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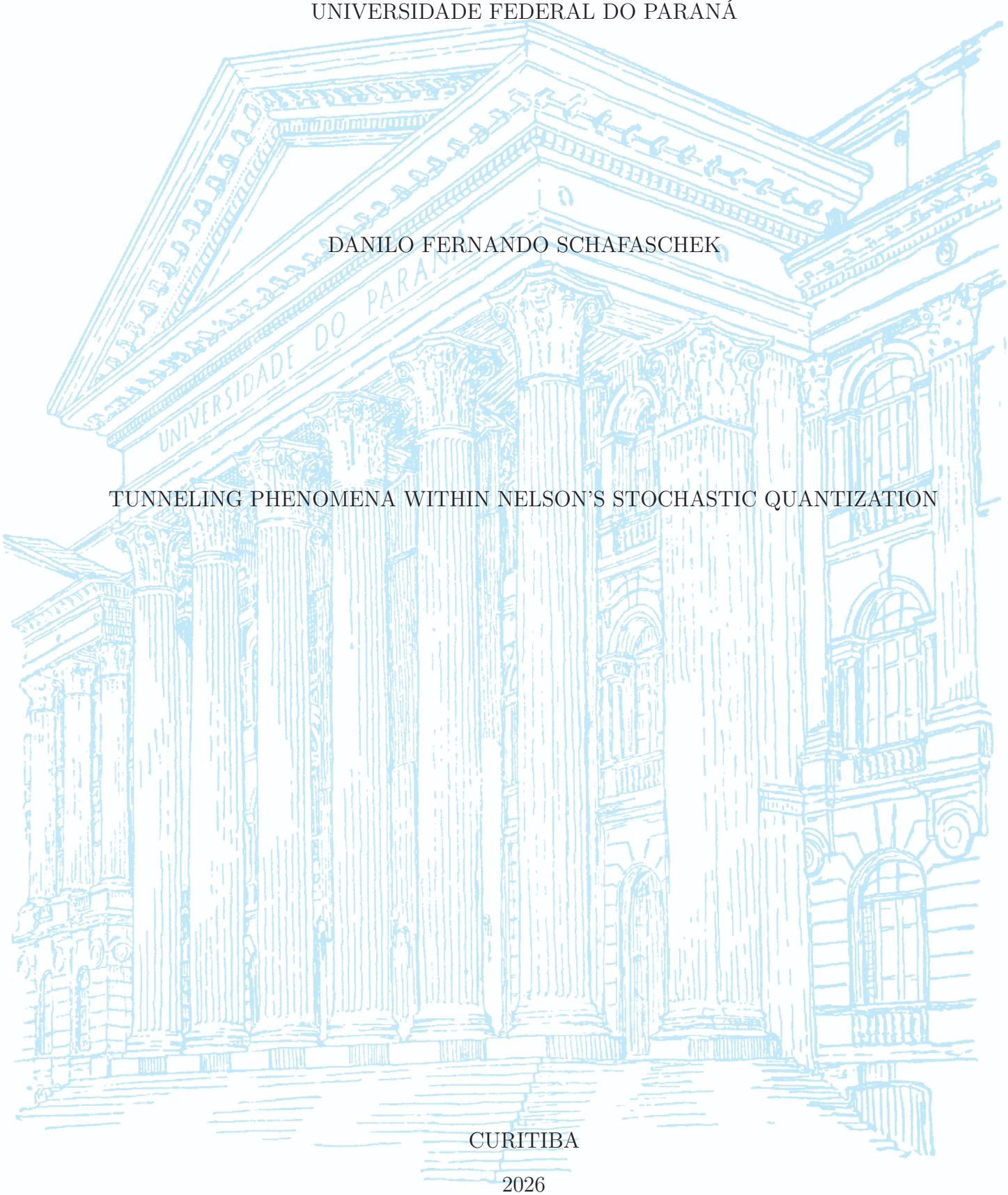

DANILO FERNANDO SCHAFASCHEK

TUNNELING PHENOMENA WITHIN NELSON'S STOCHASTIC QUANTIZATION

CURITIBA

2026

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Orientador: Prof. Dr. Giovani Lopes Vasconcelos
Co-orientador: Prof. Dr. Antônio Murilo Santos Macêdo

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"The opposite of a true statement is a false statement. But the opposite of a profound truth may well be another profound truth."

