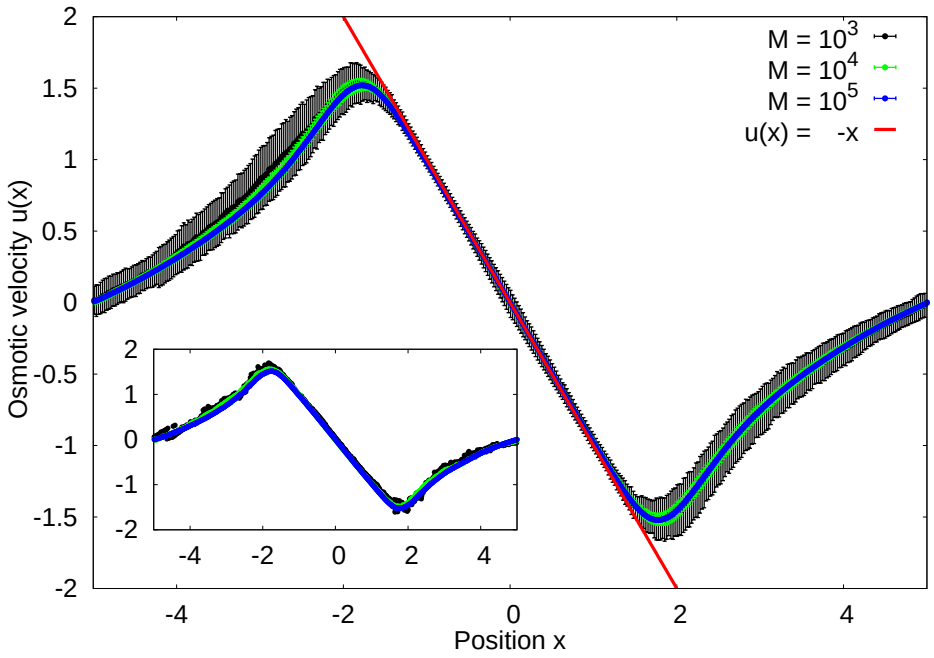

Figure 4.7.: *Osmotic velocity for the stationary one-dimensional harmonic oscillator from M trajectories, each with 10 iteration steps and 100 overall simulations that were finally averaged. The exact solution (red curve) indicates the range in which the algorithm yields correct results. Error bars reflect the spread of the 100 overall simulations underlying the here presented data. Inset: Outcome of a single simulation results out of the ensemble.*

As the next step, the effect of parameter variations on the calculated osmotic velocity is examined. Simulations with different numbers of paths M are calculated and presented in **Figure 4.7**. These simulations consist of 100 overall simulations, each of which with ten iteration steps that in turn require M trajectories to be calculated. It can be seen that the results have almost the same range of convergence; however, the standard deviation determined by repeating the simulation 100 times becomes the smaller the more trajectories are accounted for in each iteration step. In the inset of **Figure 4.7**, the outcome of *one* out of the 100 simulations relying on $M = 10^3$, 10^4 and 10^5 trajectories is shown. An increasing number of trajectories renders each simulation result more stable, as well as the simulated osmotic velocity becomes smoother (and more precise). Henceforth, testing the influence of also other parameters on the simulation outcome $u(x)$, 10^5 paths are calculated in each iteration step.

Results concerning a variation of the time increment h are plotted in **Figure 4.8**. If the time increment is too small, no suitable results will be obtained, as well as the simulation may diverge (as for the latter case, see the simulation outcome using $h = 0.002$). Nonetheless, if the time increment is set to values between 0.004 to 0.009,

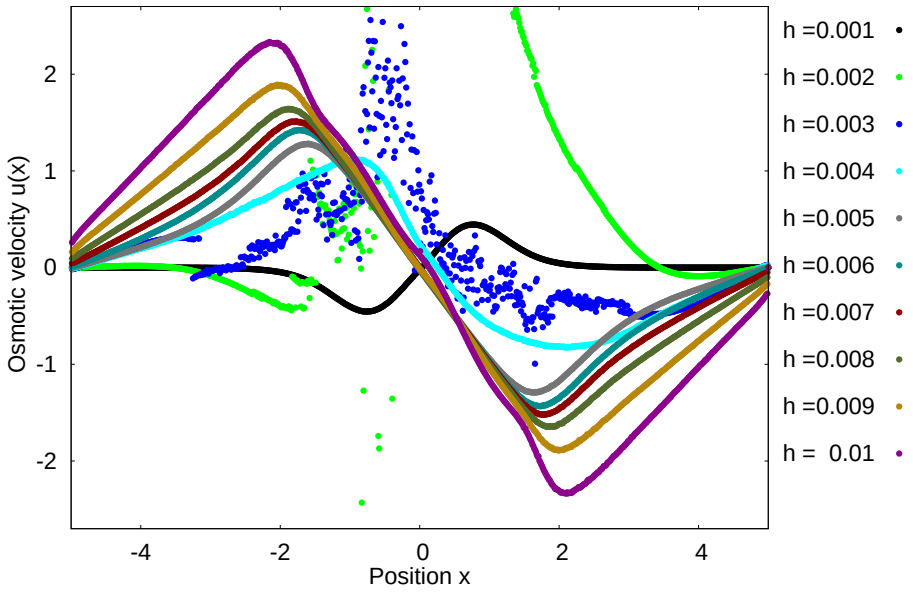

Figure 4.8.: *Osmotic velocity for the stationary one-dimensional harmonic oscillator for different time increments h after 10 iterations. The backward equation is solved by analyzing the associated ODE. The presented velocities are arithmetic averages over 100 single simulations.*

sufficient agreement with the analytically calculated osmotic velocity is obtained, where the range of convergence increases with increasing h. If h becomes larger than 0.009, significant deviations occur that are caused by the reduced precision of the Heun method underlying the here presented calculations. Similar behavior is revealed by varying the number of time steps, N. In **Figure 4.9** results for different N can be seen; the inset in **Figure 4.9** gives a rough overview over a broad range of N. Both, a small and a quite large number of steps per trajectory yield misleading results. If each path consists only a few simulation steps, the estimate stays close to zero (see, for instance, $N = 100$), while a large value of N is accompanied by divergence of the simulation.

In summary, for trajectories of a suitable length (parameter N), the range of convergence will become large with increasing $T = N \cdot h$. Simulations evaluating the ODE are quite sensitive to parameter changes, and only a small set of tuples (N, h) provides reliable simulation results. This situation is ascribed to the non-linearity of the ODE. If more paths are generated in each iteration step, each single simulation becomes more stable. This, in turn, renders longer trajectories more feasible from a technical point of view, while the number of single simulations required for sufficiently precise results can be reduced. On the other hand, computing a plethora of trajectories significantly increases the computational effort per simulation, while only modest improvements on the finally obtained velocity might be achieved.

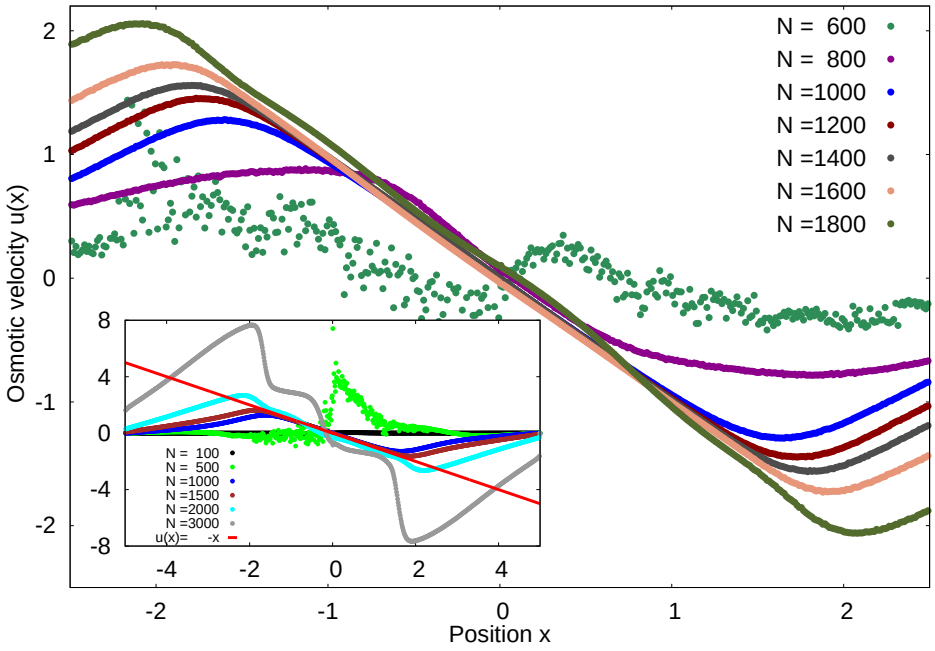

Figure 4.9.: *Osmotic velocity for the stationary one-dimensional harmonic oscillator as determined using different numbers of time steps N in each path, and using 10 iterations. The backward equation is solved by analyzing the associated ODE. The presented velocities are arithmetic averages over 100 single simulations. Inset: Simulated $u(x)$ for $100 \leq N \leq 3000$ (points) and exact solution (red curve).*

Direct evaluation of the BSDE

As mentioned above, the osmotic velocity can also be determined by solving the backward equation itself. **Figure 4.10** shows the impact of the number of iteration steps (parameter $N_{\text{Iteration}}$) on the so-obtained simulation result along with the analytical, exact solution. Because a high number of realizations of the motion process is needed for the numerical calculation of the backward equation, the forward SDE is solved using an Euler-Maruyama method to save computational time.

Within a certain range around the center of the harmonic potential, the numerical solution coincides well with the exact one. Outside this range, however, the simulation drops down to zero, which is the chosen initial estimate of $u(x)$. This situation is also reminiscent of the previous simulations. In addition, the inset in **Figure 4.10** shows part of the results after 10, 50 and 200 iteration steps. Simulation uncertainties ("error bars") stay almost the same over the entire range of x-values; already a small number of iterations (e.g. $N = 10$) turns out to be sufficient for an acceptable range of convergence. Within the range of good agreement between the simulated and the analytical result, error bars are small and have almost the same value, irrespective of the specific position. As before, the range of convergence of the osmotic velocity

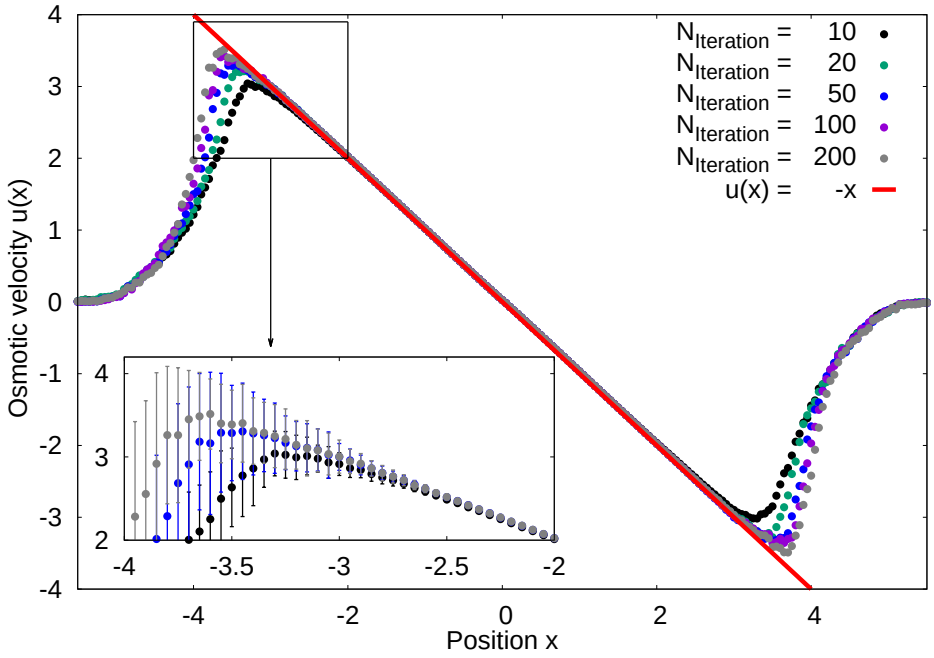

Figure 4.10.: *Numerical solution of the osmotic velocity for the one-dimensional harmonic oscillator in the stationary case after different numbers of iteration steps, and exact solution (red line). The solution to the backward equation was directly determined using a method for coupled FBSDEs. Inset: Part of the results after 10, 50 and 200 iteration steps, including the standard deviation indicated by error bars. The presented results are arithmetic averages of 100 single simulations. The displayed errors correspond to the dispersion of single simulations. In each iteration step,* 10^6 *paths of the motion process with 100 equidistant time steps* ($h = 0.01$) *are calculated.*

gets larger the more iteration steps are made during the simulation. Because of the high number of realizations, the range of convergence is larger than the corresponding domain from the ODE.

Evaluating the velocity calculated after 200 iteration steps, the probability density can be computed either by determining a position histogram of the quantum particle, or by numerical integration of equation (4.87). Results from both methods are compared to the quantum-mechanical solution in **Figure 4.11**. Here, the advantage of the numerical integration becomes obvious: the range of agreement between the simulated and the analytically calculated result is larger for the numerical integration method than for the normalized position histogram. While the accuracy of $p(x)$ determined from the position histogram is comparable for both methods available for the backward equation, the probability density determined from numerical integration is much better for the direct analysis of the BSDE. The position histograms in **Figure 4.6** and **Figure 4.11** rely on the same number of integration ("time") steps, yielding a similar quality for both cases. This is contrasted by the fact that numerical integration relies on the

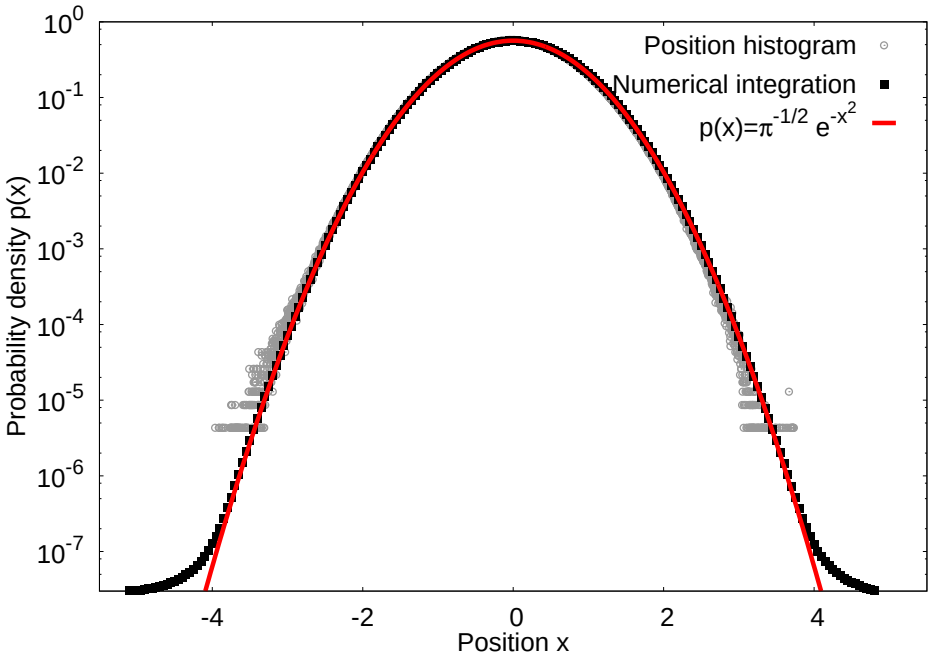

Figure 4.11.: *Probability density determined by either numerical integration (black points) or by elaborating a position histogram (gray points) are compared to the analytical result (red line) for the case of a stationary one-dimensional harmonic oscillator. Both cases rely on the osmotic velocity that is computed on the basis of 200 iteration steps. A logarithmic representation is chosen to emphasize differences between the numerical and the analytical result at regions with a small probability density.*

osmotic velocity only. Evaluating the osmotic velocity directly, $u(x)$ converges faster due to the larger number of generated trajectories during the iteration. Thus, the range of excellent agreement of the probability density with the analytical result is increased.

The larger number of generated paths is required to ensure a certain order of convergence of the solution to the backward equation [Bender and Steiner, 2012]. The simulation quality depends also on the number of steps used for calculation of each trajectory. The more steps are made, the more paths have to be calculated. Later on, correlations between the number of generated paths and other parameters (e.g. N, L) will be discussed in more detail.

Aiming for optimal computational times, it is of high technical interest to explore if simulations relying on a reduced number of trajectories will still provide suitable results. Therefore, the above simulation is repeated with $M = 10^3$, 10^4, 10^5, with the results after 10 iteration steps being presented in **Figure 4.12**. Here, the previous simulation incorporating 10^6 simulation steps serves as a reference relative to the exact solution, thus reflecting the algorithm's benchmark accuracy. As expected, increasing

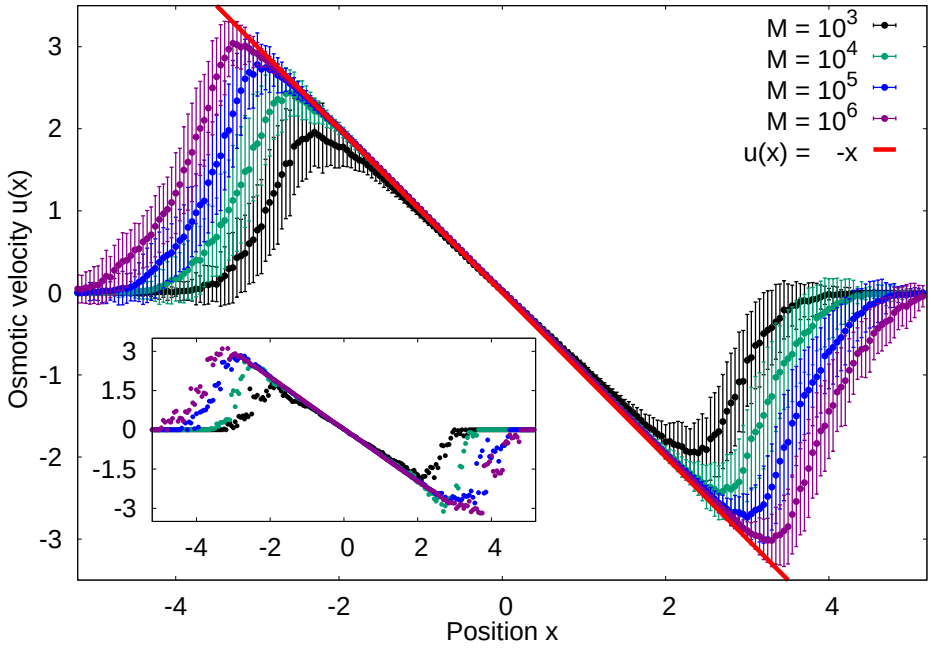

Figure 4.12.: *Osmotic velocity for the stationary one-dimensional harmonic oscillator for different M after 10 iterations, including the standard deviation reflected by error bars and the exact one (red line). The BSDE is solved directly, where 100 time steps with an increment $h = 0.01$ were calculated for each trajectory. The presented results are arithmetic averages over 100 single simulations. The displayed error is given by the spread of the single simulations. Inset: Result of a single simulation for each M.*

M yield enlarged convergence ranges. Furthermore, it should be noted that the slope is too small in the case of $M = 10^3$. Additional iteration steps do not considerable improve the simulation result. **Table 4.1** summarizes the slope and intercept of the resulting osmotic velocity as determined from a linear fit to the simulated data in the convergence region. It follows that the slope increases with an increasing number of paths generated in each iteration. As said before, the number of the minimum number of paths sufficient for precise simulation depends on the number of time steps and has to be sufficiently large in order to achieve a suitable $u(x)$ [Bender and Steiner, 2012]. For paths with 100 time steps each, at least 10^4 trajectories have to be calculated.

M	10^3	10^4	10^5	10^6
Slope	-0.933 ± 0.001	-0.984 ± 0.001	-0.990 ± 0.001	-0.993 ± 0.001
Intercept	0.025 ± 0.001	0.025 ± 0.001	0.023 ± 0.001	0.024 ± 0.001

Table 4.1.: *Slope and intercept with the ordinate for the osmotic velocity from **Figure 4.12** as determined by linear fits.*

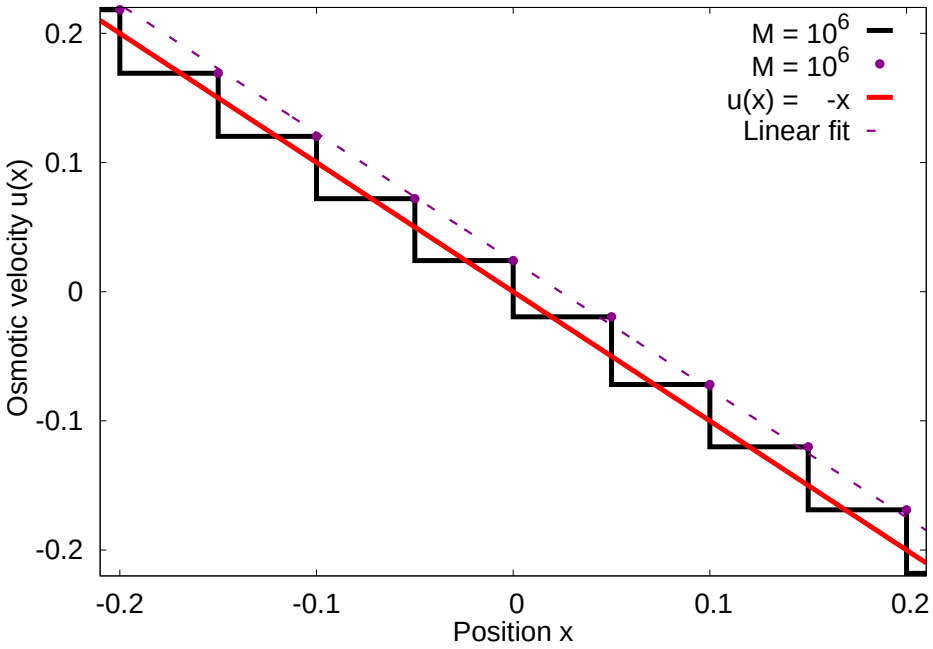

Figure 4.13.: *Osmotic velocity as a step function (black line) for the stationary one-dimensional harmonic oscillator for $M = 10^6$ as compared to the exact solution (red line). Additionally, the resulting fit function (purple dashed line) and data points (purple points) used for the linear fit are depicted. The here shown $u(x)$ is identical to that one presented in* ***Figure 4.12*** *for $M = 10^6$; however, only the x-range close to zero is shown.*

In contrast to the well-behaved slope, the osmotic velocities have an intercept different from zero. Note that the intercept is found to be about 0.025 irrespective of the choice of M, which is half of the chosen interval width δ. The intercept arises because of the step character of the resulting osmotic velocity, with particular impact of the chosen intervals length δ. In practice, the intervals are constructed using $D_l := [x_{\min} + (l-1)\,\delta\,,\, x_{\min} + l\,\delta]$ for $l = 1, \ldots,\ L$, i.e., the intervals are not symmetric around the ordinate. The data points used for the linear fit are in accordance with the (right) endpoints of the x-intervals, where the velocity has a constant value. Hence, the fit function is shifted towards higher values, leading in turn to an increased, non-zero intercept. The bias effect is determined by the interval length, thus, simulations with the same value of the data yield (almost) the same intercept. This effect is well seen in **Figure 4.13** using simulation results with $M = 10^6$ trajectories and 10 iteration steps, with the x-range being chosen in such a way that the discontinuous, steplike behavior of $u(x)$ becomes obvious. The unwanted effect of the steplike behavior of the numerical velocity can be minimized by increasing the number of intervals (reducing the interval width) and by a symmetric position of the intervals around the point of origin.