Niels Bohr

RESUMO

A quantização estocástica é uma formulação da mecânica quântica que descreve o movimento de uma partícula como um processo estocástico e que é unitariamente equivalente ao formalismo padrão no espaço de Hilbert. Ao reformular a dinâmica quântica em termos de um par de equações diferenciais estocásticas, a teoria oferece uma descrição complementar e intuitivamente atraente, com uma estrutura matemática estreitamente relacionada à mecânica clássica. Nesse contexto, a noção de trajetória estocástica fornece um meio natural de definir e calcular quantidades físicas que são de difícil tratamento na mecânica quântica convencional, como o tempo médio que uma partícula leva para atravessar uma barreira de potencial. A definição do tempo de tunelamento é notoriamente desafiadora na mecânica quântica devido à ausência de um operador tempo auto-adjunto. No entanto, ao combinar a quantização estocástica de Nelson com a teoria de tempos médios de primeira passagem, torna-se possível definir um tempo médio de tunelamento. Para estados de espalhamento, a definição estocástica de tempo médio de passagem através de uma barreira (ou poço) quadrada oferece percepções valiosas sobre o tempo envolvido em fenômenos quânticos, reproduzindo o limite clássico para barreiras desprezíveis e o crescimento exponencial característico do regime de barreiras opacas. No contexto de estados ligados em um potencial de poço duplo, o tempo de tunelamento obtido a partir da quantização estocástica apresenta uma conexão notável com o semi-período quântico de oscilação de um estado não estacionário inicialmente localizado em um dos poços. Esses dois tempos estão relacionados por um fator de proporcionalidade que tende a $\pi/2$ no limite de barreiras opacas, independentemente da forma específica do potencial. O problema da inversão da amônia também mostra excelente concordância com as previsões da mecânica estocástica para a frequência de tunelamento, reforçando a robustez do método. Além disso, simulações das trajetórias estocásticas fornecem naturalmente a distribuição completa dos tempos de tunelamento, a qual exibe a cauda exponencial típica de processos de primeira passagem. Em conjunto, este trabalho demonstra um exemplo concreto das vantagens ainda pouco exploradas da quantização estocástica e destaca seu potencial como uma ferramenta poderosa para a análise e interpretação de fenômenos quânticos.

Palavras-chaves: Quantização Estocástica; Tunelamento; Tempo na Mecânica Quântica; Difusão Conservativa.

ABSTRACT

Stochastic quantization is a formulation of quantum mechanics that describes the motion of a particle as a stochastic process and is unitarily equivalent to the standard Hilbert-space formalism. By recasting quantum dynamics in terms of a pair of stochastic differential equations, the theory provides a complementary and intuitively appealing picture with a mathematical structure closely related to classical mechanics. In this framework, the notion of a stochastic trajectory offers a natural way to define and compute physical quantities that are otherwise difficult to address in standard quantum mechanics, such as the mean time a particle spends tunneling through a potential barrier. The definition of a tunneling time is notoriously challenging in quantum mechanics due to the absence of a self-adjoint time operator. However, by combining Nelson's stochastic quantization with the theory of mean first passage times, it becomes possible to define a mean tunneling time. For scattering states, the stochastic mean passage time across a square barrier (or well) offers valuable insights into the time elapsed in quantum phenomena, reproducing the correct classical limit for negligible barriers and the exponential growth characteristic of the opaque barrier regime. In the context of bound states in a double-well potential, the tunneling time obtained from stochastic quantization exhibits a striking connection with the quantum-mechanical half-period of oscillation of a non-stationary state localized in one well. These two times are related by a proportionality factor approaching $\pi/2$ in the opaque-barrier limit, independently of the detailed shape of the potential. The ammonia inversion problem also shows excellent agreement with the stochastic predictions for the tunneling frequency, reinforcing the robustness of the method. Moreover, simulations of stochastic trajectories naturally yield the full distribution of tunneling times, which displays the expected exponential tail characteristic of first-passage processes. Altogether, this work demonstrates a concrete example of the unexplored advantages of stochastic quantization and highlights its potential as a powerful tool for the analysis and interpretation of quantum phenomena.