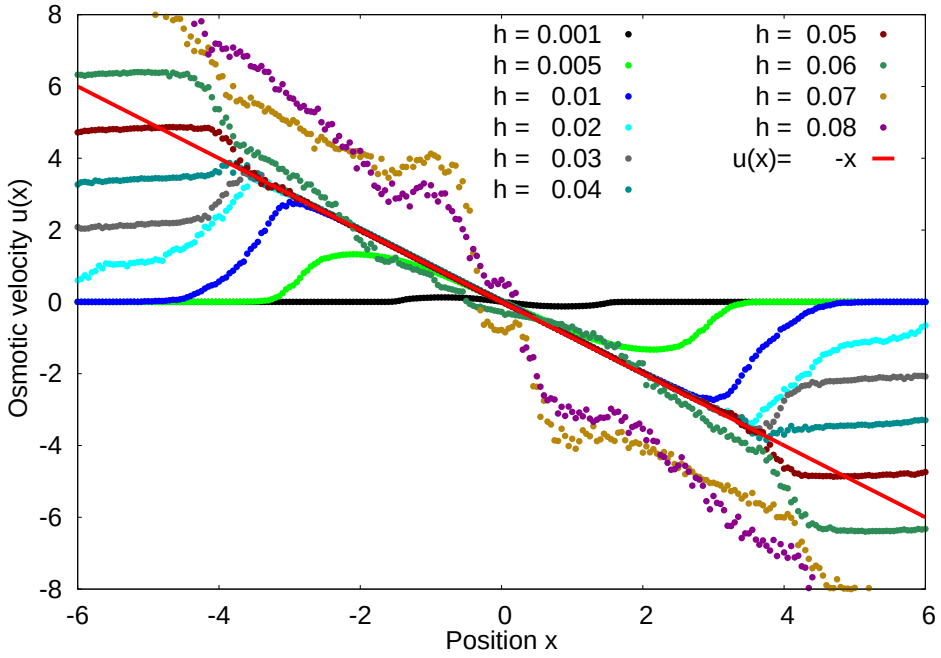

Figure 4.14.: *Osmotic velocity for the stationary one-dimensional harmonic oscillator for different values of h after 10 iteration steps, including also the exact result (red line). In each iteration step, 10^5 paths with 100 time steps are determined and the BSDE is solved directly. The presented results are arithmetic averages over 100 single simulations.*

Several aspects impact the errors accumulated during computation of the backward equation. First, the used values of the forward process are determined numerically by exploiting the Euler-Maruyama method, which has a strong order of convergence of one half.[10] At the same time, the the backward equation is discretized on the basis of an Euler-Maruyama-method, which causes numerical inaccuracy. Solving the difference equation of the backward process, the conditional expectation has to be evaluated numerically. The simulation error of the backward equation will scale as $N^{-\rho/2}$ for $\rho \in [0, 1]$, if the number of intervals L increases proportional to N^{α} ($\alpha \geq 0$), and the number of paths M increases proportional to $N^{2+2\alpha+\rho}$ [Bender and Steiner, 2012]. The number of computed paths increases quickly with a growing number of time steps. The osmotic velocity is calculated using an iterative method, i.e., the quality of the results depends also on the number of iterations. As a consequence, a quantitative estimate of the overall error of the osmotic velocity is hard to achieve and is beyond the scope of this thesis.

Finally, the influence of the length of the single path $T = h \cdot N$ on the numerical results will be studied. For this purpose, the time increment h is varied for a fixed number of

[10] More information on the convergence of SDEs can be found in the appendix, section A.4.

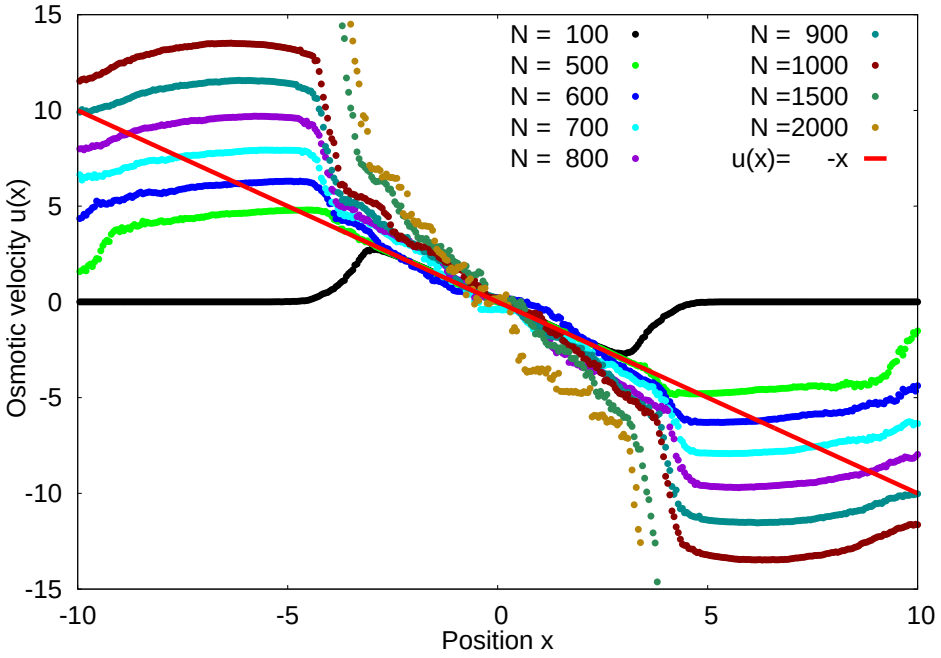

Figure 4.15.: *Osmotic velocity for the stationary one-dimensional harmonic oscillator for different N (denoting the number of time steps) after 10 iteration steps as compared to the exact result (red line). The BSDE is solved directly, where 10^5 paths are calculated in each iteration using the equidistant time increment $h = 0.01$. The presented results are arithmetic averages over 100 single simulations.*

time steps (see **Figure 4.14**), while the number of time steps is increased for a fixed h (see **Figure 4.15**). Both have nearly the same effect. If the time increment h is in a certain range ($h \in [0.01, 0.06]$), the simulations will provide suitable results, where the range of convergence increases with an increasing time increment. If h is too large, however, numerical errors will arise in the calculation of both, the forward and the backward equation. If h is too small, randomness has no effect and the particle stays allmost all the time in the classical ground state (see **Figure 4.14**, $h = 0.001$). It is recommended to extend the trajectory length by increasing the number of time steps to make use of the effect discussed above. Additional time steps are accompanied by an increased number of generated paths; otherwise, misleading results are obtained; see **Figure 4.15** ($N \geq 600$).

Concluding this section, solving the BSDE directly is the preferred method for the following reason: First, the simulation is less prone to parameter changes, rendering the calculations more stable and reducing the risk of fallacy; second, longer trajectories can be computed despite potentially high computational effort; third, solving the ODE arising from Itô's formula is nothing else than solving the gradient of the Schrödinger equation; forth, for non-stationary problems, a PDE has to be solved numerically which is very complex, and, last but not least, a method achieving the wave function without

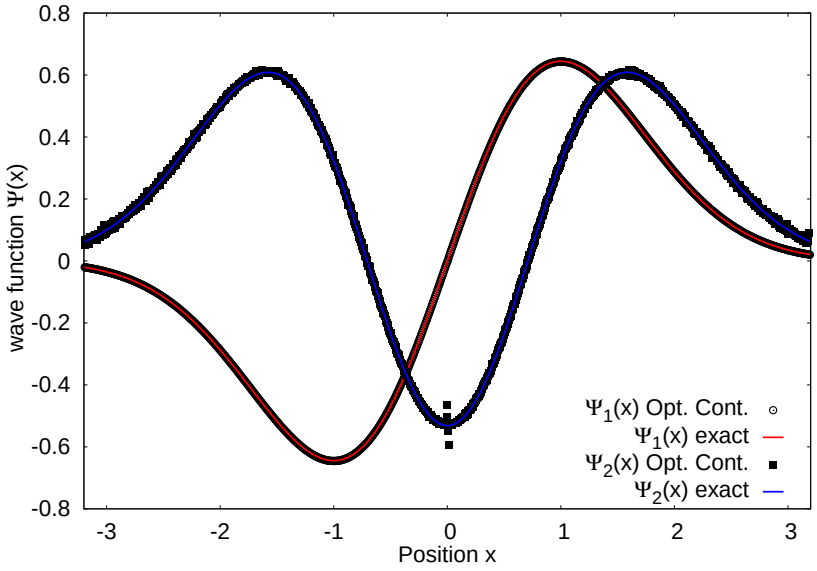

Figure 4.16.: *First and second excited state for the one-dimensional harmonic oscillator.*

using the Schrödinger equation itself has been one the major goals of this thesis.

Excited states

Figure 4.2 shows schematically how the ground-state solution can be used to find the excited states by quantifying the ground state of a modified potential [Grigorenko, 1991]. Using equation (4.43) (the equation for the superpartner of the Hamilton operator), the modified potential for the harmonic oscillator reads

$$V_1(x) = V(x) - \hbar \frac{\mathrm{d}u_0(x)}{\mathrm{d}x} = V(x) + \hbar\omega \quad . \tag{4.89}$$

Since the drift term of the BSDE for the osmotic velocity is given by the derivative of the potential, the osmotic velocity in the modified potential equals the original one. Hence, the ground state of $\hat{H}_1$ is given by the ground state in the original potential $\Psi_0(x)$. Consequently, no further optimization is required and the excited states can be directly calculated using the transformation given by equation (4.45), i.e.,

$$\Psi_1(x) = \sqrt{\frac{m}{2\,(E_1 - E_0)}} \left(-u_0(x) - \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right) \Psi_0(x) \quad , \tag{4.90}$$

$$\Psi_2(x) = \sqrt{\frac{m}{2\,(E_2 - E_1)}} \sqrt{\frac{m}{2\,(E_2 - E_0)}} \left(-u_0(x) - \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 \Psi_0(x) \quad . \tag{4.91}$$

In **Figure 4.16**, the numerical results for the first and second wave function are compared to the exact wave functions as calculated from the Schrödinger equation. The results agree well with each other.

Using the theory of supersymmetric Hamilton operators, one can determine the energy spectrum of the harmonic oscillator [Sukumar, 1985a; Cooper et al., 1995]. The n-times modified potential is given by $V_n(x) = V(x) + n\hbar\omega$, so that the energy is given by

$$\begin{aligned} E_n =& \mathrm{E}\left[\frac{m}{2}u_0^2(x) + V_n(x)\right] = \mathrm{E}\left[\frac{m}{2}u_0^2(x) + V(x) + n\hbar\omega\right] \\ =& E_0 + n\hbar\omega = \hbar\omega\,(n\,+\,1/2) \quad . \end{aligned} \tag{4.92}$$

The excited energies can also be calculated using the numerical results and are presented in **Table 4.2**. Additionally, if the exact result for the ground state wave function

$$\Psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left\{-\frac{m\omega}{2\hbar}\,x^2\right\} \tag{4.93}$$

is used, the wave function of the n-th excited state will be given by

$$\begin{aligned} \Psi_n(x) =& \prod_{i=0}^{n-1}\sqrt{\frac{m}{2\,(E_n - E_i)}}\left(\omega x\, -\, \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \Psi_0(x) \\ \overset{(4.92)}{=}& \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{\sqrt{2^n\,n!}}\sqrt{\frac{m}{\hbar\omega}}^{\,n}\left(\omega x\, -\, \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \exp\left\{-\frac{m\omega}{2\hbar}\,x^2\right\} \\ =& \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{\sqrt{2^n\,n!}}\,\exp\left\{-\frac{m\omega}{2\hbar}\,x^2\right\} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \quad , \end{aligned} \tag{4.94}$$

since $\varphi_0^n(x) = \Psi_0(x)$ for all $n \in \mathbb{N}$, with the Hermite polynomials $H_n(x)\,,\ n \in \mathbb{N}$, being defined by equation (4.83). Furthermore,

$$\begin{aligned} \hat{A}^+\Psi_n(x) =& \sqrt{\frac{m}{2}}\left(\omega x - \frac{h}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)\frac{1}{\sqrt{2^n\,n!}}\sqrt{\frac{m}{\hbar\omega}}^{\,n}\left(\omega x\, -\, \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \Psi_0(x) \\ =& \sqrt{\hbar\omega(n+1)}\,\Psi_{n+1}(x) \quad , \end{aligned} \tag{4.95}$$

$$\begin{aligned} \hat{A}^-\Psi_n(x) =& \sqrt{\frac{m}{2}}\left(\omega x + \frac{h}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)\frac{1}{\sqrt{2^n\,n!}}\sqrt{\frac{m}{\hbar\omega}}^{\,n}\left(\omega x\, -\, \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \Psi_0(x) \\ =& \sqrt{\hbar\omega n}\,\Psi_{n-1}(x) \quad . \end{aligned} \tag{4.96}$$

	E_0	E_1	E_2
Numerical result	0.49995	1.4993	2.4987
Exact value	0.5	1.5	2.5

Table 4.2.: *First three energies for the one-dimensional harmonic oscillator determined using the numerical result as compared to the exact values.*

As for the harmonic oscillator, the operators $\hat{A}^{\pm}$ coincide with the creation and annihilation operator[11]. In the literature, the ladder operators are transformed into dimensionless variables, such that the prefactor $\sqrt{\hbar\omega}$ will disappear in equations (4.95) and (4.96).

Utilizing equation (4.47), the functions $S(t)$ can be determined, and, finally, the complete wave function for the n-th state reads

$$\Psi_n(x,t) = \frac{1}{\sqrt{2^n\, n!}} \sqrt{\frac{m}{\hbar\omega}}^{\,n} \left(\omega x - \frac{\hbar}{m}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \Psi_0(x)\, \mathrm{e}^{-i\,n\,\omega\,t}\, \mathrm{e}^{-\frac{i\omega\,t}{2}} \quad . \tag{4.97}$$

4.4.2. One-dimensional double-well potential

A prime example of a Hamiltonian for which no analytically wave function is available is the one-dimensional double-well potential. This potential – shown in the inset of **Figure 4.17** – is given by

$$V(x) = \frac{V_0}{a^4}\left(x^2 - a^2\right)^2 \quad . \tag{4.98}$$

Here, the minima of the potential are located at $\pm a$, with $a = 1.5$, and the barrier height is given by $V_0 = 2.0$. In contrast to the classical solution, where the particle rests in one of the minima, a quantum particle of energy $E < V_0$ can overcome the barrier. Thus, the probability density should be different from zero at the maximum of the potential, and has a maximum in each well.

As before, the osmotic velocity is calculated using the described algorithm, with an initial estimate of the velocity given by $u^0 \equiv 0$. The starting point(s) of the motional process are randomly chosen as one of the classical stationary points of the potential (maximum at $x = 0$, minimum at $x = \pm a$). All presented results are determined by direct evaluation of the BSDE during the simulation, and are given by the mean value of 100 single simulations. The depicted error bars are thus characterized by the spread of the single simulations. Additionally, to save computational time, the forward equation is solved using an Euler-Maruyama method. The probability density is afterwards calculated by numerical integration of equation (4.87) and is plotted in **Figure 4.17** for different numbers M of generated paths. In the inset below, the related osmotic velocities are shown. For small M, one can see that $p(x)$ is determined with increased uncertainty (large error bars) at positions close to, or exactly at, its two maxima. This situation is due to highly asymmetric behavior of single simulations.

[11] The theory of the ladder operators can be found in almost every textbook for quantum mechanics; see e.g. ref. [Nolting, 2013].

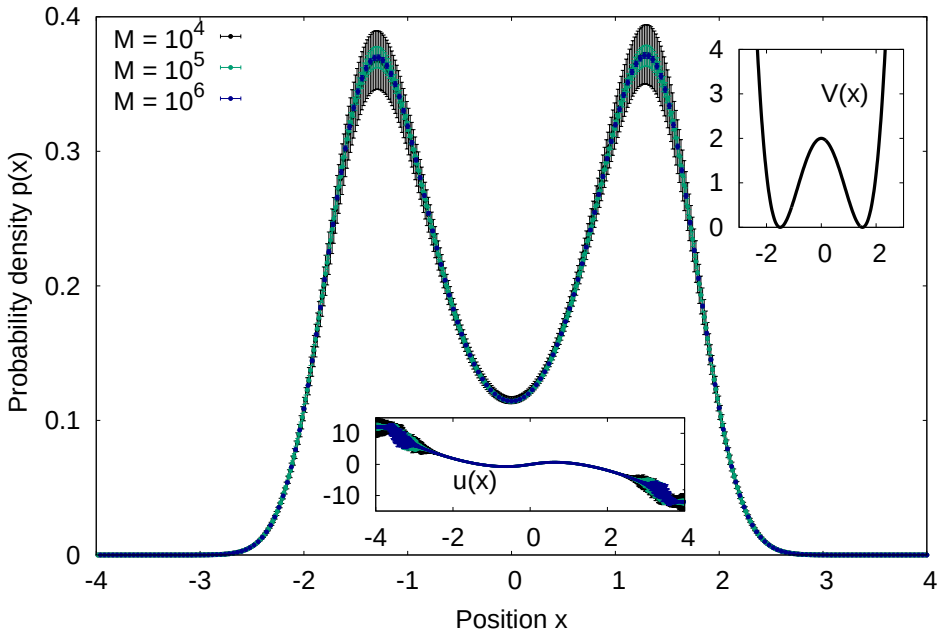

Figure 4.17.: *Probability density for the stationary one-dimensional double-well potential for different values of M (the number of trajectories calculated per iteration) and a fixed time increment $h = 0.01$. 200 iteration steps were applied. The barrier height is given by $V_0 = 2.0$ and the well position is $a = \pm 1.5$. The presented results are arithmetic averages over 100 single simulations and the displayed error is given by the dispersion of the single simulations. The potential is plotted in the inset in the right upper corner and the underlying osmotic velocities are shown in the lower inset.*

The difference of the height of the maxima becomes smaller the more trajectories are averaged. The osmotic velocity diverges for $|x| \to \infty$ and great differences between the single simulations occur in the outer x-range. In **Figure 4.18** the osmotic velocity as calculated for different numbers of iterations is shown. As in the case of the harmonic oscillator, the osmotic velocity has converged over a broad range of x-values even for a small number of iterations. The dispersion between single simulations stays comparable for different numbers of iterations; see also the inset in **Figure 4.18**. However, the more paths are generated in one iteration step, the more extended is the range in which a smooth solution occurs. It seems that there is a point at which $u(x)$, calculated after a few iterations only, experiences a kink, i.e., a point at which $u(x)$ is not differentiable. With an increasing number of iteration steps, the kink vanishes.

It is worth noting that the maxima of $p(x)$ cannot be found directly at the minima of the potential, resulting from the coupling of the two wells by tunneling.

The resulting probability density is compared to the solution calculated using the

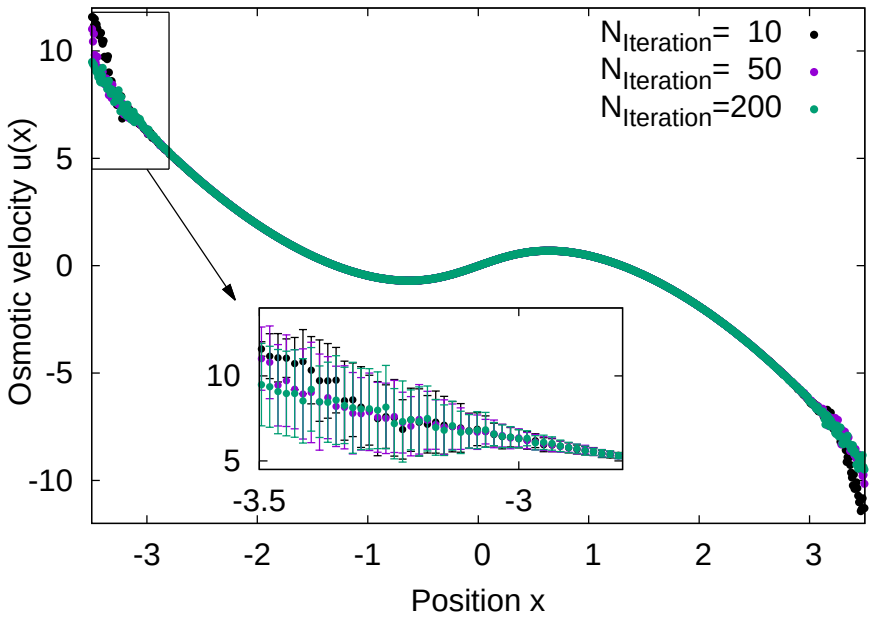

Figure 4.18.: *Osmotic velocity for the stationary one-dimensional double-well potential for different number of iterations, using a time increment $h = 0.01$ and $M = 10^6$ trajectories ($V_0 = 2.0$, $a = \pm 1.5$). Inset: Zoomed area of the main plot including standard deviations. The presented results are arithmetic averages over 100 single simulations and the displayed error is given by the spread of single simulations.*

Numerov method[12], which is a common numerical method for the solution of the stationary Schrödinger equation [Blatt, 1967; Johnson, 1977]. This method is an algorithm for second-order ODEs (without first derivative), is derived using a Taylor expansion and has a high order of convergence (convergence order of five [Blatt, 1967]). The very good agreement of the results of both simulation methods becomes apparent in **Figure 4.19**.

Going on further, the first excited state is determined by identifying the ground state in the modified potential. In contrast to the harmonic oscillator, where the potential is modified by a constant value, the ground state of the new potential has to be calculated by a new optimization run. In **Figure 4.20**, left panel, the so-obtained wave function is compared with that one resulting from the Numerov algorithm. Here, the solution to the osmotic velocity relying on $M = 10^6$ trajectories is used to modify the potential. Since the modified potential reads

$$V_1(x) = V(x) - \hbar \frac{\mathrm{d}u_0(x)}{\mathrm{d}x} \quad , \tag{4.99}$$

[12]More information about the Numerov method can be found in the Appendix, cf. section A.5.

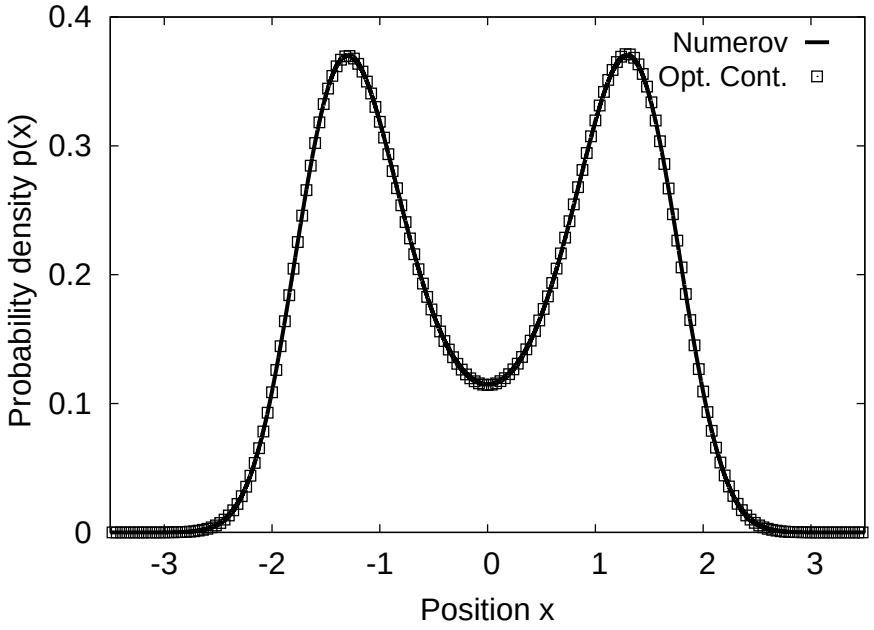

Figure 4.19.: *Probability density as determined by optimal control theory in comparison with the Numerov solution for the stationary one-dimensional double-well potential. 200 iteration steps were performed using $M = 10^6$ trajectories and a time increment of $h = 0.01$. The barrier height is given by $V_0 = 2.0$ and $a = 1.5$.*

and since the drift term of the BSDE is given by the gradient of the potential, the second derivative of the ground state osmotic velocity has to be calculated in order to find the velocity in the modified potential. Hence, fluctuations occur in the wave function (see **Figure 4.20**). For comparison, the ground-state wave function is also plotted in **Figure 4.20 (left)** and the following points should be considered: (i) the maxima of the two wave functions are located at different positions, where the maxima of the first state is closer to the well minima, and (ii), the heights of the maxima are different. Both situations can be explained by considerable coupling between the two wells that is mediated through tunneling processes.

Furthermore, the energy of the ground state[13] can be determined by numerical integration of

$$E_0 = \mathbb{E}\left[\frac{1}{2}u_0^2(x) + V(x)\right] = \int_{-\infty}^{\infty}\left\{\frac{1}{2}u_0^2(x) + V(x)\right\} p_0(x)\mathrm{d}x \quad . \tag{4.100}$$

The first two determined energies are in good agreement the those calculated on the basis of the Numerov method, but at the same time slightly deviate from the values determined by the instanton[14] method; see **Table 4.3**. The instanton method is a path

[13] Calculating E_1 is analogues to determining the ground-state energy.
[14] More information on the instanton solution can be found in the appendix, section A.7.