Key-words: Stochastic Quantization; Tunneling; Time in Quantum Mechanics; Conservative Diffusion.

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1 INTRODUCTION

After the publication of his cornerstone papers of quantum mechanics in 1926, Erwin Schrödinger (1887-1961) turned his attention to understanding and interpreting the physical meaning of the equation that now bears his name, in particular the meaning of the imaginary unit that appears there. He quickly observed that, under the substitution of real time by imaginary time, the Schrödinger equation takes the form of a heat equation. This observation establishes an immediate link between quantum mechanics and diffusion processes, which are classically described by the heat equation. Motivated by this connection, Schrödinger published in 1931 a paper titled *On the Reversal of the Laws of Nature* (direct translation from German) [1], in which he explored the idea that quantum mechanics might emerge from an underlying diffusion process.

However, a fundamental problem arises when attempting to relate quantum mechanics to classical diffusion. Quantum mechanics is a time-reversible theory: its fundamental equations remain invariant under time reversal. Diffusion processes, on the other hand, are intrinsically time-irreversible, being constrained by the second law of thermodynamics, which establishes an arrow of time as a manifestation of increasing entropy. Schrödinger's key insight in his 1931 paper was that a time-reversible diffusion process can be constructed by considering two coupled diffusion processes: one evolving forward in time and another evolving backward in time. This bidirectional construction avoids the conflict with thermodynamic irreversibility and preserves time-reversal symmetry.

This connection becomes more transparent when one examines time-reversal symmetry in the Schrödinger equation. The complex conjugate of the wave function, Ψ^*, satisfies the same Schrödinger equation as Ψ if time is reversed:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi, \tag{1.1}$$

$$i\hbar\frac{\partial\Psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi^* + V\Psi^*, \tag{1.2}$$

where the second equation follows from taking the complex conjugate of the first and performing the transformation $t \to -t$. Since Ψ^* represents the time-reversed state of Ψ, this pair of equations shows explicitly that the presence of the imaginary unit in the Schrödinger equation is essential for the preservation of time-reversal symmetry. Without the imaginary unit, the equation would resemble a diffusion equation and would lose this symmetry, resulting in irreversible dynamics.

Schrödinger recognized that this idea (known as the Schrödinger bridge problem) of a bidirectional diffusion hinted at a deep structural connection between quantum mechanics and statistical physics, but he chose not to develop the theory further, concluding the 1931

paper with the remark:

> "I do not wish to analyse these points more closely before time tells if they can really lead to a better understanding of quantum mechanics."

In 1933, Reinhold Fürth (1893-1979) demonstrated that diffusion processes satisfy uncertainty relations involving the variances of position and velocity resembling the uncertainty principle of quantum mechanics [2]. Later, inspired by Fürth's results and Schrödinger's 1931 work, Imre Fényes (1917-1977) showed, in 1952, that the Schrödinger equation can be recovered from a purely statistical framework [3]. He argued that wave-mechanical processes correspond to particular Markov processes, that is, diffusion processes without memory. Within this approach, the uncertainty relations arise naturally as consequences of the statistical description, rather than as statements about measurement-induced disturbance or a fundamental impossibility of simultaneous exact measurements.