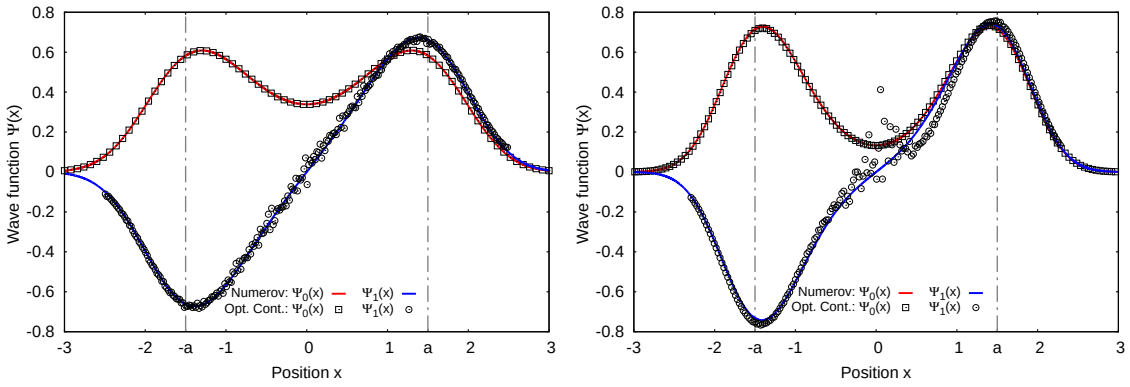

Figure 4.20.: *Wave function of the first two excited states in comparison with the Numerov solution for the stationary one-dimensional double-well potential with $a = 1.5$ and barrier height $V_0 = 2.0$ (**left**) as well as $V_0 = 5.0$ (**right**).*

integral approach with time-located solutions to the classical euclidean equations of motion, which are derived by a Wick rotation [Vaĭnshteĭn et al., 1982]. Even though the resulting Feynman paths [Feynman, 1948] are equivalent to the paths generated by the stochastic equations of motion [Nelson, 1964; Pavon, 2000], the instanton energies are different. An approach to the instanton energies can be found by making use of the following assumptions: (i) Most of the time, the particle stays in one of the two wells, meaning that transitions between the two wells are fast and require only short periods as compared to the considered time horizon, and (ii), in the vicinity of the minimum, the potential can be approximated by a harmonic-oscillator potential [Carlitz and Nicole, 1985]. The resulting energy formulas read [Vaĭnshteĭn et al., 1982]

$$E_0 = \frac{\omega}{2}\left[1 - \sqrt{\frac{2\omega^3 a^4}{\pi V_0}}\, \mathrm{e}^{-\frac{w^3 a^4}{12 V_0}}\right] \quad , \tag{4.101}$$

$$E_1 = \frac{\omega}{2}\left[1 + \sqrt{\frac{2\omega^3 a^4}{\pi V_0}}\, \mathrm{e}^{-\frac{w^3 a^4}{12 V_0}}\right] , \tag{4.102}$$

	E_0	E_1	ΔE
Optimal control	1.10345	1.2762	0.173
Numerov method	1.10342	1.2877	0.184
Instanton	1.198	1.4683	0.27

Table 4.3.: *Numerical result for E_0 and E_1 for the one-dimensional double-well potential, as compared to the outcomes of the Numerov method and the instanton solution.*

with

$$\omega = \frac{\sqrt{8\,V_0}}{a} \quad . \tag{4.103}$$

The instanton energies coincide with those determined using a WKB[15] approximation [Cooper et al., 1995; Garg, 2000]. For clearly separated wells, it is a fruitful method to determine energy splittings [Banerjee and Bhatnagar, 1978; Wang et al., 1992; Park et al., 1998; Garg, 2000]. Because of the presence of the second well, the energy levels are split in both wells, resulting in two energy levels, one lower and one higher than the ground-state energy of the single well. Thus, the ground-state energy in the two wells is considered to be reduced by $^1/_2\Delta E$, i.e. $E_0 = E_0' - {}^1/_2\Delta E$, with an energy splitting ΔE calculated using a WKB-approximation[16] [Garg, 2000] or an instanton method [Vaĭnshteĭn et al., 1982].

This approach is in contradiction to the resulting energies using optimal control theory or the Numerov method (see also **Table 4.3**). The assumptions made in both semi-classical theories are only acceptable if the wells are widely separated from each other. In **Figure 4.20 (right)**, the two first states associated with a potential barrier height of $V_0 = 5.0$ are plotted in comparison with the results using the Numerov algorithm. The more separated the two wells are, the closer the two solutions will be, i.e. the peak of the right-hand side of the potential will be almost the same for both energies. The position of the maxima are closer to the well position and the influence of tunneling becomes less significant.

Tunneling time

Before the energies and the energy splitting will be analyzed for varying potential parameters, the mean first passage time is addressed. **Figure 4.21**, upper inset, shows an example path of the motional process, including two tunneling events. As discussed in section 3.2, the mean first passage time between the two points x_i and x_f can be calculated as [Paul and Baschnagel, 2013]

$$\tau_{\mathrm{mfpt}} = 2\int_{-x_i}^{x_f} \frac{\mathrm{d}x'}{p_0(x')} \int_{-\infty}^{x'} p_0(x'')\,\mathrm{d}x'' \quad . \tag{4.104}$$

Using the associated probability density, the integral can be determined numerically, yielding the mean first passage time from displacements $-a$ to a given in **Table 4.4**. Furthermore, the calculated osmotic velocity can be used to generate a multitude of trajectories reflecting the motional process, which in turn can be used to calculate

[15] named after Wentzel Kramers and Brillouin

[16] WKB-approach is a semi-classical approach in quantum mechanics; see, for instance, ref. [Landau and Lifschitz, 1979] or appendix, section A.6.

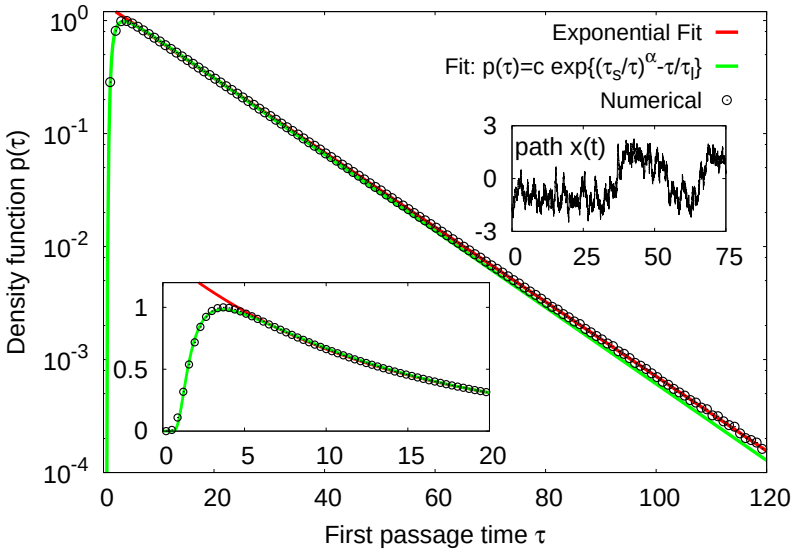

Figure 4.21.: *Density function of first passage times for the one-dimensional double-well potential with $V_0 = 2.0$ and $a = 1.5$, exponential fit (red line) and best fit using equation (4.106) (green line). The solution to the osmotic velocity for $M = 10^6$ is used to calculate 10^6 paths, each with 10^6 time steps (time increment: $h = 0.005$).*

first passage times. The resulting density function of first passage times is shown in **Figure 4.21** (black points). Except of very short periods, the first passage times of a double-well potential are exponentially distributed (see **Figure 4.21**), which is a characteristic property of tunneling processes. For instance, radioactive decays are commonly well-described by an exponential relationship. **Figure 4.21** presents a logarithmic representation of $p(\tau)$, rendering a mono-exponential relationship obvious. The initial regime can be thought to differ from the exponential behavior since high energies are required to overcome the barrier within a short period, rendering such kind of tunneling improbable. At the same time, such concept assumes that the particle moves with high velocity from one well to the other. Of course, the velocity cannot overcome a certain threshold, meaning that a maximum in the density function *must* occur.

	Mean first passage time τ	Standard deviation $\sigma(\tau)$
Definition	14.841	–
Empirical data	15.038	13.194
Exponential fit	15.258	13.042
Non-exponential fit	14.768	12.841

Table 4.4.: *Mean first passage time for the one-dimensional double-well potential determined using different methods. The density function was calculated by numerical integration using the Simpson method.*

For sufficiently large times, the density function can be described by an exponential function, i.e.,

$$p_{\mathrm{exp}}(\tau) = k\,\mathrm{e}^{-l\,\tau} \quad . \tag{4.105}$$

Its expectation value is given by k/l^2; the standard deviation equals $\sigma_{\mathrm{exp}}(\tau) = \sqrt{2k/l^3 - k^2/l^4}$.

For short times, another fitting function is required. Empirically, it turns out that the data can be well fit using

$$p(\tau) = c\,\exp\left\{-\left(\frac{\tau_s}{\tau}\right)^{\alpha} - \frac{\tau}{\tau_l}\right\} \quad . \tag{4.106}$$

The time scales τ_s and τ_l characterize the initial rise and final decay of the density function, respectively, while α describes the sharpness of the peak, and c is a normalization. The non-exponential fit (equation (4.106)) describes the data almost exactly for small tunneling times, even though the mono-exponential fit yields better accordance for the later exponential decay. For the purpose of smoothing, a moving average is used in the calculation of the presented density function.

The mean first passage time can also be calculated as the arithmetic average of all detected single tunneling times. Mean values and standard deviations as obtained from the different methods are summarized in **Table 4.4**, and are in good agreement with each other.

Bear in mind that the particle is described as a classical one. Thus, in the here discussed model, tunneling processes are enabled by (cumulative) quantum fluctuations that permit the particle to reach a spontaneous energy high enough to overcome the potential barrier. Energy splittings have been physically explained by tunneling processes, meaning that there should be a direct link between ΔE and the tunneling period. It has been assumed that $\Delta E = \hbar\pi/\tau$ [Paul and Baschnagel, 2013]). However, both methods – stochastic representation and the instanton method – do not reproduce the value of the above determined mean first passage time.

Different well positions and barrier heights

To analyze the relation between both quantities, the dependence of the energy and the mean first passage time on the potential parameters (barrier height and well position) needs to be explored. Therefore, the first two energies for different well positions (fixed barrier height $V_0 = 2.0$) and different barrier heights (fixed $a = 1.5$) are determined by

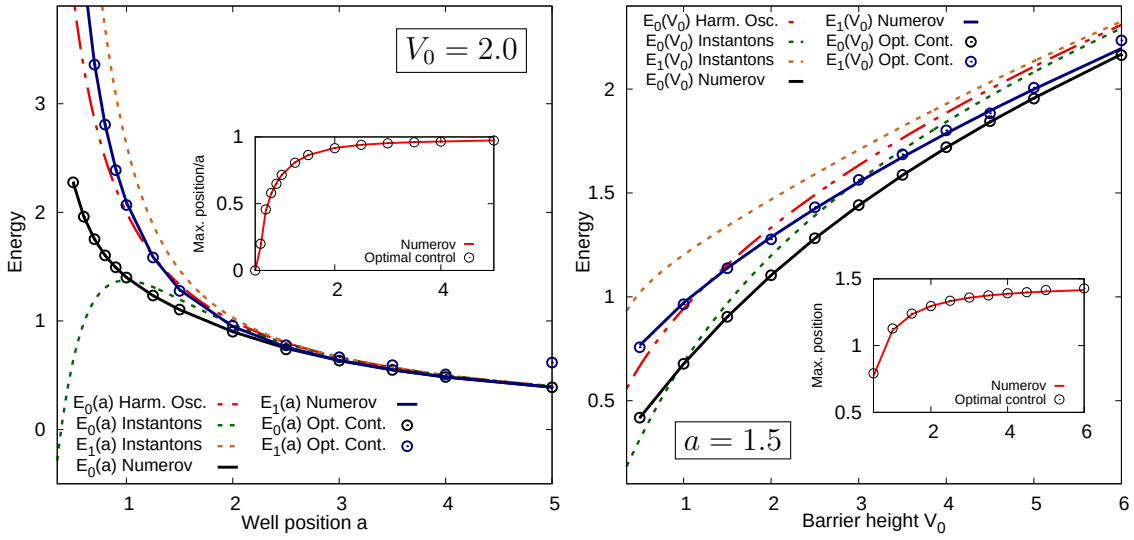

Figure 4.22.: *Energies for the ground (black) and first excited state (purple) as calculated from the quantum Hamilton equations of motion (symbols) and the Numerov algorithm (lines) for the one-dimensional double-well potential in comparison with the results of the instanton method (light blue and blue lines), and the ground-state energy of an isolated harmonic oscillator (red line).* ***Left:*** *As a function of different well-positions a.* ***Right:*** *As a function of different barrier heights V_0. The position of the maximum of the ground-state functions is depicted in the insets.*

solving the quantum Hamilton equations of motion for all different parameters. The results are compared with the energies calculated using the Numerov algorithm and the instanton method; see **Figure 4.22**. It turns out that the energies determined from the stochastic Hamilton equations of motion are in excellent agreement with those calculated from the Numerov algorithm, even if a broad range of values a and V_0 is considered. Still, deviations occur in the wave function for high values a and V_0 (cf. **Figure 4.23**). As an overview, the wave functions of the ground and the first excited state are shown in **Figure 4.23** for a plenty of different parameter combinations.

In the case of $a = 0.5$, the wave function has only one maximum. With increasing values of a, two maxima occur and separate from each other. The ground-state energy (**Figure 4.22, left panel)**) increases with a decreasing distance between the two wells. For $a \leq 0.5$, the ground-state energy exceeds the barrier, and only a single maximum remains. The calculated energy increase is explained by Heisenberg's uncertainty principle. It says that the more precisely the position of a particle is known, the less precise the momentum is defined, and thus the energy of the particle: $\Delta x \Delta p \geq \frac{\hbar}{2}$ must be fulfilled. In the case of small values of a, the two wells approach each other, leading to localized particles with increased energies.

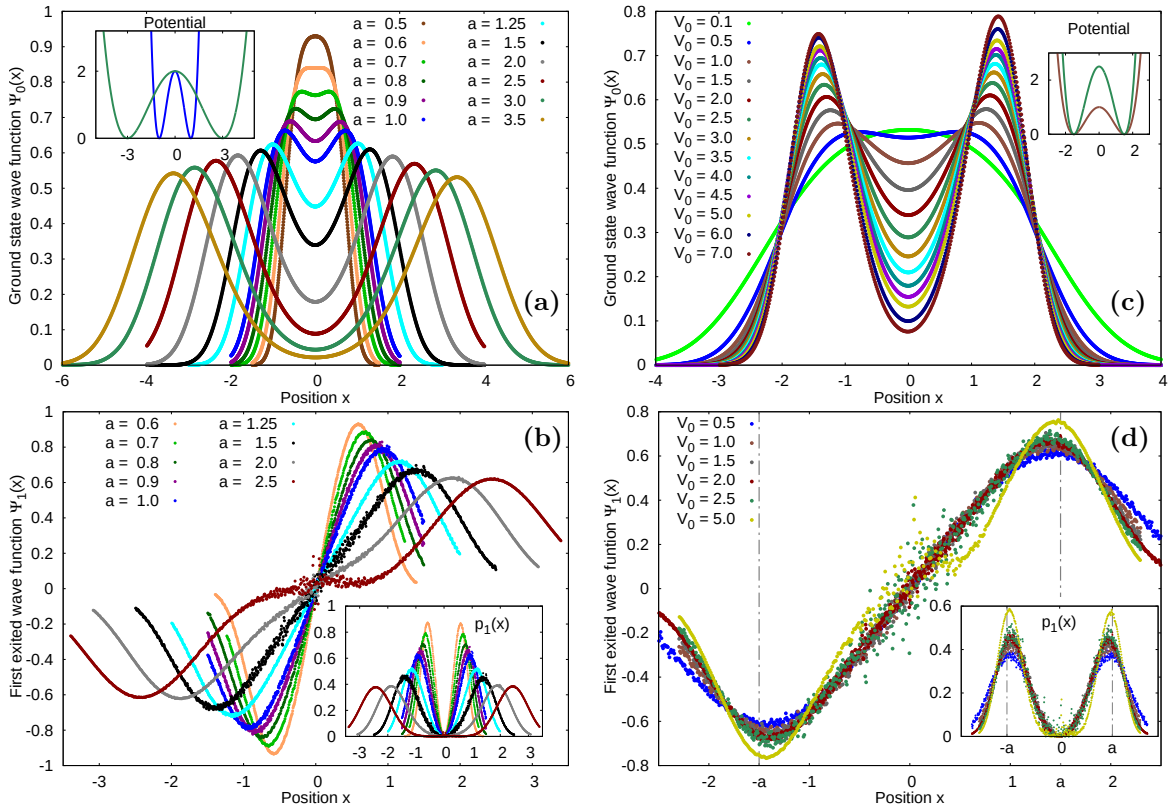

Figure 4.23.: *Ground state wave function* ***(a)*** *and first excited state wave function* ***(b)*** *for different well positions but fixed barrier height* $V_0 = 2.0$. *Ground state wave function* ***(c)*** *and first excited state wave function* ***(d)*** *for different barrier heights but a fixed well position* $a = 1.5$.

If the wells get more separated from each other, the energy becomes smaller and converges to the energy of a separated harmonic oscillator (red dot-dashed line in **Figure 4.22, left panel**),

$$V(x) = \tfrac{\omega}{2}(x \pm a)^2 \quad , \quad \omega = \tfrac{2}{a}\sqrt{2\,V_0} \quad , \tag{4.107}$$

which is localized at $\pm a$. Also the position of the maxima of the probability density shifts towards $\pm a$ for large a, which can be seen in the inset of **Figure 4.22, left panel**. Finally, it can be concluded that the double-well potential can be simplified towards two separated (isolated) harmonic potentials at moderate (but still sufficiently large) distances. This scenario becomes valid for $a \geq 3.0$ (a dimensionless; cf. equation (4.98)).

For very low barriers, the ground state energy is higher than V_0, and the wave function has only one maximum. Increasing the potential's barrier results in an energy smaller than V_0, and a wave function with two maxima. The higher the barrier is, the sharper the two maxima of the wave functions are; see **Figure 4.23, right panel**. The

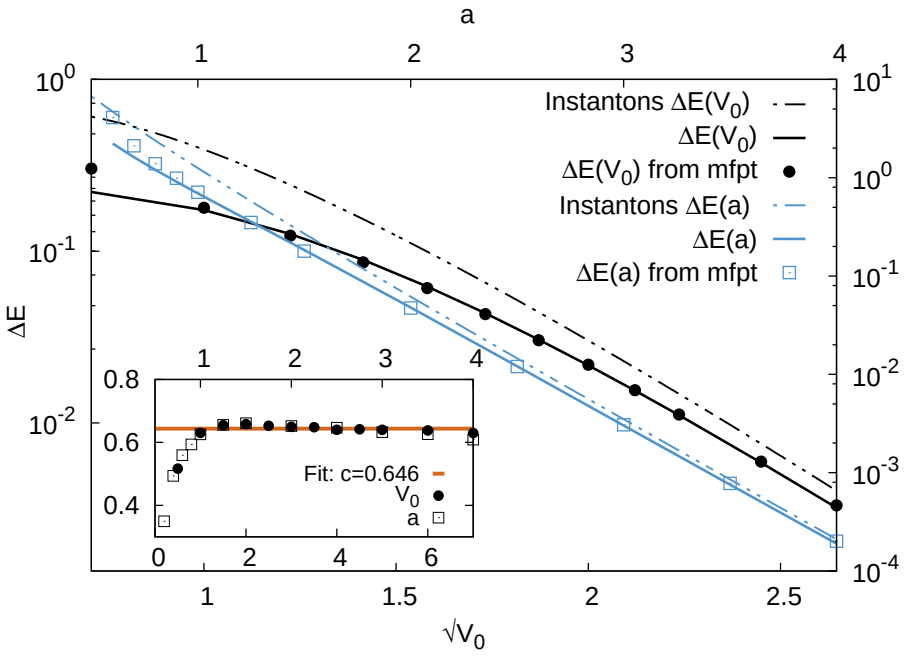

Figure 4.24.: *Energy splitting for the one-dimensional double-well potential for different well positions (blue: upper abscissa and right ordinate) and different barrier heights (black: abscissa is $\sqrt{V_0}$ and left ordinate) as calculated from the quantum Hamilton equations of motion (full lines) and the instanton method (dashed lines). Simulated data are predictions based upon the mean first passage time (symbols).* ***Inset:*** *Fit assuming a constant relation between the mean first passage time and energy splittings.*

maximum position shifts towards the well position for growing potential barriers, which is confirmed in the inset of **Figure 4.22, right panel**. Since the generated paths are too short, the wave functions are asymmetric for high barriers. In fact, it is very unlikely for the particle to overcome such a high barrier, meaning that the particle may remain at the same side of the barrier all the time. This effect can be overcome by using longer paths, but then, also more paths should be calculated to ensure numerically good results.

The above insights can be used to address the occurrence and the nature of energy splittings arising in double-well potentials. For a broad range of parameters, both the ground-state and the first exited-state energy fall below the harmonic ground-state energy. Since the probability of tunneling events drops down with increasing distances between the wells, the difference between the values of the first two energies $\Delta E = E_1 - E_0$ goes to zero; see **Figure 4.24**. Even for for well separated wells ($a \gg 1$ and/or $V_0 \gg 1$), where the instanton method predicts energy splitting reasonably well, the values of E_0 and E_1 do not match the expected relationship $^1/_2\hbar\omega \pm \Delta E$. Thus, symmetric splittings around the harmonic ground state can be disregarded: such

feature is misconception.

As a next step, the relation between so-called "tunneling splitting" and mean first passage time will be addressed. For a square barrier, the mean first passage time between entry and exit points of the barrier equals the traversal time [Chen and Wang, 1990], i.e., the time in which the particle interacts with the barrier [Büttiker and Landauer, 1982; Büttiker, 1983]. Both yield the "tunneling splitting". For the double-well potential, there is no exact point where the particle starts or stops to interact with the barrier. Therefore, it is necessary to average over all possible starting points. Suppose x_{TP} is the (smallest) positive turning point ($E - V(x_{\mathrm{TP}}) = 0$), then the averaged mean first passage time over all possible starting points, $x_i \in (-\infty, -x_{\mathrm{TP}}]$, is given by

$$\overline{\tau}_{\mathrm{mfpt}} = 2\int_{-\infty}^{-x_{\mathrm{TP}}} \left\{ \int_{x_i}^{x_{\mathrm{TP}}} \frac{\mathrm{d}x'}{p_0(x')} \int_{-\infty}^{x'} p_0(x'')\,\mathrm{d}x'' \right\} \tilde{p}_0(x_i)\,\mathrm{d}x_i \quad . \tag{4.108}$$

Here, $\tilde{p}_0(x)$ equals $p_0(x)$ except for a new normalization factor determined in a way such that $\tilde{p}_0(x)$ is a probability density on $(-\infty, -x_{\mathrm{TP}}]$. From the averaged mean first passage time, one can predict the energy splitting as $\Delta E = \pi/\overline{\tau}_{\mathrm{mfpt}}$. It turns out that they coincide with each other except for a constant prefactor $c = 0.646 \pm 0.003$. In the inset of **Figure 4.24** the energy splitting divided by $\pi/\overline{\tau}_{\mathrm{mfpt}}$ is plotted for different barrier heights (full symbols) and different well positions (empty symbols). The prefactor is calculated by a constant fit (brown line). The need of a prefactor goes back to the fact that the region in which the particle interacts with the potential barrier is not well-defined, and is in fact unknown. Averaging over all possible starting points is one possible correction to this effect; however, the end point stays fixed. Nonetheless, the resulting prediction of ΔE determined by making use of the mean first passage time (with prefactor) is in good accordance with the result from the quantum Hamilton equations of motion, or also the Numerov calculations; see **Figure 4.24**. Deviations (ΔE and c) visible for small a and V_0 occur for first excited-state energies higher than the potential barrier, where the concept of splitting due to tunneling is no longer applicable.