However, it was only in 1966 that Edward Nelson (1932-2014) significantly advanced this program by developing a rigorous mathematical formulation of quantum mechanics as a stochastic process, understood as a generalized form of diffusion. Nelson's work, titled *Derivation of the Schrödinger Equation from Newtonian Mechanics* [4], is widely regarded as the foundation of the statistical approach now known as *Nelson's stochastic quantization* or *stochastic mechanics*.

Nelson's formulation closely parallels Schrödinger's earlier insight: quantum mechanics emerges from the interplay of two stochastic processes, one evolving forward in time and the other backward in time. By coupling these two equations to render the diffusion conservative, Nelson obtained a dynamics whose statistical evolution reproduces the Schrödinger equation. In this view, the complex structure of the wave function and the appearance of the imaginary unit are not fundamental postulates, but instead arise from the combination of forward and backward stochastic motions necessary for the time-reversibility of the theory.

Nelson's construction provides an appealing reinterpretation of quantum theory: instead of postulating a wave function with abstract probabilistic meaning, one introduces a stochastic dynamics for particle trajectories whose statistical properties reproduce all predictions of nonrelativistic spinless quantum mechanics. In this framework, the wave function plays the role of a mathematical construction that guides the ensemble of stochastic trajectories, while observables emerge from averages over these trajectories. This perspective places quantum mechanics as a statistical theory emerging due to the presence of an irreducible noise of purely kinematic origin.

Despite its elegance, Nelson's stochastic quantization raises several deep questions. Among these is the physical interpretation of the forward and backward diffusion processes,

whether they are real trajectories or just a mathematical tool, and their relation to time-reversal symmetry [5, 6]. Another central issue concerns the microscopic origin of the stochastic noise that drives the particle trajectories [7]. Nelson originally regarded the noise as an intrinsic feature of the theory, unrelated to environmental interactions—what he called *the hypothesis of universal Brownian motion* [4, 5].

Nelson's stochastic reformulation of quantum mechanics also provides new tools for studying dynamical quantities that are otherwise difficult to define within the standard formulation. Notably, tunneling processes acquire a clear meaning in terms of sample paths of the underlying diffusion, making Nelson's framework particularly suitable for the investigation of such phenomena.

Tunneling is one of the most striking and counterintuitive predictions of quantum theory. In classical mechanics, a particle with energy lower than the height of a potential barrier cannot penetrate the barrier and must remain confined to the classically allowed region. In quantum mechanics, however, the situation changes: even if the particle energy is lower than the potential barrier, there is a non-zero probability for the particle to traverse the classically forbidden region. This effect, known as quantum tunneling, was first described by Friedrich Hund (1896-1997) in 1927 [8] and has since become central to the understanding of numerous physical processes, from alpha decay in nuclear physics to chemical reactions and electronic transport in nanostructures [9].

Even today, tunneling remains a vibrant area of research. A remarkable recent example is the 2025 Nobel Prize in Physics, awarded to John Clarke, Michel Devoret, and John Martinis "for the discovery of macroscopic quantum mechanical tunnelling and energy quantization in an electric circuit" [10]. In their pioneering experiments during the mid-1980s, superconducting components were separated by thin insulating layers, and quantum tunneling manifested in the form of current flowing through these non-conductive materials [11]. These studies demonstrated that tunneling is not merely a microscopic phenomenon but can occur in macroscopic quantum systems, reinforcing its fundamental importance.

Despite its significance, the notion of a "tunneling time" in quantum mechanics remains highly nontrivial. Within the conventional formalism, there is no unique expression for the time a particle spends in the barrier region, and multiple definitions coexist, each capturing different aspects of the problem [12]. This ambiguity reflects the broader difficulty of defining time observables in quantum mechanics. Furthermore, stochastic quantization has provided insights into the calculation of tunneling times [13, 14].

In the present thesis, we build upon Nelson's stochastic quantization to analyze the dynamics of particles in potential barriers and double-well potentials, focusing in particular on the calculation of tunneling times. Within the stochastic framework, a tunneling time can be defined in a natural and operational way, offering both conceptual clarity and

practical computational advantages.