In summary, there is a systematic and well observable deviation between the real energies and those predicted by the instanton solution. For the instanton method, integration over all possible paths can only be done approximately. Still, this method provides reasonably good results regarding the absolute difference between the two energies, given that the energy splitting ΔE is sufficiently small. In contrast, the here presented stochastic model yields sufficiently precise results for any of the studied potentials, irrespective of small or large energy splittings. Within numerical uncertainty,

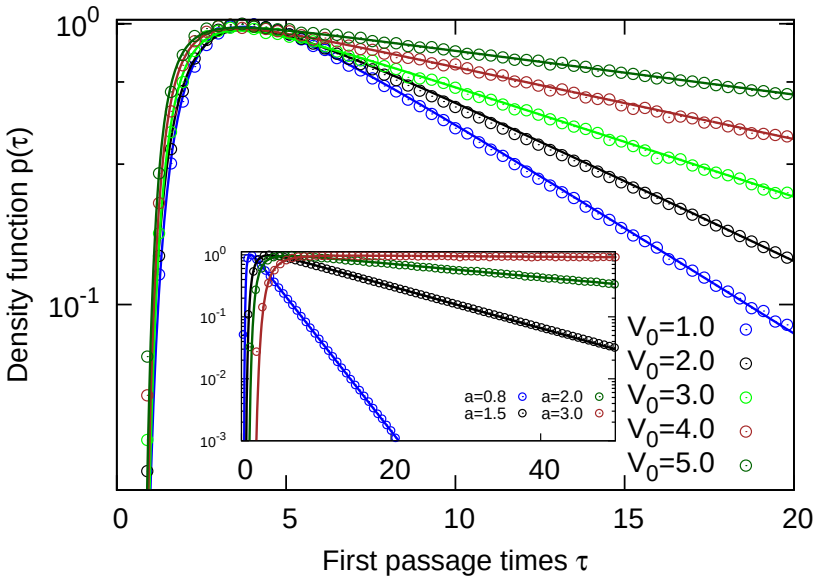

Figure 4.25.: *Density function of first passage times dependent on V_0 (main figure) and a (inset). The fit function is given by equation (4.106).*

the so-obtained results are exact.

As the last point, the behavior of the density of first passage times is analyzed. For different parameters, 10^5 paths of the motional process are generated using the associated osmotic velocity for the ground state $u_0(x)$. The first passage times from $(-a)$ to (a) are detected and the resulting density functions can be seen in **Figure 4.25**. It turns out that the position of maximum density depends only on the position of the wells, but not on the barrier height. The more separated the wells, the lower the exponential decrease. The simulated results can be fit empirically using equation (4.106), yielding excellent agreement (**Figure 4.25**), with the best-fit parameters being

a	V_0	τ_s	τ_l	α	c
1.5	1.0	1.67	9.51	1.98	1.79
1.5	2.0	1.50	12.83	2.33	1.48
1.5	3.0	1.36	18.38	2.69	1.26
1.5	4.0	1.25	28.04	3.04	1.15
1.5	5.0	1.16	46.08	3.28	1.09
0.8	2.0	0.65	2.85	3.30	1.75
2.0	2.0	2.19	39.94	2.76	1.18
3.0	2.0	3.61	533.4	3.25	1.00

Table 4.5.: *Parameters obtained from empirical fits to the first passage time density function dependent on the tuple (a, V_0). The density function is given by eq. (4.106).*

summarized in **Table 4.5**.

4.5. Non-stationary quantum systems

In the case of non-stationary systems, the current velocity is different from zero and the motion process $(X(t))_{t\in[0,T]}$ is described by the following forward as well as backward SDE:

$$\begin{cases} \mathrm{d}X(t) & = [v(X(t),t) + u(X(t),t)]\,\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\mathrm{d}W_f(t)\ , \quad t \in [0,T] \\ X(t=0) & = x_0 \in \mathbb{R} \end{cases} , \tag{4.109}$$

$$\begin{cases} \mathrm{d}X(t) & = [v(X(t),t) - u(X(t),t)]\,\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\mathrm{d}W_b(t)\ , \quad t \in [0,T] \\ X(t=T) & = x_T(\omega) \end{cases} \tag{4.110}$$

Again, the starting point of the forward motion is arbitrary and the starting point of the backward motion has to be the end point of the forward process and is affected by random events. The Wiener processes $(W_f(t))_{t\in[0,T]}$ and $(W_b(t))_{t\in[0,T]}$ were explained above. In contrast to the stationary case, the velocities are now functions of the motional process *and* the time.

As mentioned previously, the current and the osmotic velocity are given as the saddle points of the two variational problems introduced by Pavon [1995b]:

$$J_{\mathrm{R}}[\hat{v},\hat{u}] = \min_v \max_u \mathrm{E}\left[\int_0^T \left\{\frac{m}{2}\left(v^2(X(t),t) - u^2(X(t),t)\right) - V(X(t),t)\right\}\mathrm{d}t + S(x_0)\right] , \tag{4.111}$$

$$J_{\mathrm{I}}[v^*,u^*] = \max_v \min_u \mathrm{E}\left[\int_0^T m\,v(X(t),t)\,u(X(t),t)\mathrm{d}t + \hbar\,R(x_0)\right] . \tag{4.112}$$

Remember that the quantum Hamilton principle combines both principles and reads

$$J(u,v) = \mathrm{E}\left[\int_0^T \left\{\frac{m}{2}(v(X(t),t) - \mathrm{i}u(X(t),t))^2 - V(X(t),t)\right\}\mathrm{d}t + \Phi_0(x_0)\right] . \tag{4.113}$$

Here, the function $\Phi_0(x)$ is given by the initial condition of the wave function $\Psi(x,t_0) = \exp\left[\frac{\mathrm{i}}{\hbar}\,\Phi_0(x)\right]$.

Now, there are two methods available for finding the two velocities: First, both saddle-point problems are solved simultaneously by finding the Nash equilibrium and, second, the complex-valued quantum Hamilton problem is analyzed.

4.5.1. Finding the Nash equilibrium

The following treatment is based on the maximum principle for forward-backward stochastic games [Øksendal and Sulem, 2014], which was described in the beginning of this chapter. One can easily check that the osmotic velocitiy and the current velocity are given by the Nash equilibrium (see equation (4.4)-(4.5)) of the two saddle-points principles, i.e. a Nash equilibrium $\hat{u}, \hat{v}$ is a pair such that

$$J_R(u, \hat{v}) \leq J_R(\hat{u}, \hat{v}) \quad \text{for all } u \tag{4.114}$$

$$\text{and} \quad J_I(\hat{u}, v) \leq J_I(\hat{u}, \hat{v}) \quad \text{for all } v \tag{4.115}$$

is fulfilled.

In the physical system described herein, the forward controlled process equals the backward one. However, in general, the two controlled processes are given by two different random variables. Therefore, the backward process is given by a second process $(Y(t))_{t\in[0,T]}$,

$$\begin{cases} \mathrm{d}Y(t) & = [v(Y(t),t) - u(Y(t),t)]\,\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\mathrm{d}W_b(t)\ , \quad t \in [0,T] \\ Y(t=T) & = x_T(\omega) \end{cases} \quad . \tag{4.116}$$

The equivalence of the forward controlled process $(X(t))_{t\in[0,T]}$ and the backward process $(Y(t))_{t\in[0,T]}$ in each time step is included as a constraint,

$$Y(t) = X(t) \quad \forall t \in [0,T] \quad . \tag{4.117}$$

Suppose α_R and α_I are two Lagrangian parameters, then the two related Hamilton functions read

$$\begin{aligned} H_R(t,x,y,u,v) = &\frac{m}{2}(v^2 - u^2) - V(x,t) + \lambda_R(u-v) + p_R(u+v) \\ &+ \sqrt{\frac{\hbar}{m}}q_R + \alpha_R(x-y) \end{aligned} \tag{4.118}$$

and

$$H_I(t,x,y,u,v) = m\,uv + \lambda_I(u-v) + p_R(u+v) + \sqrt{\frac{\hbar}{m}}q_I + \alpha_I(x-y) \quad . \tag{4.119}$$

The adjoint processes are given by the forward SDEs,

$$\begin{cases} \mathrm{d}\lambda_R(t) &= -\alpha_R \,\mathrm{d}t \\ \lambda_R(t=0) &= S'(x_0) \end{cases} , \quad \begin{cases} \mathrm{d}\lambda_I(t) &= -\alpha_I \,\mathrm{d}t \\ \lambda_I(t=0) &= R'(x_0) \end{cases} , \tag{4.120}$$

and backward SDEs,

$$\begin{cases} \mathrm{d}p_R(t) &= \left[\frac{\partial V(x,t)}{\partial t}\Big|_{x=X(t)} - \alpha_R \right] \mathrm{d}t \,+\, q_R(t)\,\mathrm{d}W_b(t) \\ p_R(t=T) &= \lambda_R(T) \end{cases} , \tag{4.121}$$

$$\begin{cases} \mathrm{d}p_I(t) &= -\alpha_I \,\mathrm{d}t \,+\, q_I(t)\,\mathrm{d}W_b(t) \\ p_I(t=T) &= \lambda_I(T) \end{cases} . \tag{4.122}$$

Using the maximum principle [Øksendal and Sulem, 2014], i.e., finding the roots of the partial derivatives of H_R and H_I with respect to u and v, one gets

$$m\,u(t) = \lambda_R + p_R \quad , \quad m\,v(t) = \lambda_R - p_R \tag{4.123}$$

$$m\,u(t) = \lambda_I - p_I \quad , \quad m\,v(t) = -\lambda_I - p_I \quad . \tag{4.124}$$

One of the two relations for each velocity can now be used to determine a backward SDE for the respective velocity; knowledge on the two Lagrangian parameters is not required. Using the integral representation

$$\lambda_R(t) = S'(x_0) - \int_0^t \alpha_R \,\mathrm{d}s \quad \text{and} \quad \lambda_I(t) = R'(x_0) - \int_0^t \alpha_I \,\mathrm{d}s \tag{4.125}$$

of the forward adjoint processes and the integral representation of the backward adjoint processes, the following BSDE describing the current velocity $v(t)$ is determined:

$$\begin{aligned} p_R(t) &= \lambda_R(T) - \int_t^T \left[\frac{\partial V}{\partial x}(X(s),s) - \alpha_R \right] \mathrm{d}s \,-\, \int_t^T q_R(s) \mathrm{d}W_b(s) \\ &= S'(x_0) - \int_0^T \alpha_R \,\mathrm{d}s - \int_t^T \left[\frac{\partial V}{\partial x}(X(s),s) - \alpha_R \right] \mathrm{d}s - \int_t^T q_R(s) \mathrm{d}W_b(s) \\ &= \underbrace{S'(x_0) \,-\, \int_0^t \alpha_R \,\mathrm{d}s}_{\lambda_R(t)} - \int_t^T \frac{\partial V}{\partial x}(X(s),s) \mathrm{d}s \,-\, \int_t^T q_R(s)\,\mathrm{d}W_b(s) \\ \Rightarrow\; m\,v(t) &= p_R(t) - \lambda_R(t) = -\int_t^T \frac{\partial V}{\partial x}(X(s),s) \mathrm{d}s \,-\, \int_t^T q_R(s)\,\mathrm{d}W_b(s) \end{aligned} \tag{4.126}$$

Analogously, the osmotic velocity is given by

$$\begin{aligned} p_I(t) =& \lambda_I(T) + \int_t^T \alpha_I \,\mathrm{d}s \; - \int_t^T q_I(s)\mathrm{d}W_b(s) \\ =& \underbrace{R'(x_0) - \int_0^t \alpha_I \,\mathrm{d}s}_{\lambda_I(t)} \; - \int_t^T q_I(s)\,\mathrm{d}W_b(s) \\ \Rightarrow \; m\,u(t) =& \lambda_I(t) - p_I(t) = \int_t^T q_I(s)\,\mathrm{d}W_b(s) \quad , \end{aligned} \tag{4.127}$$

with the abbreviation

$$\frac{\partial V}{\partial x}(X(s),s) = \left.\frac{\partial V(x,s)}{\partial x}\right|_{x=X(s)} \quad . \tag{4.128}$$

Similar to the stationary case, the adjoint processes $q_R(t)$ and $q_I(t)$ can be found using an Itô formula, i.e.

$$\frac{q_R(t)}{m} = \sqrt{\frac{\hbar}{m}}\left.\frac{\partial v(x,t)}{\partial x}\right|_{x=X(t)} \quad \text{and} \quad \frac{q_I(t)}{m} = \sqrt{\frac{\hbar}{m}}\left.\frac{\partial u(x,t)}{\partial x}\right|_{x=X(t)} \quad . \tag{4.129}$$

The BSDEs for the two velocities thus read

$$m\,\mathrm{d}v(t) = \left.\frac{\partial V(x,t)}{\partial x}\right|_{x=X(t)} \mathrm{d}t \; + \sqrt{\hbar\, m}\;\partial_x\, v(x,t)|_{x=X(t)}\;\mathrm{d}W_b(t) \quad , \tag{4.130}$$

$$m\,\mathrm{d}u(t) = \sqrt{\hbar\, m}\;\partial_x\, u(x,t)|_{x=X(t)}\;\mathrm{d}W_b(t) \quad . \tag{4.131}$$

PDEs quantifying the two velocities can be determined from the adjoint processes. $p_R(t)$ is an adjoint process to the forward motional process. Equation (4.121) shows that $p_R(t)$ has the same mathematical structure as $p_R(X(t),t)$. Suppose the partial derivatives $\partial_t p_R(x,t)$, $\partial_x p_R(x,t)$ and $\partial_{xx} p_R(x,t)$ are continuous, then – using a forward (normal) Itô formula – the function $p_R(x,t)$ is the solution of

$$\frac{\partial p_R}{\partial t} + \Big(v(x,t) + u(x,t)\Big)\frac{\partial p_R}{\partial x} + \frac{\hbar}{2m}\frac{\partial^2 p_R}{\partial x^2} - \frac{\partial V}{\partial x} + \alpha_R = 0 \quad , \tag{4.132}$$

where $x \in \mathbb{R}$ and $t \geq 0$. Analogously, $\lambda_R(X(t),t)$ is an adjoint process to the backward motional process and fulfills a backward-Itô equation [Pavon, 1995b]. The function $\lambda_R(x,t)$ fulfills

$$\frac{\partial \lambda_R}{\partial t} + \Big(v(x,t) - u(x,t)\Big)\frac{\partial \lambda_R}{\partial x} - \frac{\hbar}{2m}\frac{\partial^2 \lambda_R}{\partial x^2} + \alpha_R = 0,\; x \in \mathbb{R},\; t \leq 0 \quad . \tag{4.133}$$

This PDE for the adjoint process $\lambda_R(t)$ is trivially true. Using the same relation for the current velocity as before, i.e., $m\,v = \lambda_R - p_R$, the PDE characterizing the current

velocity is found by taking the difference of equations (4.133) and (4.132), that is,

$$0 = \underbrace{\frac{\partial \lambda_R}{\partial t} - \frac{\partial p_R}{\partial t}}_{\partial_t v(x,t)} + v(x,t) \underbrace{\frac{\partial \lambda_R}{\partial x} - \frac{\partial p_R}{\partial x}}_{\partial_x v(x,t)} - u(x,t) \underbrace{\frac{\partial \lambda_R}{\partial x} + \frac{\partial p_R}{\partial x}}_{\partial_x u(x,t)} - \frac{\hbar}{2m} \underbrace{\left[\frac{\partial^2 \lambda_R}{\partial x^2} + \frac{\partial^2 p_R}{\partial x^2} \right]}_{\partial_{xx} u(x,t)} - \frac{1}{m} \frac{\partial V(x,t)}{\partial x} \tag{4.134}$$

$$\Rightarrow \quad 0 = \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} - u \frac{\partial u}{\partial x} - \frac{\hbar}{2m} \frac{\partial^2 u}{\partial x^2} + \frac{1}{m} \frac{\partial V}{\partial x} \quad . \tag{4.135}$$

Note that the Lagrangian parameter is unknown and that the relation for the osmotic velocity is needed in the derivation. Thus, both relations (equation (4.123)) are necessary to derive the PDE for the current velocity.
In the same way, the PDE for the osmotic velocity can be calculated using the relations derived from the entropy production principle, $J_I[u, v]$. $\lambda_I(X(t), t)$ is the adjoint process to the backward motion process and

$$\frac{\partial \lambda_I}{\partial t} + (v(x,t) - u(x,t)) \frac{\partial \lambda_I}{\partial x} - \frac{\hbar}{2m} \frac{\partial^2 \lambda_I}{\partial x^2} + \alpha_I = 0 \tag{4.136}$$

holds for $\lambda_I(x,t)$, $x \in \mathbb{R}$, $t \geq 0$. $p_I(X(t), t)$ is a function of the forward process and $p_I(x,t)$, $x \in \mathbb{R}$, $t \geq 0$ fulfills

$$\frac{\partial p_I}{\partial t} + (v(x,t) + u(x,t)) \frac{\partial p_I}{\partial x} + \frac{\hbar}{2m} \frac{\partial^2 p_I}{\partial x^2} + \alpha_I = 0 \quad . \tag{4.137}$$

Subtracting equation (4.137) from equation (4.137), the PDE for the osmotic velocity

$$0 = \frac{\partial u}{\partial t} + v \frac{\partial u}{\partial x} + u \frac{\partial v}{\partial x} + \frac{\hbar}{2m} \frac{\partial v^2}{\partial x^2} \tag{4.138}$$

can be derived.

Nonetheless, difficulties arise at a more detailed level concerning the interpretation of the above method: In principle, two additional PDEs can be derived by taking the sum of equation (4.133) and (4.132), and (4.136) and (4.137),

$$\frac{\partial u}{\partial t} + v \frac{\partial u}{\partial x} - u \frac{\partial v}{\partial x} - \frac{\hbar}{2m} \frac{\partial^2 v}{\partial x^2} - \frac{\partial V}{\partial x} + 2\alpha_r = 0 \quad , \tag{4.139}$$

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + u \frac{\partial u}{\partial x} - \frac{\hbar}{2m} \frac{\partial^2 u}{\partial x^2} + 2\alpha_I = 0 \quad . \tag{4.140}$$

Technically, the resulting equations are as meaningful as the previous ones resulting from summation. However, the Lagrangian parameters still occur in these equations, which is not in accordance with the Madelung equations. Also, the physical interpretation of these PDEs remains unclear.

Circumventing this issue, the quantum Hamilton principle can be directly evaluated.

4.5.2. Analyzing the quantum Hamilton principle

In the following, a maximum principle for BDSDE systems [Bahlali and Gherbal, 2010] is used to analyze the quantum Hamilton principle directly. Defining a complex valued optimal control, $v_q := v(t) - \mathrm{i}\, u(t)$, the action functional reads

$$J(u,v) = \mathrm{E}\left[\int_0^T \left\{ \tfrac{m}{2} v_q(t)^2 - V(X(t),t)\right\}\mathrm{d}t + \Phi_0(x_0)\right] \tag{4.141}$$

and is structurally similar to the least-action principle in classical mechanics.

Using an Itô formula, Pavon [1995b] showed that the SDEs for the motional process can be also written as

$$\mathrm{d}X(t) = v(t)\mathrm{d}t + \frac{1}{2}\sqrt{\frac{\hbar}{m}}\left[\mathrm{d}W_f(t) + \mathrm{d}W_b(t)\right] \quad , \tag{4.142}$$

$$0 = u(t)\mathrm{d}t + \frac{1}{2}\sqrt{\frac{\hbar}{m}}\left[\mathrm{d}W_f(t) - \mathrm{d}W_b(t)\right] \quad . \tag{4.143}$$

Multiplying equation (4.143) with i, $\mathrm{i}^2 = -1$, and afterwards subtracting the resulting equation (4.142), the so-obtained SDE depends only on the control v_q, i.e. [Pavon, 1995b]

$$\mathrm{d}X(t) = v_q(t)\mathrm{d}t + \frac{1}{2}\sqrt{\frac{\hbar}{m}}\left[\left(1-\mathrm{i}\right)\mathrm{d}W_f(t) + \left(1+\mathrm{i}\right)\mathrm{d}W_b(t)\right] \quad . \tag{4.144}$$

This equation characterizes the controlled process to the quantum Hamilton principle, and consists of a forward and backward Wiener process.

The associated Hamilton function reads

$$H(t,x,v_q,p,q) = -\frac{1}{2}v_q^2 + V(x,t) + p\, v_q - \sqrt{\frac{\hbar}{m}}\frac{(1+\mathrm{i})\, q}{2} \quad , \tag{4.145}$$

with the adjoint processes $p(t)$, $q(t)$ being defined by

$$\begin{cases} \mathrm{d}p(t) & = -\left.\frac{\partial V(x,t)}{\partial x}\right|_{x=X(t)} \mathrm{d}t \; - q(t)\,\mathrm{d}W_b(t) \\ p(t=0) & = \phi_0(x_0) \end{cases} \quad . \tag{4.146}$$

Since the considered performance functional $J[v_q]$ and the control v_q are complex-valued variables, the Hamilton function is also a complex function. The search for the optimal control extremizing the Hamilton function is thus reminiscent of finding the roots of the derivative of H. One can easily check that the optimal control is given by the adjoint process, i.e. $p(t) = m\, v_q(t)$. The deterministic part of equation (4.146) is forward in time; however, this equation can be transformed into the BSDE

$$\begin{cases} m\,\mathrm{d}v_q(t) & = \left.\frac{\partial V(x,t)}{\partial x}\right|_{x=X(t)} \mathrm{d}t \; - q(t)\,\mathrm{d}W_b(t) \\ v_q(t=T) & = 0 \end{cases} \quad , \tag{4.147}$$

where, in any case, the adjoint process $q(t)$ is zero for $t = T$.

The adjoint process $p(t)$ is a function of the controlled process (and time). Pavon [1995b] presented an Itô-type formula leading to a PDE for the control $v_q(t)$,

$$\frac{\partial v_q}{\partial t} + v_q \frac{\partial v_q}{\partial x} - \frac{\mathrm{i}\hbar}{2m}\frac{\partial^2 v_q}{\partial x^2} + \frac{1}{m}\frac{\partial V(x,t)}{\partial x} = 0 \quad . \tag{4.148}$$

Separating the real and the imaginary part, one gets

$$0 = \frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} - u\frac{\partial u}{\partial x} - \frac{\hbar}{2m}\frac{\partial^2 u}{\partial x^2} + \frac{1}{m}\frac{\partial V(x,t)}{\partial x} \quad , \tag{4.149}$$

$$0 = \frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} + u\frac{\partial v}{\partial x} + \frac{\hbar}{2m}\frac{\partial v^2}{\partial x^2} \quad , \tag{4.150}$$

which are equivalent to the PDEs (equation (4.135) and (4.138)) derived in the section before.

The second adjoint process is given by

$$q(t) = -\sqrt{\frac{\hbar}{m}}\frac{\partial v_q}{\partial x} \quad , \tag{4.151}$$

which can be determined using the same Itô-type formula. Separating again the real and the imaginary part in equation (4.147), one can determine the same stochastic backward equations for the two velocities as in the previous section.

Concluding this section, both methods presented herein lead to the same BSDEs for the two velocities. The equation for the physical momentum $p = m\,(v + u)$ is given by

$$\mathrm{d}\, m\,[v(t) + u(t)] = \frac{\partial V(x(t), t)}{\partial x}\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\frac{\partial m\,[v(x(t), t) + u(x(t), t)]}{\partial x}\,\mathrm{d}W_b(t) \quad . \tag{4.152}$$

This equation is also applicable to the stationary case, i.e., inserting $v(x, t) \equiv 0$ leads to the same equation for the osmotic velocity as determined from the stationary optimal control problem.

Besides that, Pavon [1995a] derived a SDE for the quantum velocity $v_q(t)$, which is

$$\mathrm{d}v_q(t) = -\left.\frac{\partial V(x, t)}{\partial x}\right|_{x=X(t)} \mathrm{d}t + \partial_x v_q(t)\,\mathrm{d}W_q(t) \quad , \tag{4.153}$$

where the quantum noise reads

$$\mathrm{d}W_q(t) = \frac{1}{2}\sqrt{\frac{\hbar}{m}}\Big[(1 - \mathrm{i})\,\mathrm{d}W_f(t) + (1 - \mathrm{i})\,\mathrm{d}W_b(t)\Big] \quad . \tag{4.154}$$

The deterministic part of the quantum velocity is forward in time, as is the equation for the adjoint process. Still, they are distinct from each other by the different kind of noise underlying the diffusion process. The reason why the two methods lead to different results is not evident at the moment. Moreover, the individual equations for the velocities are not valid for the stationary case, which can be considered as being a special case of the more general, time-dependent system.