Over the years, stochastic quantization has been successfully applied and generalized in a wide range of theoretical developments. Notable advances include the formulation of variational principles within the stochastic framework [15, 16], the construction of quantum Hamilton equations that extend the classical structure to the stochastic domain [17, 18], and the incorporation of degrees of freedom related to spin [19]. More recent efforts have expanded the formalism to relativistic settings, including stochastic dynamics on Lorentzian manifolds and extensions compatible with relativistic theories [20, 21]. These developments collectively highlight the versatility of stochastic quantization as a framework capable of bridging classical, quantum, and relativistic domains.

Another formulation relating stochastic processes to quantum mechanics is the *quantum state diffusion*, in which the Gisin-Percival-Itô stochastic Schrödinger equation describes norm-preserving diffusive evolution of pure quantum states driven by Wiener noise, i.e., the state vector has a stochastic evolution in the Hilbert space [22, 23, 24].

In this sense, one may say that Schrödinger's early intuition has indeed stood the test of time. His 1931 attempt to describe quantum mechanics through a diffusive process ultimately contributed to a deeper understanding of the theory. The developments by Fényes and Nelson not only gave substance to Schrödinger's original idea, but also opened new perspectives on the interpretation, structure, and computational treatment of quantum mechanics.

Aiming to examine the applicability of stochastic mechanics, this thesis is organized as follows:

- **Chapter 2** introduces the mathematics and physics of stochastic processes, with special attention to Brownian motion, the most fundamental stochastic process in physics. The mathematical tools necessary for the remainder of the thesis are presented there.
- **Chapter 3** explores Nelson's stochastic quantization in detail, together with the subsequently variational formalism later derived by others from Nelson's framework. In this chapter, we show how quantum mechanics acquires a mathematical structure closely analogous to classical mechanics under the stochastic description. We also discuss the equivalence between Nelson's formulation and the standard quantum-mechanical formalism.
- **Chapter 4** presents the theory of mean first-passage times and its application to the definition and computation of temporal quantities in quantum mechanics, including tunneling times.

- **Chapters 5 and 6** contain the main results of this thesis. Chapter 5 analyzes passage times for scattering states, focusing on tunneling through potential barriers. Some results from the literature are reproduced, and new results are also presented. Chapter 6 extends the analysis to bound states in double-well potentials, examining tunneling times associated with transitions between wells and comparing with the quantum-mechanical prediction for the oscillation of localized states. The stochastic approach is also used to compute the frequency of ammonia inversion. In this chapter, the main original results are presented.
- **Chapter 7** is devoted to the conclusions, where we summarize the main results obtained in the thesis.

Parts of this thesis were revised with the assistance of artificial intelligence tools, which were used exclusively to improve grammar, clarity, and style. All scientific content, analyses, and conclusions presented in this work are entirely the author's responsibility.

2 INTRODUCTION TO STOCHASTIC PROCESSES

This chapter begins by presenting an adaptation of the derivation made by Albert Einstein (1879-1955) in 1905 and by Paul Langevin (1872-1946) in 1908 for the description of Brownian motion [25]. Their works were fundamental to the consolidation of the atomic hypothesis [26, 27] defended by Ludwig Boltzmann (1844-1906) [28] and serve as a foundation for understanding the mathematics behind stochastic processes. In the following section, the mathematics of stochastic calculus will be formally presented. We then return to the discussion of Brownian motion, applying the mathematical tools introduced previously.

2.1 BROWNIAN MOTION: AN INTRODUCTION

In this section, we present an adaptation of Einstein's derivation of Brownian motion. Subsequently, we introduce Langevin's derivation, which incorporates a random force into the equation of motion—a formulation now known as the Langevin equation.