The momentum equation (equation (4.152)) is a promising instrument to describe the motion of the particle and delivers (together with the FBSDE system for the motional process) a generalization to the classical canonical equations,

$$\dot{q_\mathrm{c}} = \frac{\partial H_\mathrm{c}}{\partial p_\mathrm{c}} = \frac{p_\mathrm{c}}{m} \quad , \tag{4.155}$$

$$\dot{p_\mathrm{c}} = -\frac{\partial H_\mathrm{c}}{\partial q_\mathrm{c}} = -\frac{\partial V}{\partial q_\mathrm{c}} \quad , \tag{4.156}$$

with the Hamilton function $H_\mathrm{c} = {p_\mathrm{c}^2}/{2m} + V(x, t)$.

It is noted that the equation for the physical momentum taken on its own, equation (4.152), cannot uniquely describe the motion of the particle since only the sum of the two velocities can be determined. Hence, it would be impossible to solve the

backward equation of the motion process and calculate the complete wave function. That suggests that a forward equation to the momentum process and the velocities exists. The resulting process would be time-reversible. Though, up to now, only the backward equations could be found and it is not clear whether there is a need for a forward equation for the velocity processes, or not. Nevertheless, the dynamics of a quantum particle can be uniquely described by the individual equations for the velocities.

Exploiting the integral representation of the SDEs for the velocities and taking the expectation value, one gets

$$m\,\mathrm{E}\left[v(t)\right] = -\,\mathrm{E}\left[\int_t^T \frac{\partial V(x,s)}{\partial x}\,\mathrm{d}s\right] - \sqrt{\hbar\, m}\,\mathrm{E}\left[\int_t^T \frac{\partial v}{\partial x}\,\mathrm{d}W(s)\right] \quad , \tag{4.157}$$

$$m\,\mathrm{E}\left[u(t)\right] = -\,\sqrt{\hbar\, m}\,\mathrm{E}\left[\int_t^T \frac{\partial u}{\partial x}\,\mathrm{d}W(s)\right] \quad . \tag{4.158}$$

Since the expectation value of an Itô-integral equals zero, $\mathrm{E}[u] = 0$ holds. Using Fubini's theorem, the expectation value of the current velocity reads

$$m\,\mathrm{E}\left[v(t)\right] = -\mathrm{E}\left[\int_t^T \frac{\partial V(x,s)}{\partial x}\,\mathrm{d}s\right] = -\int_t^T \mathrm{E}\left[\frac{\partial V(x,s)}{\partial x}\right]\mathrm{d}s \quad . \tag{4.159}$$

Finally, going back to a differentially form, the equations for the expectation values[17] read

$$\mathrm{d}\,\mathrm{E}\left[X(t)\right] = \mathrm{E}\left[v(X(t),t)\right]\mathrm{d}t \quad , \tag{4.160}$$

$$m\,\mathrm{d}\,\mathrm{E}\left[v(t)\right] = -\,\mathrm{E}\left[\left.\frac{\partial V(x,t)}{\partial x}\right|_{x=X(t)}\right]\mathrm{d}t \quad , \tag{4.161}$$

which resembles Ehrenfest's theorem [Ehrenfest, 1927]. This theorem for the dynamic laws dictates the time evolution to the quantum-mechanical expectation values of the position and the momentum operator.

Example - Force-free motion of a particle

Force-free motion resembles Brownian motion in absence of the drift term, i.e., $\partial_x V(x,t) = 0$. Hence, the momentum reads

$$\mathrm{d}\,m\left[v(t)+u(t)\right] = \sqrt{\frac{\hbar}{m}}\,\frac{\partial m\left[v(x(t),t)+u(x(t),t)\right]}{\partial x}\,\mathrm{d}W_b(t) \quad . \tag{4.162}$$

[17] The derivation for the motional process is analogous to that one of the current velocity.

One obvious solution to this equation is given by $v(x,t) + u(x,t) = v_0 + u_0 = const.$ However, the expectation value of the osmotic velocity has to be zero, hence $u_0 = 0$. The motional process is thus characterized by

$$\mathrm{d}X(t) = v_0\,\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\mathrm{d}W_f(t) \quad . \tag{4.163}$$

Using $m\,v(x,t) = \partial_x\,S(x,t)$ and $\Psi(x,t) \propto \mathrm{e}^{\mathrm{i}/\hbar S(x,t)}$, the wave function equals a plane wave, i.e.,

$$\Psi(x,t) \propto \exp\left\{\mathrm{i}\,m\,\hbar^{-1}\,v_0\,x\right\} \quad . \tag{4.164}$$

4.6. Further developments

4.6.1. The efficiency of the numerical algorithm for the stationary case

In order to find a numerical approach to the backward equation of the (stationary) osmotic velocity,

$$m\,\mathrm{d}u(t) = \partial_x\,V(x)|_{x=X(t)} + q(t)\,\mathrm{d}W_b(t) \quad , \tag{4.165}$$

it is required to calculate $q(t)$ by conditional expectations that are determined by a least-square Monte Carlo scheme [Bender and Steiner, 2012].

Again, the equation characterizing the osmotic velocity is discretized using the Euler-Maruyama method. In each time step, $q(t)$ is calculated by equation (4.77), where the functional basis $\eta(\cdot)$ reads [Gobet et al., 2005]

$$\eta(\cdot) = (\mathbb{1}_{D_l}(\cdot))_{l=1,\ldots,L} \ , \text{ with } \mathbb{1}_{D_l}(x) = \begin{cases} 1\ , & x \in D_l \\ 0\ , & \text{else} \end{cases} \quad . \tag{4.166}$$

The intervals D_l are defined above. The presented algorithm is highly efficient since a multitude of realizations are determined in each iteration step. The new estimate of the osmotic velocity is calculated by taking the arithmetic average of those values $u(t)$ that have an associated argument $X(t)$ located in the desired interval. (Note that $u = u(t, X(t))$, where all u belonging to the same x-value should yield the same result. Deviations reflect numerical/technical uncertainties, and are compensated for by calculating average values.)

It turned out that the efficiency of the numerical algorithm can be highly improved by (i) changing the functional basis for the projection of the conditional expectation

from an orthogonal system to an orthonormal one, and (ii), taking the conditional expectation directly from equation (4.165). The resulting scheme for the discrete process becomes

$$u_{t_i}^{\pi,j} = \mathrm{E}\left[u_{t_{i+1}}^{\pi,j} \middle| X_{t_i}^{\pi,j} \right] - {}^1\!/_m \, \partial_x V(x)|_{x=X_{t_i}^{\pi,j}} \quad . \tag{4.167}$$

The m-th realization in the j-th iteration step of the conditional expectation

$$h_{i+1}^{j,m} := \mathrm{E}\left[u_{t_{i+1}}^{\pi,j} \middle| X_{t_i}^{\pi,j} = x_i^{j,m} \right] \tag{4.168}$$

is then given by

$$h_{i+1}^{j,m} = \alpha_0^{j,i} \, \eta_0(x_i^{j,m}) \quad , \; \alpha_0^{j,i} = \frac{1}{M} \sum_{m=1}^{M} \eta(x_i^{m,j}) \, u_{t_{i+1}}^{m,j} \quad . \tag{4.169}$$

Here, $x_i^{j,m}$ is the value of the m-th path of the discrete process $X_{t_i}^{\pi,j}$ at time t_i in the j-th iteration step. The functional basis $\eta_0(\cdot)$ reads

$$\eta(\cdot) = \sqrt{\frac{M}{card(D_l)}} \; (\mathbb{1}_{D_l}(\cdot))_{l=1,\ldots,L} \quad . \tag{4.170}$$

$card(D_l)$ gives the number of all $x_i^{j,m}$ which are at time t_i in the interval D_l [Bachouch et al., 2014, 2016]. It should be emphasized that the conditional expectation of equation (4.165) leads to a scheme in which the adjoint process[18] $q(t)$ is no longer necessary. Furthermore, the functional basis is, in contrast to the work of Gobet et al. [2005], normalized by $card(D_l)$.

In **Figure 4.26**, single realizations of the backward equation (black points) are compared to the resulting estimate of the osmotic velocity (blue points) as obtained from both methods and both analyzed systems. Here, the efficiency of the new method becomes obvious. Bender and Steiner [2012] argued that there are two error sources to the numerical procedure. First, systematic errors induced by the choice of the basis functions and, second, the simulation error itself. Hence, the right choice of the functional basis is very beneficial as it increases the simulation's quality and reliability. In fact, for the new algorithm much less paths are necessary to achieve much better results, and the computational time decreases dramatically. As for the double-well potential, this situation permits to analyze a broader parameter range.

The range of convergence can be further increased by making use of uniformly dis-

[18] The drift in the backward equation depends only on $X(t)$.

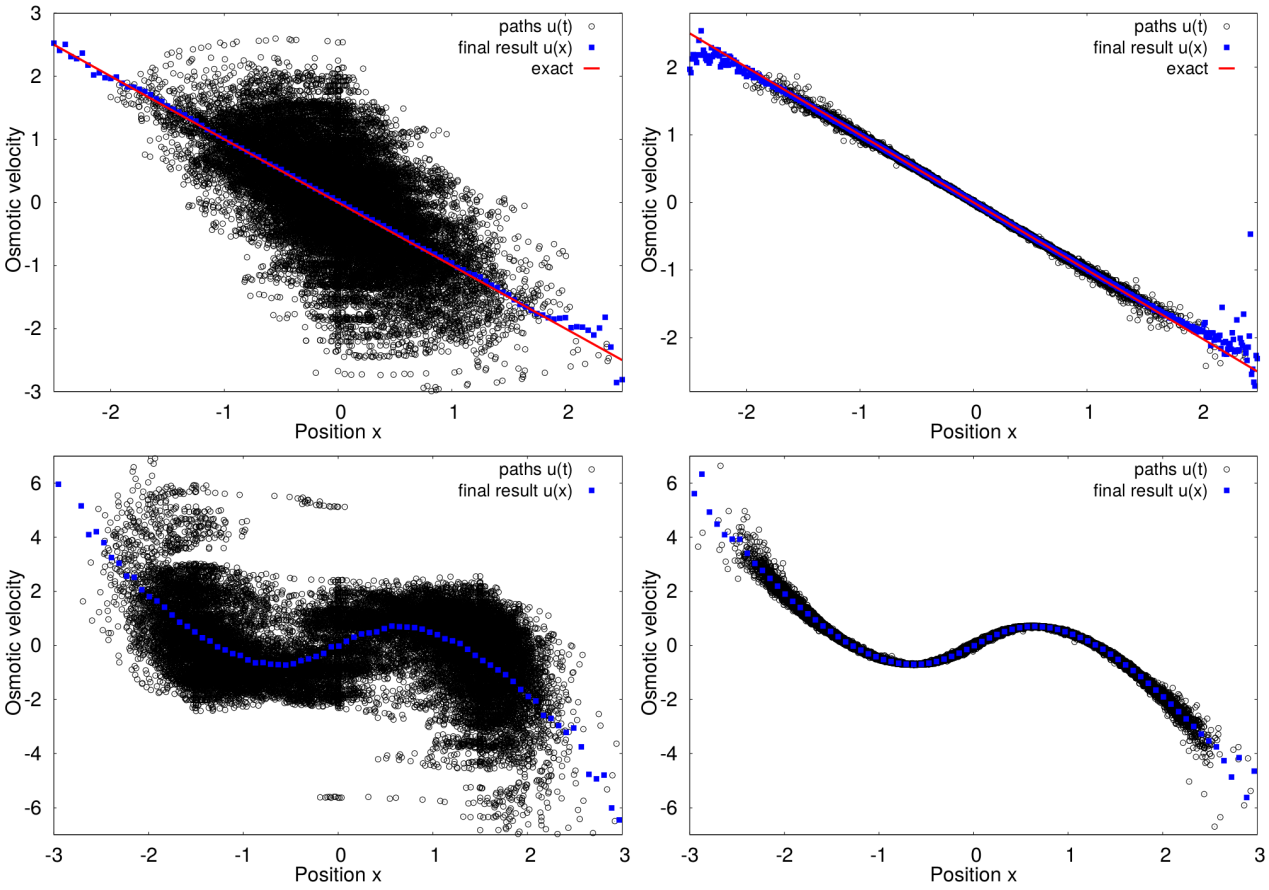

Figure 4.26.: *Efficiency of the numerical algorithm for stationary systems: Comparison between single paths of the osmotic velocity (solution to the backward equation) $u(t)$ and result from the hole algorithm $u(x)$.*
Top: *harmonic oscillator in comparison with the exact solution.*
Bottom: *Double-well potential.*
Left: *Used method.* ***Right:*** *More efficient method.*

tributed[19] starting points. Uniformly distributed starting points are physically reasonable, noting that the starting point might be imprecisely known from an observation (measurement). More information on further developments to the algorithm can be found in ref. [Beyer, 2018].

4.6.2. Higher dimensions

In principle, all equations can be extended to the multidimensional case, i.e. describing more than one particle in higher dimensions. Suppose the process $(\mathbf{X}(t))_{t\in[0,T]}$ takes

[19] Uniformly distributed across the chosen domain.

values in $\mathbb{R}^d$, then the SDEs read

$$\begin{cases} \mathrm{d}\boldsymbol{X}(t) & = [\boldsymbol{v}(\boldsymbol{X}(t),t) + \boldsymbol{u}(\boldsymbol{X}(t),t)]\,\mathrm{d}t + \underline{\boldsymbol{\sigma}}\,\mathrm{d}\boldsymbol{W}_f(t)\,, \quad t \in [0,T] \\ \boldsymbol{X}(t=0) & = \boldsymbol{x}_0 \in \mathbb{R} \end{cases} , \tag{4.171}$$

$$\begin{cases} \mathrm{d}\boldsymbol{X}(t) & = [\boldsymbol{v}(\boldsymbol{X}(t),t) - \boldsymbol{u}(\boldsymbol{X}(t),t)]\,\mathrm{d}t + \underline{\boldsymbol{\sigma}}\,\mathrm{d}\boldsymbol{W}_b(t)\,, \quad t \in [0,T] \\ \boldsymbol{X}(t=T) & = \boldsymbol{x}_T(\omega) \end{cases} . \tag{4.172}$$

Here, $\boldsymbol{W}_f$ ($\boldsymbol{W}_b$) is a d-dimensional forward (backward) Wiener process and the diffusion coefficient is given by a diagonal matrix, i.e. $\underline{\boldsymbol{\sigma}} := \sqrt{\hbar/m}\,\mathbb{I}_d$, where $\mathbb{I}_d$ is the d-dimensional identity matrix.

The maximum principle can be used in the same way as before. However, since the diffusion coefficient is given by a matrix, the related adjoint process is also a matrix, and the Hamilton function is given by scalar products [Li and Zheng, 2015; Zhuang, 2017]. For instance, the Hamilton function to the stationary case reads

$$H(\boldsymbol{x},\boldsymbol{u},\boldsymbol{\lambda},\boldsymbol{p},\underline{\boldsymbol{q}}) = \frac{m}{2}\boldsymbol{u}^2 - V(\boldsymbol{x}) + \langle\boldsymbol{\lambda},\boldsymbol{u}\rangle + \langle\boldsymbol{p},\boldsymbol{u}\rangle + \left\langle\underline{\boldsymbol{\sigma}}\,,\,\underline{\boldsymbol{q}}\right\rangle \quad . \tag{4.173}$$

The scalar product for matrices is given by the trace of the matrix product, meaning that

$$\left\langle\underline{\boldsymbol{\sigma}}\,,\,\underline{\boldsymbol{q}}\right\rangle = \mathrm{Tr}\left(\underline{\boldsymbol{\sigma}}^T\,\underline{\boldsymbol{q}}\right) \quad . \tag{4.174}$$

The equation for the physical momentum is thus given by

$$\mathrm{d}\,m\,[\boldsymbol{v}(t)+\boldsymbol{u}(t)] = \nabla_{\boldsymbol{x}}\,V(\boldsymbol{x}(t),t)|_{\boldsymbol{x}=\boldsymbol{X}(t)}\,\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\,\underline{\boldsymbol{J}}_{m(\boldsymbol{v}+\boldsymbol{u})}\left(\boldsymbol{X}(t)\right)\,\mathrm{d}\boldsymbol{W}_b(t) \quad , \tag{4.175}$$

with $\underline{\boldsymbol{J}}_{m(\boldsymbol{v}+\boldsymbol{u})}(\boldsymbol{x})$ being the Jacobian matrix of the momentum.

The stochastic Hamilton equations of motion for higher dimensions resemble those of the one-dimensional case. Difficulties arise for cases in which a change of variables is necessary, e.g., due to central forces [Beyer, 2018].

Finally, it is noted that excited states for non-Cartesian (stationary) systems are an interesting, non-trivial issue, the quantification of which might be challenging, but manageable using the here presented approach; see also ref. [Patzold, 2018].

4.6.3. Outlook – time-dependent case

Thus far, there is no algorithm feasible for time-dependent stochastic Hamilton equations. The PDEs for the two velocities can be solved in each iteration step [Milstein and Tretyakov, 2006], yet such treatment would be highly inefficient, with no benefit compared to a numerical solution of the time-dependent Schrödinger equation itself. In fact, such concept resembles a numerical approach to the Schrödinger equation.

Apart from that, the algorithm developed herein can indeed be adapted to cases in which the two velocities are given by non-stationary equations. Applications are restricted to the paths of the velocities instead of addressing the functions $\boldsymbol{u}(\boldsymbol{x}, t)$ and $\boldsymbol{v}(\boldsymbol{x}, t)$, as well as the backward equation of the motional process cannot be considered.

It would be highly interesting to extend the here presented concepts and algorithms to relativistic systems and spin-carrying particles, and to study multi-body systems by making use of a multi-dimensional approach. The thesis at hand might provide a fruitful basis for such applications.

CHAPTER 5

Conclusion

Non-relativistic particles can be described on the basis of Nelson's stochastic mechanics, yielding a feasible alternative approach to quantum systems. Grounded on Nelson's pioneering work in 1966, variational principles have been established from which kinematic laws and the Schrödinger equation could be derived, ultimately stressing the equivalence of the different theories [Yasue, 1981a; Guerra and Morato, 1983]. Finally, Pavon [1995b] presented the so-called quantum Hamilton principle in a way consistent with classical analytical mechanics, and using the kinematic equations of Nelson [1966] as constraints in the search for the optimal path, thus extremizing the action functional. Nevertheless, the wave function was, up to now, a prerequisite for applying these theories.

Opposed to previous approaches, the thesis at hand deals with the variational problem in terms of stochastic optimal control. That is, instead of searching for the optimal *path*, optimal *controls* are addressed, namely the osmotic and current velocity. These extremize the given cost functions. Putting the considerations into effect leads to the following two major aspects:

1. **The Schrödinger equation**
   The Madelung equations were derived as the Hamilton-Jacobi-Bellman equations of the considered variational problem, which are, for the ground state of a quantum system, equivalent to the Schrödinger equation [Madelung, 1927].

2. **Quantum Hamilton equations of motion**
   Using a maximum principle for forward-backward differential games [Øksendal and Sulem, 2014], or rather a maximum principle for optimal control problems with the controlled process being given by a backward doubly stochastic differential equation [Bahlali and Gherbal, 2010], quantum dynamical equations were derived. The latter equations can be considered as a generalization of the classical Hamilton equations of motion. The associated forward-backward stochastic differential

equations are the central result of the thesis at hand, and offer a complete and unique description of quantum systems. This approach is in accordance with, but independent from, the time-dependent Schrödinger equation.

In detail, the thesis was divided into two main parts, that is, stationary and non-stationary systems.

In the stationary case, the mathematical problem was reduced to a zero-sum case and only the real part of the quantum Hamilton principle had to be taken into account. The resulting coupled forward-backward stochastic differential equations characterize the position and the osmotic velocity of the particle. Furthermore, the Madelung equations of the stationary Schrödinger equation were derived as the Hamilton-Jacobi-Bellman equation of the related least-action principle. The stochastic optimal control problem provided the ground state of the system; however, using the approach of supersymmetric Hamiltonians, all excited states, and therefore the complete spectrum of eigenfunctions and eigenvalues, can be calculated from the ground state. The dynamic equations were solved numerically with an iterative algorithm, hence it was possible to find a numerical approach to the osmotic velocity and the wave function for two different systems. Especially in the case of a one-dimensional (quartic) double-well potential – a system without an exactly known wave function – tunneling processes were analyzed by evaluating the mean first passage time. Furthermore, a direct relation between the mean first passage time and energy splittings, i.e., the difference between the first excited-state energy and the ground-state energy, was derived. It turns out that the assumption of symmetric splitting of the first two energy levels around the harmonic-oscillator energy is not right for basically the entire parameter set.

For non-stationary systems, two distinct derivations of the stochastic Hamilton equations of motion were presented. One the one hand, the real and imaginary part of the quantum Hamilton principle were considered as two variational problems, and the two velocities were then given as their Nash equilibrium. One the other hand, the complex-valued principle was analyzed directly, with optimal conditions for backward doubly stochastic differential equations [Bahlali and Gherbal, 2010]. Both methods provided the same backward stochastic differential equations of the two velocities. Additionally, Nelson's PDEs for the velocities were derived as the Hamilton-Jacobi-Bellman equations to the variational problems. The equation for the momentum is also applicable to the stationary case. Furthermore, the derived quantum Hamilton equations of motion satisfy the correspondence principle, and can be reduce to classical Hamilton equations.

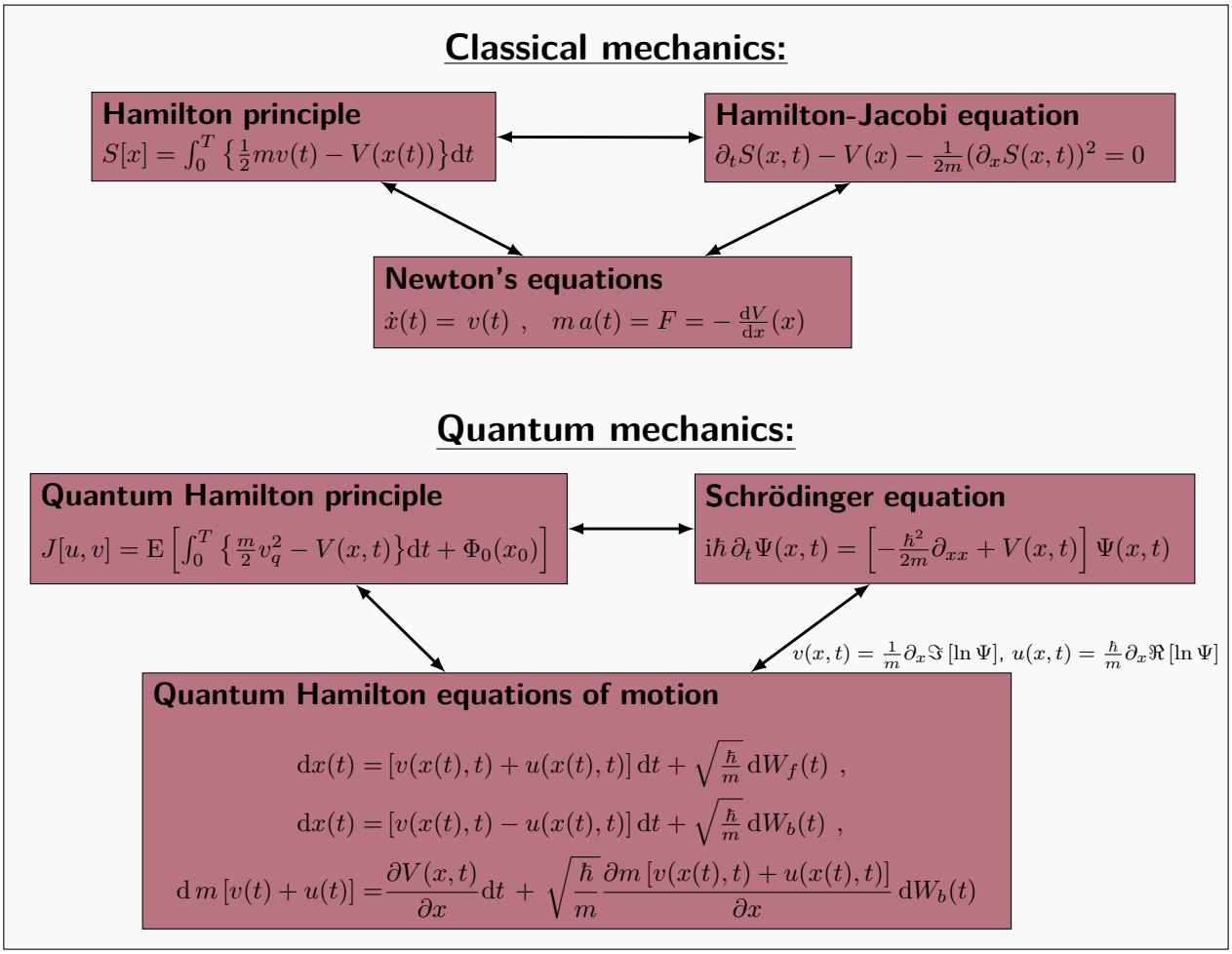

Figure 5.1.: *Schematic representation of the three equivalent theories, which describes the motion of a particle uniquely and independently from each other. Top: For classical particles. Bottom: For quantum particles.*

In summary, the derived quantum Hamilton equations of motion provide a beneficial theory for describing quantum systems independently of the Schrödinger equation. Consequently, the Schrödinger equation is one, but not the only, complete description of quantum systems. This situation is reminiscent of different ways to formulate classical analytical mechanics; cf. **Figure 5.1**. Now being also able to describe systems lacking an analytical wave function, stochastic mechanics, with its more intuitive way of representing quantum-mechanical systems, permits to analyze and illustrate quantum-mechanical phenomena in a way that is in accordance with our every-day experience, and avoids the often complicated interpretation of quantum-mechanical results in the usual sense.

APPENDIX A

Appendix

A.1. General definitions

The following definitions can be found in many textbooks of stochastic analysis; see e.g. ref. [Arnold, 1973; Øksendal, 2000; Meintrup and Schäffler, 2005].

Definition A.1 (Filtration) *Let* $\mathbb{F} = (\mathcal{F}_t)_{t\in I}$ *be an increasing sequence of sub-*σ*-algebras, i.e.,*

$$\mathcal{F}_s \subset \mathcal{F}_t\,,\ \forall\, s,t \in I\,,\ s \leq t \quad , \tag{A.1}$$

then $\mathbb{F}$ *is called filtration.*

Definition A.2 (Measurable function) *Let* $(\Omega, \mathcal{F}, P)$ *be a given probability space, then a function* $f\colon \Omega \to \mathbb{R}^d$ *will be called* $\mathcal{F}$*-measurable, if*

$$f^{-1}(U) := \{\omega \in \Omega\,;\ f(\omega) \in U\} \in \mathcal{F} \tag{A.2}$$

for all open sets $U \subset \mathbb{R}^d$.

Definition A.3 (Adapted process) *A stochastic process* $(X(t))_{t\in I}$ *is called adapted with respect to* $\mathcal{F}_t$ *(or* $\mathcal{F}_t$*-adapted), if* $X(t)$ *is* $\mathcal{F}_t$*-measurable for all* $t \in I$.

Markov processes are introduced in Definition 2.5. The following theorem gives equivalent formulations to the Markov property.

Theorem A.4 *Each of the following conditions are equivalent to the Markov property given by Definition (2.5):*

1. $P\{A|\mathcal{F}_s\} = P\{A|X(s)\}$ *is fulfilled for all* $0 \leq s < t \leq T$ *and* $A \in \mathcal{F}_t$.
2. *Let* $\mathcal{F}_{[t,T]}$ *be the* σ*-algebra generated by the process* $(X(t))_{t\in[0,T]}$ *from time* t *up to* T *and let* Y *be* $\mathcal{F}_{[t,T]}$*-measurable and integrable, then* $\mathrm{E}\,[Y|\,\mathcal{F}_s] = \mathrm{E}\,[Y|\,X(s)]$ *for all* $0 \leq s < t \leq T$.

3. *Let* $A_1 \in \mathcal{F}_{t_1}$ *and* $A_2 \in \mathcal{F}_{[t_2,T]}$*, then*

$$P\{(A_1 \cap A_2)|X(t)\} = P\{A_1|X(t)\}\ P\{A_2|X(t)\} \tag{A.3}$$

for $0 \le t_1 \le t \le t_2 \le T$.

4. *For* $n \ge 1$, $0 < t_1 < t_2 < \cdots < t_n < t \le T$ *and* $B \in \mathcal{B}^d$ *one has*

$$P\{X(t) \in B|X(t_1), X(t_2), \ldots, X(t_n)\} = P\{X(t) \in B|X(t_n)\} \quad . \tag{A.4}$$

The proof of Theorem A.4 can be found in the textbook by Arnold [1973].

Definition A.5 (Martingale) *A stochastic process* $(M_t)_{t\ge0}$ *is called martingale with respect to a family* $(\zeta_t)_{t\ge0}$ *of* σ*-algebras* $\zeta_t \subset \mathcal{F}$*, where* $\zeta_s \subseteq \zeta_t$ *for* $s \le t$*, if:*

1. $\{\omega\colon M(t,\omega) \le C\} \in \zeta_t\ ,\quad \forall C \in \mathbb{R}\ ,\quad \forall t \ge 0.$
2. $\mathrm{E}\Big(|M(t)|\Big) < \infty\ ,\quad \forall t \ge 0.$
3. $\forall s \le t\colon\ \mathrm{E}\left[M(t)|\,\zeta_s\right] = M(s).$

Theorem A.6 (The martingale representation theorem) *Suppose* $M(t)$ *being square integrable, i.e.* $E\Big(|M^2(t)|\Big) < \infty$*, and* $M(t)$ *being a* $\mathcal{F}_t$*-martingale. Then, a unique stochastic process* $g(s,\omega)$ *can be defined such that* $g \in \mathcal{V}(t)$ *(see also Definition 2.6 for* $\mathcal{V}(t)$*) for all* $t \ge 0$*, and*

$$M(t,\omega) = \mathrm{E}(M_0) + \int_0^t g(s,\omega)\mathrm{d}W(s) \quad a.s.^1 \quad \forall t \ge 0 \quad . \tag{A.5}$$

The proof of theorem A.6 can be found in ref. [Øksendal, 2000].

Theorem A.7 (Solution of a linear SDE) *The linear stochastic differential equation*

$$\mathrm{d}X(t) = \Big(B(t)\,X(t) + b(t)\Big)\,\mathrm{d}t\ +\ \sigma(t)\,\mathrm{d}W(t)\quad ,\ X(t=0) = x_0 \tag{A.6}$$

has the following solution for $t \in [0,T]$*,*

$$X(t) = \Phi(t)\left(x_0 + \int_0^t \Phi^{-1}(s)\,b(s)\,\mathrm{d}s + \int_0^t \Phi^{-1}(s)\,\sigma(s)\,\mathrm{d}W(s)\right) \quad , \tag{A.7}$$

[1] almost sure

where $\Phi(t)$ is the fundamental matrix of the deterministic equation $\dot{x} = B(t)\,x$. Especially, if the function $B(t)$ is independent of t, i.e. $B(t) = B$, then the solution becomes

$$X(t) = x_0\,\mathrm{e}^{B\,t} + \int_0^t \mathrm{e}^{B(t-s)} b(s)\,\mathrm{d}s + \int_0^t \mathrm{e}^{B(t-s)} \sigma(s)\,\mathrm{d}W(s) \quad . \tag{A.8}$$

The proof of theorem A.7 can be found in ref. [Arnold, 1973].

In probability theory, there are different notations of convergence of random variables as will be presented in the following. Let X, X_n, $n \geq 1$ be $\mathbb{R}^d$-valued random variables on the probability space $(\Omega, \mathcal{F}, P)$.

Definition A.8 (Stochastic convergence) *A sequence $(X_n)_{n\geq 1}$ of random variables converges in probability towards a random variable X, if*

$$P\left\{\omega \in \Omega\colon\ |X_n(\omega) - X(\omega)| > \varepsilon\right\} \to 0 \quad (n \to \infty) \tag{A.9}$$

holds for all $\varepsilon > 0$. The common notation is

$$\operatorname*{P\text{-}lim}_{n\to\infty} X_n = X \quad \textit{or} \quad X_n \xrightarrow{P} X \quad (n \to \infty) \quad . \tag{A.10}$$

Definition A.9 (Convergence in distribution) *Let F and F_n be the cumulative distribution function of X and X_n, respectively. A sequence $(X_n)_{n\geq 1}$ of random variables is said to converge in distribution (or converge weakly) towards X, if*

$$\lim_{n\to\infty} F_n(x) = F(x) \tag{A.11}$$

holds for all $x \in \mathbb{R}^d$ at which $F(x)$ is continuous.

Definition A.10 (Almost sure convergence) *If a null set $N \in \mathcal{F}$ can be defined in such a way that the sequence $(X_n)_{n\geq 1}$ converges in the usual sense towards x for all $\omega \notin N$, i.e.,*

$$P\left\{\omega \in \Omega\colon\ \lim_{n\to\infty} X_n(\omega) = X(\omega)\right\} = 1 \quad , \tag{A.12}$$

then $(X_n)_{n\geq 1}$ converges almost surely, or almost everywhere, or with probability one towards X. Almost sure convergence is often denoted by the abbreviation a.s., i.e., writing

$$X_n \xrightarrow{a.s.} X \quad (n \to \infty) \quad \textit{or} \quad \operatorname*{a.s.\text{-}lim}_{n\to\infty} X_n = X \quad . \tag{A.13}$$

Definition A.11 (Convergence in p-th mean) *If $X, X_n \in L^p$ and $\mathrm{E}|X_n - X|^p \to 0$ $(n \to \infty)$ holds, then the sequence $(X_n)_{n\geq 1}$ is said to converge in the*

p-th mean towards X. For p = 1 one says that X_n converges in mean towards X. For p = 2, it is common to say that X_n converges in mean square to X as is expressed via

$$\underset{n\to\infty}{\text{ms-lim}} X_n = X \quad . \tag{A.14}$$

The relation between the different terms of convergence is presented in **Figure A.1**.

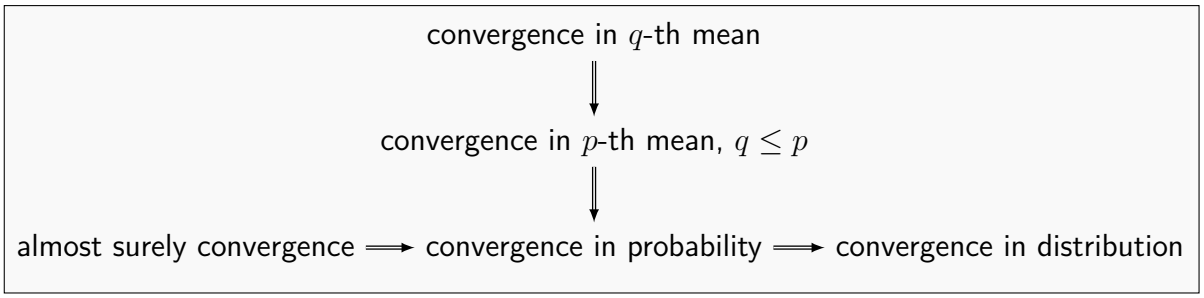

Figure A.1.: *Relation between different terms of convergence. Scheme adopted from ref. [Arnold, 1973].*

A.2. Necessary and sufficient conditions for the maximum principle

In the following, necessary and sufficient optimal conditions for a forward-backward stochastic differential game are presented. The zero-sum case used for stationary systems is a special case of this class of problems. Thus, all statements are also transferable to the zero-sum case. The following conditions are presented and proven in the paper of Øksendal and Sulem [2014]. Consider the (forward) controlled process

$$\mathrm{d}X(t) = b(t, X(t), u(t), \omega)\,\mathrm{d}t + \sigma(t, X(t), u(t), \omega)\,\mathrm{d}W(t)\ , \quad X(0) = x_0 \in \mathbb{R} \tag{A.15}$$

and its associated backward controlled processes

$$\begin{cases} \mathrm{d}Y_i(t) = & -g_i(t, X(t), Y_i(t), Z_i(t), u(t), \omega)\mathrm{d}t + Z_i(t)\mathrm{d}W(t) \ , \ t \in [0, T] \\ Y_i(T) = & h_i(X(T), \omega)\ , \ i = 1, 2 \quad , \end{cases} \tag{A.16}$$

where $u(t) = (u_1(t), u_2(t))$ is related to the two players $i = 1, 2$. As before, $(W(t))_{t\in[0,T]}$ is a Wiener process forward in time, where the time horizon $T > 0$ is fixed. $b(t, x, u)$, $\sigma(t, x, u)$, $g_i(t, x, y, z, u)$ and $h_i(x)$ are known functions in such a way that a unique solution to the forward and the backward equations exists.
The two sub-filtrations $\mathcal{E}_t^{(i)} \subseteq \mathcal{F}_t$, $t \in [0, T]$ represent the information available to the player $i = 1, 2$ at time t. $\mathcal{A}_i$ are the sets of admissible control processes for the player

i and are contained in the set of $\mathcal{E}_t^{(i)}$-predictable processes for $i = 1, 2$, with values $A_i \subset \mathbb{R}$. The optimal controls $u_1(t)$ and $u_2(t)$ are sought as the Nash equilibrium of

$$J_i(u) := \mathrm{E}\left[\int_0^T f_i(t, X^u(t), u(t), \omega)\mathrm{d}t \, + \, \phi_i(X^u(T), \omega) \, + \, \Psi_i(Y_i^u(0))\right] \quad , \; i = 1, 2 \quad , \tag{A.17}$$

i.e. searching for the optimal control $\hat{u}_1, \hat{u}_2$

$$J_1(u_1, \hat{u}_2) \leq J_1(\hat{u}_1, \hat{u}_2) \quad \text{for all } u_1 \in \mathcal{A}_1 \tag{A.18}$$

$$\text{and} \qquad J_2(\hat{u}_1, u_2) \leq J_2(\hat{u}_1, \hat{u}_2) \quad \text{for all } u_2 \in \mathcal{A}_2 \tag{A.19}$$

are fulfilled. The associated Hamilton functions are defined by

$$\begin{aligned} H_i(t, x, y, z, u_1, u_2, \lambda_i, p_i, q_i) := f_i(t, x, y, z, u_1, u_2) \, + \, \lambda_i \, g_i(t, x, y, z, u_1, u_2) \\ + \, p_i \, b(t, x, u_1, u_2) \, + \, q_i \, \sigma(t, x, u_1, u_2) \quad , \end{aligned} \tag{A.20}$$

with the adjoint processes $\lambda_i(t), p_i(t), q_i(t)$ being defined by a forward,

$$\begin{cases} \mathrm{d}\lambda_i(t) &= \lambda_i(t)\left[\frac{\partial g_i}{\partial y}(t)\,\mathrm{d}t \, + \, \frac{\partial g_i}{\partial z}(t)\,\mathrm{d}W(t)\right] \quad , \; t \in [0, T] \; , \\ \lambda_i(0) &= \Psi_i'\left(Y_i(0)\right) \quad , \end{cases} \tag{A.21}$$

as well as a backward SDE,

$$\begin{cases} \mathrm{d}p_i(t) &= \frac{\partial H_i}{\partial x}(t)\,\mathrm{d}t \, + \, q_i(t)\,\mathrm{d}W(t) \; , \; t \in [0, T] \; , \\ p_i(T) &= \phi_i'\left(X(T)\right) \, + \, h_i'(X(T))\,\lambda_i(T) \quad . \end{cases} \tag{A.22}$$

The functions $f_i(t, x, u)$, $\phi_i(x)$ and $\Psi_i(x)$ are fixed functions in such a way that the integrand and the expectation value in equation (A.17) exist.

Theorem A.12 (Sufficient maximum principle) *Let $(\hat{u}_1, \hat{u}_2) \in \mathcal{A}_1 \times \mathcal{A}_1$ be optimal controls with the associated solutions $\hat{X}(t)$, $\hat{Y}_i(t)$, $\hat{Z}_i(t)$, $\hat{\lambda}_i(t)$, $\hat{p}_i(t)$ and $\hat{q}_i(t)$ for $i = 1, 2$. Suppose that the following statements hold [Øksendal and Sulem, 2014]:*

1. *(Concavity I) The functions $x \to h_i(x)$, $x \to \phi_i(x)$, $x \to \Psi_i(x)$ are concave.*

2. *(Conditional maximum principle) It holds that*

$$\begin{aligned} &\operatorname*{ess\,sup}_{v \in \mathcal{A}_1} \mathrm{E}\left[H_1(t, \hat{X}(t), \hat{Y}_1(t), \hat{Z}_1(t), v, \hat{u}_2(t), \hat{\lambda}_1(t), \hat{p}_1(t), \hat{q}_1(t))\middle| \mathcal{E}_t^{(1)}\right] \\ &= \mathrm{E}\left[H_1(t, \hat{X}(t), \hat{Y}_1(t), \hat{Z}_1(t), \hat{u}_1(t), \hat{u}_2(t), \hat{\lambda}_1(t), \hat{p}_1(t), \hat{q}_1(t))\middle| \mathcal{E}_t^{(1)}\right] \end{aligned} \tag{A.23}$$

and, similarly,

$$\begin{aligned} &\operatorname*{ess\,sup}_{v\in\mathcal{A}_2} \mathrm{E}\left[H_2(t,\hat{X}(t),\hat{Y}_2(t),\hat{Z}_2(t),\hat{u}_1(t),v,\hat{\lambda}_2(t),\hat{p}_2(t),\hat{q}_2(t))\Big|\,\mathcal{E}_t^{(2)}\right] \\ &= \mathrm{E}\left[H_2(t,\hat{X}(t),\hat{Y}_2(t),\hat{Z}_2(t),\hat{u}_1(t),\hat{u}_2(t),\hat{\lambda}_2(t),\hat{p}_2(t),\hat{q}_2(t))\Big|\,\mathcal{E}_t^{(2)}\right] \quad . \end{aligned} \tag{A.24}$$

3. *(Concavity II) (Arrow conditions) The functions*

$$\hat{\mathcal{H}}_1(x,y,z) := \operatorname*{ess\,sup}_{v_1\in\mathcal{A}_1} \mathrm{E}\left[H_1(t,x,y,z,v_1,\hat{u}_2(t),\hat{\lambda}_1(t),\hat{p}_1(t),\hat{q}_1(t))\Big|\,\mathcal{E}_t^{(1)}\right] \tag{A.25}$$

and

$$\hat{\mathcal{H}}_2(x,y,z) := \operatorname*{ess\,sup}_{v_2\in\mathcal{A}_2} \mathrm{E}\left[H_2(t,x,y,z,\hat{u}_1(t),v_2,\hat{\lambda}_2(t),\hat{p}_2(t),\hat{q}_2(t))\Big|\,\mathcal{E}_t^{(1)}\right] \tag{A.26}$$

are concave for all $t\in[0,T]$ almost surely. Assume that the following condition is fulfilled:

$$\begin{aligned} \mathrm{E}\Bigg[\int_0^T \Big\{ &\hat{p}_i^2(t)\,(\sigma(t)-\hat{\sigma}(t))^2 + \hat{q}_i^2(t)\left(X(t)-\hat{X}(t)\right)^2 \\ &\left(Y_i(t)-\hat{Y}_i(t)\right)^2 \left(\tfrac{\partial\hat{\mathcal{H}}_i}{\partial z}\right)^2(t) + \hat{\lambda}_i^2(t)\left(Z_i(t)-\hat{Z}_i(t)\right)^2\Big\}\,\mathrm{d}t\Bigg] < \infty \end{aligned} \tag{A.27}$$

for $i=1,2$.

Then, $\hat{u}(t)=(\hat{u}_1(t),\hat{u}_2(t))$ is a Nash equilibrium for equation (A.15)–(A.17).

Furthermore, it is also possible to prove a version of the maximum principle without concavity conditions [Øksendal and Sulem, 2014]. A necessary maximum principle [Øksendal and Sulem, 2014] can be formulated and understood as an extension to that one presented in refs. [Øksendal and Sulem, 2009; An and Øksendal, 2012].

Theorem A.13 (Necessary maximum principle) *Let $(\hat{u}_1,\hat{u}_2)\in\mathcal{A}_1\times\mathcal{A}_1$ be optimal controls with the associated solutions $\hat{X}(t)$, $\hat{Y}_i(t)$, $\hat{Z}_i(t)$, $\hat{\lambda}_i(t)$, $\hat{p}_i(t)$, $\hat{q}_i(t)$ for $i=1,2$. Suppose that the following statements hold [Øksendal and Sulem, 2014]:*

1. *For all $t_0\in[0,T]$ and all bounded $\mathcal{E}_i^{(i)}$-measurable random variables $\alpha_i(\omega)$, the control $\beta_i(t):=\mathbb{1}_{(t_0,T)}(t)\,\alpha_i(\omega)$ belongs to $\mathcal{A}_i$, $i=1,2$.*

2. *For all u_i, $\beta_i\in\mathcal{A}_i$ with β_i bounded, there exists a $\delta_i>0$ such that the control $\tilde{u}_i(t):=u_i(t)+s\,\beta_i(t)$, $t\in[0,T]$ belongs to $\mathcal{A}_i$ for all $s\in(-\delta_i,\delta_i)$, $i=1,2$.*

3. *The derivative processes*

$$x_1(t) = \frac{\mathrm{d}}{\mathrm{d}s} X^{(u_1+s\beta_1,u_2)}(t)\Big|_{s=0} \quad ,$$
$$y_1(t) = \frac{\mathrm{d}}{\mathrm{d}s} Y^{(u_1+s\beta_1,u_2)}(t)\Big|_{s=0} \quad ,$$
$$z_1(t) = \frac{\mathrm{d}}{\mathrm{d}s} X^{(u_1+s\beta_1,u_2)}(t)\Big|_{s=0} \quad ,$$

and, similarly,

$$x_2(t) = \frac{\mathrm{d}}{\mathrm{d}s} X^{(u_1u_2+s\beta_2)}(t)\Big|_{s=0} \quad , \quad \textit{etc.}$$

exist and belong to $L^2([0,T]\times\Omega)$.

4. *Suppose*

$$\mathrm{E}\Bigg[\int_0^T \Bigg\{ p_i^2(t)\left(\frac{\partial\sigma}{\partial x}(t)\,x_i(t) + \frac{\partial\sigma}{\partial u_i}(t)\,\beta_i(t)\right)^2 + x_i^2(t)\,q_i^2(t) + \lambda_i^2(t)\,z_i^2(t) + y_i^2(t)\left(\frac{\partial H_i}{\partial z}\right)^2(t)\Bigg\}\mathrm{d}t\Bigg] < \infty \quad ,$$

$i = 1, 2$.

Then, the following statements are equivalent [Øksendal and Sulem, 2014]:

$$\frac{\mathrm{d}}{\mathrm{d}s} J_1(u_1 + s\beta_1, u_2)\Big|_{s=0} = \frac{\mathrm{d}}{\mathrm{d}s} J_2(u_1, u_2 + s\beta_2)\Big|_{s=0} = 0 \tag{A.28}$$

for all bounded $\beta_1 \in \mathcal{A}_1$, $\beta_2 \in \mathcal{A}_2$.

$$\mathrm{E}\left[\frac{\partial}{\partial v_1} H_1(t, X(t), Y_1(t), Z_1(t), v_1, u_2(t), \lambda_1(t), p_1(t), q_1(t))\,\middle|\,\mathcal{E}_t^{(1)}\right]$$
$$= \mathrm{E}\left[\frac{\partial}{\partial v_2} H_1(t, X(t), Y_2(t), Z_2(t), u_1(t), v_2, \lambda_2(t), p_2(t), q_2(t))\,\middle|\,\mathcal{E}_t^{(2)}\right] = 0 \quad . \tag{A.29}$$

A.3. Malliavin derivative

The algorithm for solving the backward SDE used in this thesis is based upon the projection property of conditional expectations. However, it is also possible to find an algorithm using the Malliavin derivative.