2.1.1 Einstein's Theory of Brownian Motion

In 1905, Einstein published his first work related to the erratic motion performed by tiny particles expelled from pollen grains over a liquid medium. This phenomenon is called Brownian Motion after its discovery in 1827 by Robert Brown (1773-1858) [29]. Einstein's idea was to assume this erratic motion as a result of a large number of collisions with the molecules of the medium [25, 30]. His paper titled *On the movement of small particles suspended in stationary liquids required by the molecular-kinetic theory of heat* (direct translation from German) was fundamental to the confirmation of the existence of atoms and molecules [26]. Three years later, in 1908, Jean Perrin (1870-1942) confirmed experimentally the theory [31], being laureate with the Nobel prize in Physics in 1926 "for his work on the discontinuous structure of matter [...]" [32]. In Fig. 1, it is possible to see an example of a Brownian motion trajectory in two dimensions [1].

The hypothesis adopted by Einstein was that by considering a very large number of particles suspended in a medium, such as water, for example, we could treat them independently as an ideal gas exerting an additional pressure on the medium, which he called osmotic pressure. In this way, using the ideal gas law, we can express the pressure P as a function of temperature T by

$$P = k_B n T, \tag{2.1}$$

[1] Unless otherwise indicated, all figures in this thesis were produced by the author.

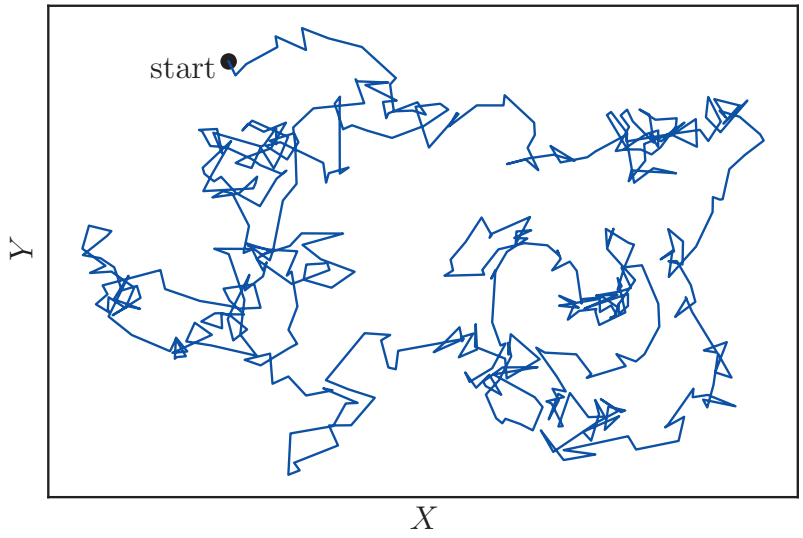


FIGURE 1 – Trajectory of a Brownian particle in two dimensions. This trajectory was generated simulating a standard Brownian motion or Wiener process, as presented in Sec. 2.2.1, in the horizontal and vertical displacements.

where $n = N/V$ is the number of particles per unit of volume and k_B is the Boltzmann constant. From (2.1) we can relate the force acting on the Brownian particles to the temperature, since, in the steady state, the force density can be calculated by the pressure gradient, that is,

$$F_n = -k_B T \nabla n. \tag{2.2}$$

Therefore, the force acting on each particle will be, on average

$$F = -\frac{k_B T}{n} \nabla n. \tag{2.3}$$

Now, let us treat the Brownian particles as macroscopic particles and assume that Stokes' law is valid in this case. Stokes' law relates the friction force exerted by a fluid on a spherical body immersed inside it [33]. For a particle of radius a and velocity v, we will have for the friction force

$$F_{\text{drag}} = -6\pi\eta a v = -\gamma v, \tag{2.4}$$

where η is the *viscosity coefficient* of the fluid. In this way, the movement differential equation of the Brownian particle can be written as

$$M\frac{dv}{dt} = -\gamma v + F, \tag{2.5}$$

where M is the mass of the Brownian particle. The steady-state solution (v constant) happens when