The conditional expectation $\mathrm{E}\left[Y^{\pi}_{t_{i+1}} | X^{\pi}_{t_i} = x\right]$ can be defined using delta distributions, namely

$$\mathrm{E}\left[Y^{\pi}_{t_{i+1}} \middle| X^{\pi}_{t_i} = x\right] := \frac{\mathrm{E}\left(\delta_x(X^{\pi}_{t_i})\, Y^{\pi}_{t_{i+1}}\right)}{\mathrm{E}\left(\delta_x(X^{\pi}_{t_i})\right)} \quad , \text{ with } \delta_x(X) = \begin{cases} 1 \ , & X = x \\ 0 \ , & \text{else} \end{cases} \quad . \tag{A.30}$$

Since the delta distribution is only different from zero for $x \in \mathbb{R}$, and since $x \in \mathbb{R}$ is drawn with probability zero, the delta distribution cannot be calculated during the simulation[2]. Therefore, one aims for an expression for the conditional expectation in which the antiderivative $\mathbb{1}_{x \leq X}$ is used instead of the delta function. The revised expression reads

$$\mathrm{E}\left[Y^{\pi}_{t_{i+1}} \middle| X^{\pi}_{t_i} = x\right] = \frac{\mathrm{E}\left(\mathbb{1}_{x \leq X^{\pi}_{t_i}}\, S^h(1)\, Y^{\pi}_{t_{i+1}}\right)}{\mathrm{E}\left(\mathbb{1}_{x \leq X^{\pi}_{t_i}}\, S^h(1)\right)} \quad . \tag{A.31}$$

The new random variable $S^h(1)$ will be defined later.

In short notations, $f'(\cdot) := \delta_x(\cdot)$ is written, and the wanted expectation value reads

$$\mathrm{E}(f'(X)\, Y) = \mathrm{E}(f(X)\, Z) \quad . \tag{A.32}$$

The following definition and chain rule will be necessary to eliminate the derivative (or finding the new random variable Z). Further information and the proof of the chain rule can be found in the textbook by Nualart [2006].

Definition A.14 *Let $(W(t))_{t\in[0,T]}$ be an n-dimensional Brownian-motion process on a complete probability space $(\Omega, \mathcal{F}, P)$, and let $\mathcal{F}_t$ be the complete filtration generated by the Brownian motion up to time t. The set $\mathcal{S}$ is the set of all smooth random variables F of the form*

$$F = f\left(\int_0^T h_1(t)\, \mathrm{d}W_1(t)\, , \ldots , \int_0^T h_n(t)\, \mathrm{d}W_n(t)\right) \quad , \tag{A.33}$$

where $f\colon \mathbb{R}^n \to \mathbb{R}$ is an infinitely often continuously differentiable function, and $h_i \in L^2(\Omega \times \mathbb{R}_+)$, $i = 1, \ldots, n$. The derivation of a smooth random variable F is the stochastic process $(D_t F)_{t\in[0,T]}$ in $L^2(\omega \times \mathbb{R}_+)$ given by

$$D_t F = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\left(\int_0^T h_1(t)\, \mathrm{d}W_1(t)\, , \ldots , \int_0^T h_n(t)\, \mathrm{d}W_n(t)\right) h_i(t) \quad . \tag{A.34}$$

[2]The process X^{π} is a real number in a specified interval.

Example A.15 *Let $f(x) = x$, then the derivative of the random variable $F = f\left(\int_0^T h(t)\,\mathrm{d}W(t)\right)$ reads*

$$D_t F = \left.\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right|_{x=\int_0^T h(t)\,\mathrm{d}W(t)} \cdot h(t) = h(t) \quad . \tag{A.35}$$

The domain of the derivative in $L^2(\Omega)$ is denoted by $\mathbb{D}^{1,2}$, meaning that the Hilbert space $\mathbb{D}^{1,2}$ is the closure of the class of smooth random variables $\mathcal{S}$ with respect to the norm [Nualart, 2006]

$$\|F\|_{1,2} = \sqrt{\mathrm{E}\Big(|F|^2\Big) + \mathrm{E}\Big(\|DF\|^2\Big)} \quad . \tag{A.36}$$

The following theorem [Nualart, 2006] will be very useful to find the desired random variable Z.

Theorem A.16 (Chain rule) *Let $\varphi\colon \mathbb{R}^m \to \mathbb{R}$ be a continuously differentiable function with bounded partial derivatives. Suppose that $F = (F^1, \ldots, F^m)$ is a random vector whose components belong to $\mathbb{D}^{1,2}$. Then, $\varphi(F) \in \mathbb{D}^{1,2}$ and*

$$D_t\,\varphi(F) = \sum_{i=1}^{m} \frac{\partial \varphi}{\partial x_i}(F)\, D_t\, F^i \quad . \tag{A.37}$$

Assuming that $\mathrm{E}\int_0^T \|X(t)\|_{1,2}^2\,\mathrm{d}t < \infty$ holds for a one-dimensional process X, the derivative of the considered function $f(X)$ is given by

$$D_t\, f(X) = f'(X) D_t\, X \quad . \tag{A.38}$$

Multiplying this equation with $Y\,h(t)$ on both sides leads to

$$Y\,h(t)\, D_t\, f(X) = f'(X) D_t X\, Y\, h(t) \quad . \tag{A.39}$$

Here, the function $h(t)$ fulfills the conditions [Bouchard et al., 2004]

$$\int_0^T D_t X_{t_i}^{\pi}\, h(t)\,\mathrm{d}t = 1 \quad , \quad \int_0^T D_t X_{t_{i+1}}^{\pi}\, h(t)\,\mathrm{d}t = 0 \quad . \tag{A.40}$$

Integrating equation (A.39) with respect to t and using the condition given in equation (A.40), one gets

$$f'(X_{t_i}^{\pi}) Y = \int_0^T Y\, h(t)\, D_t f(X_{t_i}^{\pi})\,\mathrm{d}t \quad . \tag{A.41}$$

Hence, the expectation value reads

$$\mathrm{E}\left(f'(X_{t_i}^{\pi}) Y\right) = \mathrm{E}\left(\int_0^T Y\, h(t)\, D_t f(X_{t_i}^{\pi})\,\mathrm{d}t\right) \quad . \tag{A.42}$$

The right-hand side of this equation is given the definition presented below [Nualart, 2006].

Definition A.17 (Divergence operator) *Let u be a stochastic process such that*

$$\left|\mathrm{E}\left(\int_0^T D_t F\, u(t)\mathrm{d}t\right)\right| \leq c\|F\|_{1,2} \tag{A.43}$$

holds for all $F \in \mathbb{D}^{1,2}$, with $c \in \mathbb{R}$ being constant. Then, the divergence operator $\delta(u)$, also called Skohorod integral, is a random variable defined by

$$\mathrm{E}\left(F\,\delta(u)\right) = \mathrm{E}\left(\int_0^T D_t F\, u(t)\,\mathrm{d}t\right) \quad , \forall F \in \mathbb{D}^{1,2} \quad . \tag{A.44}$$

For an adapted process $(u(t))_{t\in[0,T]}$ the Skohorod integral equals the Itô integral [Nualart, 2006].

Going back to the specific problem, i.e. $f'(\cdot) = \delta_x(\cdot)$, the wanted conditional expectation reads

$$\mathrm{E}\left[Y^\pi_{t_{i+1}}\middle|\, X^\pi_{t_i} = x\right] = \frac{\mathrm{E}\left(\mathbb{1}_{x\leq X^\pi_{t_i}}\, S^h(1)\, Y^\pi_{t_{i+1}}\right)}{\mathrm{E}\left(\mathbb{1}_{x\leq X^\pi_{t_i}}\, S^h(1)\right)} \quad . \tag{A.45}$$

Here, $S^h(F)$ denotes the general Skohorod integral of the random variable F and is commonly denoted as

$$S^h(F) := \int_0^T F\, h(t)\, \delta W(t) \quad . \tag{A.46}$$

Consequently, one has to calculate Skohorod integrals numerically in each time step, and a beneficial function h is needed. One attempt to this function can be found in ref. [Bouchard and Touzi, 2004].

A.4. Numerical solution of stochastic differential equations

In this section, some general statements about the numerical solution of SDEs are made. A numerical approximation to the solution process is given by time-discrete stochastic processes that converge to the exact solution. In this context, fundamental terms (e.g. convergence or global error) are explained and the used numerical approximation schemes (the Euler-Maruyama method and the Heun method) are analyzed. All definitions and statements can be also found, for instance, in the textbook by Kloeden and Platen [1992].

Suppose that the stochastic process $(X(t))_{t\in[0,T]}$ is given by the SDE

$$\mathrm{d}X(t) = b(t, X(t))\,\mathrm{d}t + \sigma(t, X(t))\,\mathrm{d}W(t) \quad X(t=0) = x_0 \quad , \tag{A.47}$$

where the coefficients $b, \sigma\colon [0,T] \times \mathbb{R} \to \mathbb{R}$ are known functions in such a way that a unique solution exists (see theorem 2.14). For the sake of simplicity, only one-dimensional processes are considered. In fact, all statements are also applicable to higher dimensions.

Let $0 \le t_0 < t_1 < \cdots < t_N = T$ be a partition of the given time interval $[0,T]$ with time increments $\Delta_i = t_{i+1} - t_i$, $i = 0, \ldots, N-1$. The simplest approximation scheme is given by the Euler-Maruyama method characterized by the difference equation

$$\begin{aligned} Y_0 &= x_0 \\ Y_{t_{i+1}} &= Y_{t_i} + b(t_i, Y_{t_i})\,\Delta_i + \sigma(t_i, Y_{t_i})\,\Delta W_i \quad , \end{aligned} \tag{A.48}$$

with $\Delta W_i := W(t_{i+1}) - W(t_i)$, $i = 0, \ldots, N-1$ being discrete increments of the Wiener process. The time discrete process[3] $(Y_{t_i})_{i=0,\ldots,N}$ is a numerical approximation to the exact (continuous) process $(X(t))_{t\in[0,T]}$.

Strong convergence

Definition A.18 (Global error) *Let $(X(t))_{t\in[0,T]}$ be the exact solution of equation (A.47), and let $(Y_{t_i})_{i=0,\ldots,N}$ be an approximation of the exact solution as determined, for instance, by use of the Euler-Maruyama method. Then, the global error is defined by the expectation value of the difference between the exact and the numerical solution at the terminal time T, i.e.,*

$$\epsilon = \mathrm{E}\Big(X(T) - Y_{t_N}\Big) \quad . \tag{A.49}$$

Definition A.19 (Strong convergence) *Let $\delta := \max_i(\delta_i)$ be the maximum step size. The numerical approximation converges strongly to the exact solution at the terminal time T, if*

$$\lim_{\delta\to 0} \mathrm{E}\left(X(T) - Y^{\delta}_{t_N}\right) = 0 \quad . \tag{A.50}$$

In order to validate the numerical approximation, the rate of convergence has to be known.

[3] In the main part of this thesis, the process used to approximate the actual mechanism is denoted by X^{π}; however, for the sake of clarity, a new variable is used.

Definition A.20 *The approximation process converges strongly with the order* $\gamma > 0$*, if there exists a constant* $C > 0$ *independent of* δ*, and a* $\delta_0 > 0$*, such that*

$$\epsilon \leq C\,\delta^{\gamma}\ , \quad \forall \delta \in (0, \delta_0) \quad . \tag{A.51}$$

This definition is the generalization of the deterministic order of convergence and can be found in many textbooks of numerical solutions to ordinary differential equations (see, for instance, ref. [Strehmel et al., 2012]).

However, the global error to the approximation is in general difficult to determine. Thus, it would be beneficial to use the concept of consistency, which is – like the deterministic methods – linked to the concept of convergence. Since the exact solution of the SDE does not occur in the following conditions, strong consistency of an approximation is often easier to verify [Kloeden and Platen, 1992].

Definition A.21 (Strong consistency) *Let* $\mathcal{F}_t$*,* $t \in [0, T]$*, be the* σ*-algebra generated by Brownian motion (or the Itô process) up to time* t*. The approximation* Y^{δ} *corresponding to the time discretization* $0 = t_0 < t_1 < \cdots < t_N = T$ *is strongly consistent, if there is a non-negative function* $c = c(\delta)$ *with* $\lim_{\delta \to 0} c(\delta) = 0$*, such that*

$$\mathrm{E}\left(\left|\mathrm{E}\left[\Delta_i^{-1}\,\left(Y^{\delta}_{t_{i+1}} - Y^{\delta}_{t_i}\right)\middle|\,\mathcal{F}_{t_i}\right]\,-\,b\left(t_i, Y^{\delta}_{t_i}\right)\right|^2\right) \leq c(\delta) \tag{A.52}$$

and

$$\mathrm{E}\left(\Delta_i^{-1}\left|Y^{\delta}_{t_{i+1}} - Y^{\delta}_{t_i}\,-\,\mathrm{E}\left[Y^{\delta}_{t_{i+1}} - Y^{\delta}_{t_i}\middle|\,\mathcal{F}_{t_i}\right]\,-\,\sigma\left(t_i, Y^{\delta}_{t_i}\right)\,\Delta W_i\right|^2\right) \leq c(\delta) \tag{A.53}$$

hold for all fixed $Y^{\delta}_{t_i} = y$ *and* $i = 0, \ldots, N$*.*

The first condition requires the average of the increments of the approximation to converge to that of the Itô process. For vanishing noise, this situation is equivalent to the deterministic definition of consistency of a one-step-scheme. From the second condition (equation (A.53)) it follows that the variance of the difference between the random parts of the approximation and the random parts in the Itô process converges to zero [Kloeden and Platen, 1992]. Hence, strong consistency gives an indication of pathwise closeness and implies strong convergence of the time-discrete approximation to the Itô process. This proposition is explicitly proven in ref. [Kloeden and Platen, 1992] for one-dimensional, autonomous SDEs ($b(t, x) = b(x)$, $\sigma(t, x) = \sigma(x)$) with an equidistant discretization $\Delta_i = \delta$ for all i.

Weak convergence

For some practical applications, only the approximation of the probability distribution (or the moments) of the Itô process (instead of the pathwise convergence) is of interest, and weaker conditions are acceptable.

Definition A.22 (Weak convergence) *Let $\delta > 0$ be the maximum step size. The discrete time approximation Y^δ converges weakly to the Itô process X at time T with respect to a class $\mathcal{C}$ of test functions $g\colon \mathbb{R} \to \mathbb{R}$, if*

$$\lim_{\delta \to 0} \left| \mathrm{E}(g(X(T)) \, - \, \mathrm{E}\left(g\left(Y_T^\delta\right)\right)\right| = 0 \tag{A.54}$$

for all $g \in \mathcal{C}$.

If the class $\mathcal{C}$ includes all polynomials, then the convergence of all moments will be required in the above definition. As for the case of strong solutions, it is useful to consider the order of weak convergence.

Definition A.23 *The numerical approximation Y^δ will converge weakly with the order $\beta > 0$ at time T, if there exists a constant $C > 0$ independent of δ such that*

$$\left|\mathrm{E}(g(X(T)) \, - \, \mathrm{E}\left(g\left(Y_T^\delta\right)\right)\right| \leq C\,\delta^\beta \tag{A.55}$$

holds for all $g \in \mathcal{C}$.

Definition A.24 (Weak consistency) *The approximation is weakly consistent, if there exists a non-negative function $c = c(\delta)$ with $\lim_{\delta \to 0} c(\delta) = 0$, such that*

$$\mathrm{E}\left(\left|\mathrm{E}\left[\Delta_i^{-1}\,\left(Y_{t_{i+1}}^\delta - Y_{t_i}^\delta\right)\middle|\,\mathcal{F}_{t_i}\right] \, - \, b\left(t_i, Y_{t_i}^\delta\right)\right|^2\right) \leq c(\delta) \tag{A.56}$$

and

$$\mathrm{E}\left(\left|\mathrm{E}\left[\Delta_i^{-1}\,(Y_{t_{i+1}}^\delta - Y_{t_i}^\delta)^2\middle|\,\mathcal{F}_{t_i}\right] \, - \, \sigma(t_i, Y_{t_i}^\delta)^2\right|^2\right) \leq c(\delta) \tag{A.57}$$

hold for all fixed values $Y_{t_i}^\delta = y$ and $i = 0, \ldots, N$.

The first requirement equals the first condition for strong consistency (see equation (A.52)). The second condition, however, is much weaker than that in equation (A.53): only the variance of the increment of the approximation has to be close to that one of the Itô process [Kloeden and Platen, 1992]. A weakly consistent scheme is also weakly convergent.

Using the above described concepts, one can easily check that the Euler-Maruyama scheme (equation (A.48)) has a strong convergence order of $\gamma = 0.5$, and is weakly convergent with the order $\beta = 1$.

The last point of this section, the Heun method is analyzed, which is also used to determine the paths of the motion process.

Example A.25 (Heun method) *The Heun scheme for the equation (A.47) is given by*

$$\begin{aligned} Y_0 = x_0 \quad , \quad \tilde{Y}_{t_i} &= Y_{t_i} + b(t_i, Y_{t_i}) + \sigma(t_i, Y_{t_i})\Delta W_i \quad , \\ Y_{t_{i+1}} = Y_{t_i} &+ \frac{\Delta_i}{2}\Big(b(t_i, Y_{t_i}) + b(t_{i+1}, \tilde{Y}_{t_i})\Big) + \frac{\Delta W_i}{2}\Big(\sigma(t_i, Y_{t_i}) + \sigma(t_{i+1}, \tilde{Y}_{t_i})\Big) \quad . \end{aligned} \tag{A.58}$$

In general, this method is neither strongly nor weakly convergent. Only for additive noise ($\sigma(t, x) = \sigma$ is a constant), strong consistency and strong convergence of the method can be proven [Kloeden and Platen, 1992; Kloeden, 2002]. For additive noise, the method has a weak convergence order of $\beta = 2$ [Szymczak and Ladd, 2003] and is strongly convergent with the order of $\gamma = 1$ [Kloeden, 2002].

A.5. Numerov method for the stationary Schrödinger equation

The Numerov method is a common method for solving the one-dimensional stationary Schrödinger equation [Blatt, 1967; Johnson, 1977]. As a considerable advantage, the energy eigenvalues can be calculated, as was done for different potentials by Fack and Vanden Berghe [1987].

The following derivation of the algorithm can be found in the paper of Blatt [1967]. As a first step, the Schrödinger equation is written as

$$\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} = f(x)\,\Psi(x) \quad , \text{ with } f(x) := \tfrac{2m}{\hbar}\,(V(x) - E) \quad . \tag{A.59}$$

Next, the Taylor expansion at the point x is constructed, and reads

$$\Psi(x + h) = \sum_{n=0}^{\infty} \frac{h^n}{n!}\,\Psi^{(n)} \quad . \tag{A.60}$$

Here, $\Psi^{(n)}$ is the n-th derivative of $\Psi(x)$ evaluated at the point x. Hence, one can write

$$\tfrac{1}{2}\left[\Psi(x+h)+\Psi(x-h)\right] = \Psi + \tfrac{h^2}{2}\Psi^{(2)} + \tfrac{h^4}{4!}\Psi^{(4)} + \tfrac{h^6}{6!}\Psi^{(6)} + \ldots \tag{A.61}$$

and, differentiating twice, one gets

$$\tfrac{1}{2}\left[\Psi^{(2)}(x+h)+\Psi^{(2)}(x-h)\right] = \Psi^{(2)} + \tfrac{h^2}{2}\Psi^{(4)} + \tfrac{h^4}{4!}\Psi^{(6)} + \ldots \quad . \tag{A.62}$$

If equation (A.62) is multiplied by the factor $\frac{1}{12}h^2$, and the result is subtracted from equation (A.61), the term proportional to $\Psi^{(4)}$ will be eliminated. Using $\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi(x) = f(x)\,\Psi(x)$, one ends up with

$$\begin{aligned}\Psi(x+h)\,\left(1-\tfrac{h^2}{12}\,f(x+h)\right) = {} & 2\,\Psi(x)\left(1+\tfrac{5h^2}{12}\,f(x)\right) \\ & -\Psi(x-h)\,\left(1-\tfrac{h^2}{12}\,f(x-h)\right)+\mathcal{O}(h^6) \quad .\end{aligned} \tag{A.63}$$

If $\Psi(x)$ and $\Psi(x-h)$ are known, $\Psi(x+h)$ can be determined uniquely. The method has a convergence order of five, which is higher than other two-step schemes or also Runge-Kutta methods [Blatt, 1967].

Now, there are two problems in dealing with this equation. First, the function $f(x)$ has to be a known function, i.e. the energy has to be calculated, and, second, two initial points are needed to solve the equation uniquely.

Suppose that the wave function is searched within an interval $[-b, b]$, where b has to large enough to account for the position of even the most-distant classical turning point, i.e., positions at which $E = V(x)$ is fulfilled.

If the potential is symmetric, i.e. $V(x) = V(-x)$, the wave function must be either symmetric, $\Psi(x) = \Psi(-x)$, or antisymmetric,$\Psi(x) = -\Psi(-x)$.
For an even solution, $\Psi_0 = \Psi(x=0)$ is arbitrary and $\Psi_1 = \Psi(h)$ can be determined by the Numerov method,

$$\Psi_1 = \frac{1+\frac{5}{12}\,h^2\,f(0)}{1-\frac{h^2}{12}\,f(h)} \quad . \tag{A.64}$$

For an odd wave function, on the other hand, Ψ_0 has to be zero and Ψ_1 is arbitrary (one may choose $\Psi_1 = h$). The choice of the arbitrary initial value has no influence on the result since the resulting function is normalized ($\int |\Psi(x)|^2 \mathrm{d}x \stackrel{!}{=} 1$). As the solution is symmetric (or antisymmetric), Equation (A.63) will only be integrated over the positive x-range.

If the energy is unknown, the wave function has to be calculated iteratively. At the beginning, an upper (Q_1) and lower bound (Q_2) have to be chosen such that the wanted energy is in between. The first estimate for the energy is given by a bisection of the energy range, i.e.

$$E^0 = \tfrac{1}{2}\left[Q_1 + Q_2\right] \quad . \tag{A.65}$$

Next, one has to figure out whether the estimate for the energy is higher or lower than the wanted energy. If E^0 is too high, the estimate will give the new upper bound of the energy interval ($Q_1 = E^0$). If E^0 is too low, E^0 will be the new lower bound ($Q_2 = E^0$). In order to decide whether the estimate of the energy is too high or too low, equation (A.63) is integrated forward (starting at $x = 0$) and backward (starting at b) until the arbitrary point x_a is reached. $\Psi_L(x)$ is the solution of the forward (outwards) and $\Psi_R(x)$ is the solution of the backward (inwards) integration. After suitable normalizations, the two functions have the same value at x_a. Still, the derivatives of the two functions are different from each other at the point x_a if the energy is not accurately determined. One can show that the correction term of the energy ($\Delta E = E^0 - E$) is proportional to $\Psi'_R(x_a) - \Psi'_L(x_a)$ [Blatt, 1967]. The two derivatives can be calculated using again a Taylor expansion at x_a,

$$\Psi_L(x_a - h) = \Psi_L(x_a) - h\Psi'_L(x_a) + \frac{1}{2}\Psi''_L(x_a) + \mathcal{O}(h^3) \quad , \tag{A.66}$$

$$\Psi_R(x_a + h) = \Psi_R(x_a) + h\Psi'_R(x_a) + \frac{1}{2}\Psi''_R(x_a) + \mathcal{O}(h^3) \quad . \tag{A.67}$$

Since $\Psi_R(x_a) = \Psi_L(x_a) =: \Psi(x_a)$ and $\Psi''_R(x_a) = \Psi''_L(x_a) = f(x_a)\Psi(x_a)$, the difference of the derivative at x_a is given by

$$\Psi'_R(x_a) - \Psi'_L(x_a) = \frac{-\left[2 + h^2 f(x_a)\right]\Psi(x_a) + \Psi_L(x_a - h) + \Psi_R(x_a + h)}{h} + \mathcal{O}(h^2) \quad . \tag{A.68}$$

Be aware that the estimate of the energy is used in the function $f(x)$, cf. equation (A.59). Hence, if $\Delta E > 0$, then $Q_1 = E^0$, and if $\Delta E < 0$, then $Q_2 = E^0$. The correct energy will be found if the correction term equals zero.

The next estimate for the energy is given by equation (A.65), where one of the interval bounds is replaced by E^0. The described procedure is repeated until the correction term of the energy is smaller than a certain tolerance.

It has to be taken into account that the approach of the wave function associated with the energy estimate E^i (after i iterations) is composed of the solution of the forward

and backward integration, i.e.,

$$\Psi(x) = \begin{cases} \Psi_L(x) \ , & |x| \in [0, x_a] \\ \Psi_R(x) \ , & |x| \in (x_a, b] \end{cases} \quad . \tag{A.69}$$

Here, $\Psi_L(0) = \Psi_0$ and $\Psi_L(h) = \Psi_1$ (the choice of the initial points was explained above), $\Psi_R(b) = h$, and

$$\Psi_R(b-h) = \frac{2\Psi_R(b)\left(1 + \frac{5}{12}h^2 f(b)\right)}{1 - \frac{h^2}{12}f(b-h)} \quad . \tag{A.70}$$

After inwards integration, the solution $\Psi_R(x)$ is multiplied by the factor $\frac{\Psi_L(x_a)}{\Psi_R(x_a)}$. As the last step, the approximation to the wave function is normalized in such a way that

$$\int_{-b}^{b} |\Psi(x)|^2 \mathrm{d}x = 1 \quad . \tag{A.71}$$

The algorithm converges reasonable well to the desired wave function. Still, in the article by Blatt [1967], an even more precise algorithm for the energy is presented.

A.6. WKB-Approximation

The WKB-approximation – named after Wentzel, Kramer and Brillouin – is a semi-classical approach and can be found in many textbooks of theoretical physics; see, for instance, ref. [Landau and Lifschitz, 1979]. If the De Broglie wave-length[4] is small compared to the size of the system, the quantum system will have nearly classical features. Suppose that the solution to the one-dimensional, time-independent Schrödinger equation for a particle in a potential $V(x)$ is searched. The wave function is written as

$$\Psi(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)} \quad , \tag{A.72}$$

hence the function $S(x)$ fulfills

$$\frac{1}{2m}\left(\frac{\mathrm{d}S(x)}{\mathrm{d}x}\right)^2 - \frac{\mathrm{i}\hbar}{2m}\frac{\mathrm{d}^2 S(x)}{\mathrm{d}x^2} = E - V(x) \quad . \tag{A.73}$$

[4]Because of the wave-particle duality, every particle with a certain momentum is correlated with a wave length, which is called De Broglie wave-length.

According to the condition that the particle has nearly classical properties, the function is written as a power series in $\hbar$, i.e.,

$$S(x) = S_0(x) + \frac{\hbar}{\mathrm{i}} S_1(x) + \left(\frac{\hbar}{\mathrm{i}}\right)^2 S_2(x) + \ldots \quad . \tag{A.74}$$

In the first approximation, the function $S(x) = S_0(x)$ and the term including $\hbar$ is omitted in equation (A.73) [Landau and Lifschitz, 1979], resulting in

$$\frac{1}{2m}\left(\frac{\mathrm{d}S_0(x)}{\mathrm{d}x}\right)^2 = E - V(x) \quad . \tag{A.75}$$

The solution is given by the classical momentum and reads

$$S_0(x) = \pm \int \sqrt{2m(E - V(x))}\mathrm{d}x = \pm \int p(x)\mathrm{d}x \quad . \tag{A.76}$$

Neglecting the first-order term is only possible if the term is small compared to the other ones, meaning that

$$\left|\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\hbar}{S'(x)}\right)\right| \ll 1 \quad . \tag{A.77}$$

Consequently, using the definition of the De Broglie wave-length, $\lambda(x) = \hbar/p(x)$, one gets the condition

$$\left|\frac{1}{2\pi}\frac{\mathrm{d}\lambda}{\mathrm{d}x}\right| \ll 1 \quad , \tag{A.78}$$

and the system can be considered as being a semi-classical one [Landau and Lifschitz, 1979]. However, near the classical turning points, the wave length diverges and using the semi-classical approach is not permitted.

Going further, the next term of the power series $S_1(x)$ (see equation (A.74)) is determined. The term of the order of $\hbar$ in equation (A.73) reads

$$S_0'(x)S_1'(x) + \frac{S_0''(x)}{2} = 0 \quad , \tag{A.79}$$

and hence,

$$S_1'(x) = -\frac{S_0''(x)}{2\,S_0'(x)} = -\frac{p'(x)}{2\,p(x)} \quad . \tag{A.80}$$

Integrating this equation, the wave function can be written as [Landau and Lifschitz, 1979]

$$\Psi(x) = \frac{c_1}{\sqrt{p(x)}} \exp\left\{\frac{\mathrm{i}}{\hbar}\int p(x)\mathrm{d}x\right\} + \frac{c_2}{\sqrt{p(x)}} \exp\left\{-\frac{\mathrm{i}}{\hbar}\int p(x)\mathrm{d}x\right\} \quad . \tag{A.81}$$

In the classically forbidden region, i.e., the region where $E < V(x)$, the exponent becomes real.

A.7. Instantons

The so-called instanton approach will be explained on the example of a spinless particle confined in a one-dimensional double-well potential. The method can be directly extended to field theory, while the standard method (WKB approximation) cannot [Vaĭnshteĭn et al., 1982]. For the sake of simplicity, the mass of the particle is taken to be equal to unity, i.e. $m = 1$, and the potential is given by

$$V(x) = \frac{V_0}{a^4}\left(x^2 - a^2\right)^2 \quad , \tag{A.82}$$

where V_0 is the barrier height between the two wells located at $\pm a$. The potential is also presented in **Figure A.2 (left)**.

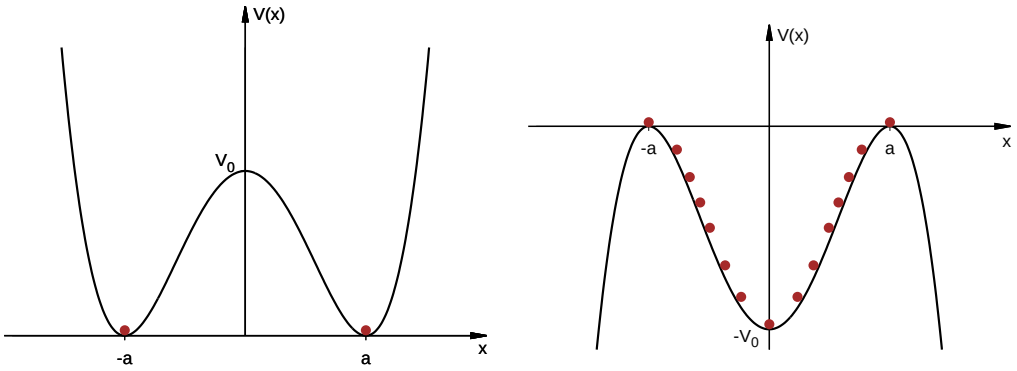

Figure A.2.: ***Left:*** *Double-well potential and classical solutions (red points).* ***Right:*** *Double-hill potential generated by Wick rotation. The two maxima can be connected by a classical trajectory (red points).*

The total energy and the Lagrange function of the particle are given by

$$E = \frac{1}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 + V(x) \quad \text{and} \quad L(x,\dot{x}) = \frac{1}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x) \quad , \tag{A.83}$$

respectively. The classical ground state ($E = 0$) is twofold degenerate and the two quantum-mechanical solutions are connected with each other via tunneling processes. This is in contrast to a classical particle, where the particle is located in one of the wells for the whole time ($E < V_0$)). The stationary points for the ground state of a classical particle are also shown in **Figure A.2 (left)**.

Suppose $\Psi_R(x)$ is the ground state of a particle located at a and $\Psi_L(x)$ is the ground state of a particle located at $-a$. The quantum-mechanical ground state of the double-

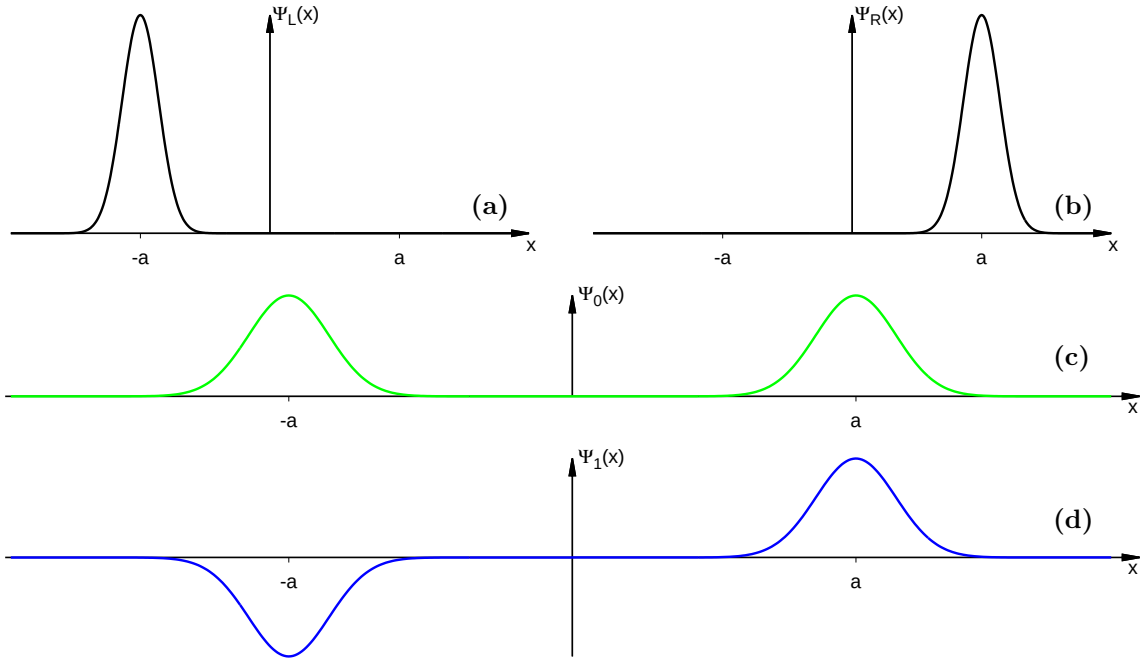

Figure A.3.: *Schematic representation of the ground-state wave function for a particle located in the left* ***(a)*** *and right* ***(b)*** *well. The ground state* ***(c)*** *as well as the first excited state of a quantum particle in a double well are given by a superposition.*

well potential and the first excited state are then supposed to be given by a superposition of the two states (see **Figure A.3**), i.e.

$$\Psi_{E_0}(x) = \frac{1}{\sqrt{2}}\Big(\Psi_R(x) + \Psi_L(x)\Big) \quad , \tag{A.84}$$

$$\Psi_{E_1}(x) = \frac{1}{\sqrt{2}}\Big(\Psi_R(x) - \Psi_L(x)\Big) \quad . \tag{A.85}$$

It is also common to use the Dirac notations for the states, i.e.

$$|-a\rangle = \Psi_L(x) \quad , \quad |a\rangle = \Psi_R(x) \quad ,$$
$$|0\rangle = \Psi_{E_0}(x) \quad , \quad |1\rangle = \Psi_{E_1}(x) \quad .$$

The probability of a transition from x_i to x_f (e.g. from $-a$ to a) using the Feynman path integral formalism [Feynman, 1948] is given by the integration over all possible paths $[\mathrm{D}x]$, with the boundaries $x(-T/2) = x_i$ and $x(T/2) = x_f$, weighted by the associated action $S(x)$ [Vaĭnshteĭn et al., 1982],

$$\langle x_f|\mathrm{e}^{-\mathrm{i}\hat{H}T}|x_i\rangle = N\int_{x_i}^{x_f}[\mathrm{D}x]\mathrm{e}^{\mathrm{i}S[x(t)]} \quad . \tag{A.86}$$

$\hat{H}$ is the Hamilton operator of the system, $\mathrm{e}^{-\mathrm{i}\hat{H}T}$ is the ordinary evolution operator and N is a normalization factor. It should be noted that the Feynman paths and the Nelson paths are equivalent [Nelson, 1964; Pavon, 2000]. The action is given by the Lagrangian function and reads

$$S[x] = \int_{-T/2}^{T/2} L(x(t), \dot{x}(t))\mathrm{d}t \quad . \tag{A.87}$$

If the states with well-known position are transformed into states with a well-known energy,

$$\hat{H}|n\rangle = E_n|n\rangle, \tag{A.88}$$

the sum of oscillating exponents

$$\langle x_f|\mathrm{e}^{-\mathrm{i}\hat{H}T}|x_i\rangle = \sum_n \mathrm{e}^{-\mathrm{i}E_nT}\,\langle x_f|n\rangle\langle n|x_i\rangle \tag{A.89}$$

will emerge [Vaĭnshteĭn et al., 1982]. However, it is clear that there is no non-trivial classical solution $x(t)$ for a particle whose total energy (see equation (A.83)) equals zero. Nevertheless, using a so-called Wick rotation, it is possible to construct non-trivial solutions by replacing the real-valued time in the Minkowski space by a complex-valued (euclidean) time, i.e. $t \to \mathrm{i}\tau$ [Vaĭnshteĭn et al., 1982]. By transition into the euclidean space, the total energy becomes

$$E = -\frac{1}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + V(x) \quad \Leftrightarrow \quad -E = \frac{1}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 - V(x) \quad , \tag{A.90}$$

which corresponds (for $E = 0$) to a rotation of the potential from $V(x)$ to $-V(x)$. Hence, the double-well potential is transformed into a "double-hill" potential and the particle can move from one maximum to the other (see red points in **Figure A.2 (right)**). The solution is given by [Vaĭnshteĭn et al., 1982]

$$x(\tau) = \pm a\,\tanh\left(\sqrt{2V_0}(\tau - \tau_0)\right) \quad , \tag{A.91}$$

with an arbitrary parameter τ_0. Such solution is called instanton solution (+), presented in **Figure A.4 (a)**, or anti-instanton solution (−). Tunneling processes can be described by an instanton or anti-instanton solution. In **Figure A.4 (b)** the derivative of x is shown, which is centered at τ_0. Suppose that the particle located by $x_i = -a$ at time $-T/2$, while it is at $x_f = a$ at time $T/2$. If the time period is shifted to infinity ($T \to \infty$), then the tunneling process will happen almost instantaneously, i.e. with a very short period as compared to T. Furthermore, the solution exponentially approximates the trivial classical solution ($\pm a$) [Kleinert, 2012].

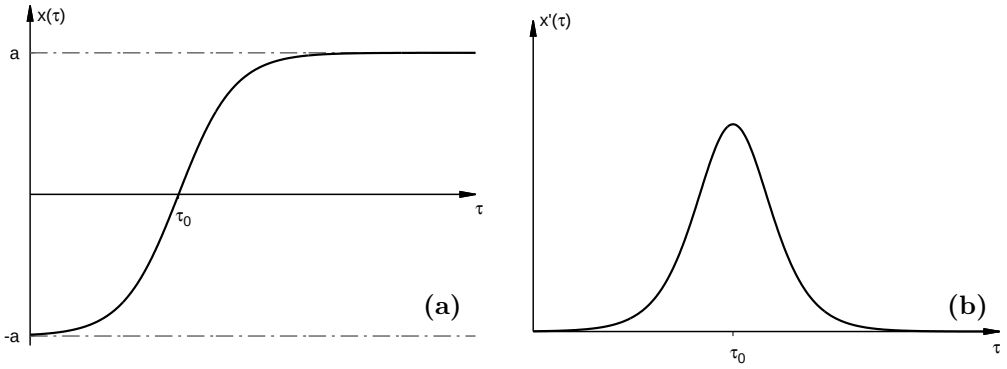

Figure A.4.: *Instanton solution of the euclidean equation of motion.* ***(a)*** *As a function of imaginary time;* ***(b)*** *time derivative.*

In the euclidean space, the action reads [Vaĭnshteĭn et al., 1982]

$$\mathrm{i}S[x] \to \int_{-T/2}^{-T/2} \left[-\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 - V(x) \right] \mathrm{d}\tau =: S_E[x] \quad . \tag{A.92}$$

Exploiting the euclidean action S_E, equation (A.86) becomes

$$\langle x_f | \mathrm{e}^{-\hat{H}\tau_T} | x_i \rangle = N \int_{x_i}^{x_f} [\mathrm{D}x]\, \mathrm{e}^{-S_E[x(\tau)]} \quad . \tag{A.93}$$

The Wick rotation, i.e., the transition towards an imaginary time axis, is possible for all Feynman integrals, since the integrand does not contain any singularities [Huang, 2007].
Consequently, if the instanton solution (equation (A.91)) is used, the action for one instanton is given by [Vaĭnshteĭn et al., 1982]

$$S_0 = \int_{-\infty}^{\infty} \dot{x}^2 \mathrm{d}\tau = \int_{-a}^{a} \left(-\frac{\sqrt{2V_0}}{a^2} \right) \left(x^2 - a^2\right) \mathrm{d}x = \frac{\omega^3 a}{12\, V_0} \quad , \tag{A.94}$$

where $\omega = \sqrt{8V_0}/a$.

As a next step, the measure of the paths has to be calculated. With considerable mathematical effort, the one-instanton contribution of equation (A.86) is found to be [Vaĭnshteĭn et al., 1982]

$$\langle -a | \mathrm{e}^{-\hat{H}\tau_T} | a \rangle_{\text{one-inst.}} = \left(\sqrt{\frac{\omega}{\pi}}\, \mathrm{e}^{-\omega\tau_T/2} \right) \left(\sqrt{\frac{6}{\pi}} \sqrt{S_0}\, \mathrm{e}^{-S_0} \right) \omega \int_{-\tau_T/2}^{\tau_T/2} \mathrm{d}\tau_0 \quad . \tag{A.95}$$

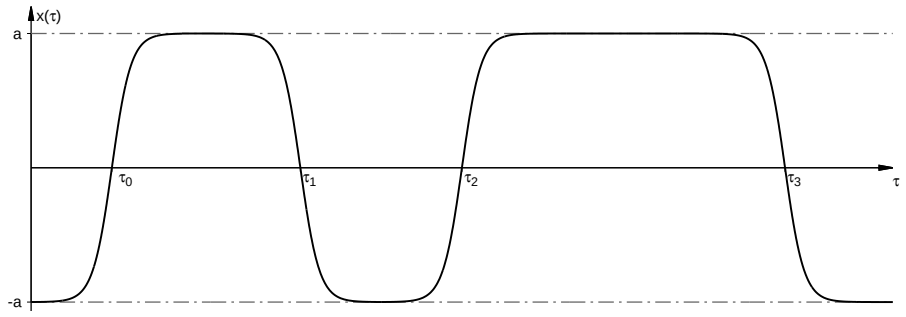

Figure A.5.: *A chain of separated instanton/anti-instantons solutions.*

For very large τ_T, multiple transitions between the two states are possible, which has to be considered in the calculation of the amplitude. To determine the energy of the lowest states, the limit $\tau_T \to \infty$ of the transition amplitude is used. Though, the limit cannot be calculated in a straightforward way using equation (A.95) [Vaĭnshteĭn et al., 1982]. Since the particle spends only a short time inside the barrier, and since the time between two crossovers is large, a solution constructed by more that one instanton/anti-instanton is again a classical solution. Suppose there are n instantons/anti-instantons with centers

$$-\frac{\tau_T}{2} < \tau_1 < \tau_2 < \cdots < \tau_n < \frac{\tau_T}{2} \quad . \tag{A.96}$$

A chain of instanton/anti-instanton solutions is shown in **Figure A.5**. If the transitions are separated from each other, i.e. $|\tau_i - \tau_j| \gg \omega^{-1}$ is fulfilled for two arbitrary centers τ_i, τ_j, then the associated action of such a path is given by $n\,S_0$, where S_0 is the action of a path with a single transition only [Vaĭnshteĭn et al., 1982]. Consequently, one has to determine n integrals (one over each center τ_i) to determine the amplitude. Vaĭnshteĭn et al. [1982] showed that

$$\begin{aligned} &\sqrt{\frac{\omega}{\pi}}\,\mathrm{e}^{-\omega\tau_T/2}\alpha^n \int_{-\tau_T/2}^{\tau_T/2} \omega \mathrm{d}\tau_n \int_{-\tau_T/2}^{\tau_n} \omega \mathrm{d}\tau_{n-1} \cdots \int_{-\tau_T/2}^{\tau_2} \omega \mathrm{d}\tau_1 \\ &= \sqrt{\frac{\omega}{\pi}}\,\mathrm{e}^{-\omega\tau_T/2}\alpha^n \frac{(\omega\tau_T)^n}{n!} \quad , \end{aligned} \tag{A.97}$$

with the instanton density being given by

$$\alpha = \sqrt{\frac{6}{\pi}}\sqrt{S_0}\,\mathrm{e}^{-S_0} \quad . \tag{A.98}$$

There are two possible amplitudes, $\langle -a|\mathrm{e}^{-\hat{H}\tau_T}|a\rangle$ and $\langle -a|\mathrm{e}^{-\hat{H}\tau_T}|-a\rangle$, each of which can be determined by the summation over all possible n. First, starting in the left well at $x_i = -a$, the particle arrives at $x_f = a$, which means that the number of transitions

n has to be odd for this transition, and second, the path ends in the left well, meaning that an even number of transitions are made. The two amplitudes read

$$\langle -a|\mathrm{e}^{-\hat{H}\tau_T}|a\rangle = \sum_{n=1,3,\ldots}^{\infty} \sqrt{\frac{\omega}{\pi}}\mathrm{e}^{-\omega\tau_T/2}\,\frac{(\omega\alpha)^n}{n!} = \sqrt{\frac{\omega}{\pi}}\mathrm{e}^{-\omega\tau_T/2}\,\sinh\left(\omega\,\tau_T\,\alpha\right) \quad , \tag{A.99}$$

$$\langle -a|\mathrm{e}^{-\hat{H}\tau_T}|-a\rangle = \sum_{n=0,2,\ldots}^{\infty} \sqrt{\frac{\omega}{\pi}}\mathrm{e}^{-\omega\tau_T/2}\,\frac{(\omega\alpha)^n}{n!} = \sqrt{\frac{\omega}{\pi}}\mathrm{e}^{-\omega\tau_T/2}\,\cosh\left(\omega\,\tau_T\,\alpha\right) \quad . \tag{A.100}$$

In the limit $\tau_T \to \infty$, only the two lowest states have to be taken into account in equation (A.89), resulting in

$$\langle -a|\mathrm{e}^{-\hat{H}\tau_T}|a\rangle = \mathrm{e}^{-\mathrm{i}E_0T}\,\langle a|0\rangle\langle 0|-a\rangle + \mathrm{e}^{-\mathrm{i}E_1T}\,\langle a|1\rangle\langle 1|-a\rangle \quad , \tag{A.101}$$

$$\langle -a|\mathrm{e}^{-\hat{H}\tau_T}|-a\rangle = \mathrm{e}^{-\mathrm{i}E_0T}\,\langle -a|0\rangle\langle 0|-a\rangle + \mathrm{e}^{-\mathrm{i}E_1T}\,\langle -a|1\rangle\langle 1|-a\rangle \quad . \tag{A.102}$$

Finally, by assessing the coefficients, the two lowest energies read

$$E_0 = \frac{\omega}{2}\left[1 - \sqrt{\frac{2\omega^3\,a^4}{\pi\,V_0}}\,\mathrm{e}^{-\frac{\omega^3\,a^4}{V_0}}\right] \quad , \tag{A.103}$$

$$E_1 = \frac{\omega}{2}\left[1 + \sqrt{\frac{2\omega^3\,a^4}{\pi\,V_0}}\,\mathrm{e}^{-\frac{\omega^3\,a^4}{V_0}}\right] \quad . \tag{A.104}$$

The two energies are symmetric around the harmonic oscillator energy. The energy splitting is given by

$$\Delta E = E_1 - E_0 = \sqrt{\frac{2\omega^3\,a^4}{\pi\,V_0}}\,\mathrm{e}^{-\frac{\omega^3\,a^4}{V_0}} \quad . \tag{A.105}$$

Carlitz and Nicole [1985] showed (and later also Garg [2000]) that this formula coincides with the energy splitting determined by a second order WKB-approximation.

These formulas are derived under two assumptions: (i) the potential can be approximated by the harmonic oscillator close to the minima, and (ii), the particle is located at $\pm a$ except for short periods during which the particle moves through the barrier. This formalism of path integrals results in good values for very small splittings, which cannot be described by a first order perturbation theory.

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Eidesstattliche Erklärung

Hiermit versichere ich, die vorliegende Arbeit selbständig und ohne fremde Hilfe verfasst und keine anderen als die von mir angegebenen Quellen und Hilfsmittel verwendet zu haben. Die den benutzten Werken wörtlich oder inhaltlich entnommenen Stellen habe ich als solche kenntlich gemacht.

Ich erkläre keine anderweitigen Promotionsversuche unternommen und die vorliegende Dissertation weder in der jetzigen noch in einer anderen Fassung einer anderen wissenschaftlichen Einrichtung vorgelegt zu haben.

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