$$v = \frac{F}{\gamma} = \mu F, \tag{2.6}$$

where $\mu = 1/\gamma$ is known as *mobility coefficient* [34]. Therefore, the steady-state particle flux density is written as

$$J = nv = n\mu F = -\mu k_B T \nabla n. \tag{2.7}$$

If we assume that individual particles perform a diffusive movement, then the Fourrier-Fick's law will be valid and the particle flux density can be calculated by [35]

$$J = -D\nabla n, \tag{2.8}$$

where D is the *diffusion coefficient*. Comparing Eqs. (2.7) and (2.8) is possible to conclude that

$$D = \mu k_B T. \tag{2.9}$$

Equation (2.9) is known as *Einstein relation* or *Einstein-Smoluchowski relation* [36]. Let's see now how the diffusion process can be related to the probability distribution of the particle position.

Consider a particle moving in one dimension subjected to independent and random impacts that occur at times $i\tau$, for $i = 1, 2, \ldots$. As a consequence of these impacts, the particle has a probability p of moving a distance ℓ to the right and a probability $q = 1 - p$ of moving a distance ℓ to the left. We will denote by $f(x, t)$ the probability of finding the particle at position x at time $t = N\tau$ as a result of N impacts, after starting at position $x = 0$ at time $t = 0$. We can then establish that $f(x, t)$ satisfies the following equation, known as master equation [37, 38]:

$$f(x, t + \tau) = pf(x - \ell, t) + qf(x + \ell, t). \tag{2.10}$$

Equation (2.10) is characteristic of a one-dimensional random walk. Subtracting $f(x, t)$ from both sides of Eq. (2.10) gives us

$$f(x, t + \tau) - f(x, t) = p\left[f(x - \ell, t) - f(x, t)\right] + q\left[f(x + \ell, t) - f(x, t)\right], \tag{2.11}$$

remembering that $p+q = 1$. Let us take τ/t, $\ell/x \ll 1$ and perform Taylor series expansions, getting

$$f(x, t + \tau) - f(x, t) = \tau\frac{\partial f}{\partial t} + \mathcal{O}(\tau), \tag{2.12}$$

$$f(x - \ell, t) - f(x, t) = -\ell\frac{\partial f}{\partial x} + \frac{1}{2}\ell^2\frac{\partial^2 f}{\partial x^2} + \mathcal{O}(\ell^2), \tag{2.13}$$

$$f(x + \ell, t) - f(x, t) = \ell\frac{\partial f}{\partial x} + \frac{1}{2}\ell^2\frac{\partial^2 f}{\partial x^2} + \mathcal{O}(\ell^2). \tag{2.14}$$

Then, Eq. (2.11) can be written as

$$\tau\frac{\partial f}{\partial t} = -(p - q)\ell\frac{\partial f}{\partial x} + \frac{1}{2}\ell^2\frac{\partial^2 f}{\partial x^2}. \tag{2.15}$$

Setting $\tau, \ell \to 0$ and $N \to \infty$ and furthermore that x and $t = N\tau$ stay finite, and

$$\frac{\ell^2}{\tau} \to 2D, \qquad (p-q)\frac{\ell}{\tau} \to \nu, \tag{2.16}$$

where ν and D are constants called *drift coefficient* and *diffusion coefficient*, respectively. Therefore, in the limit $\tau, \ell \to 0$, Eq. (2.10) takes the form of a second-order partial differential equation:

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2} - \nu\frac{\partial f}{\partial x} \tag{2.17}$$

with initial condition $f(x, 0) = \delta(x)$.

If we take $\nu = 0$ and extend Eq. (2.17) to the three-dimensional case we will have

$$\frac{\partial f}{\partial t} = D\nabla^2 f. \tag{2.18}$$

We can interpret $f = f(\mathbf{r}, t)$ in Eq. (2.18) as the probability of finding a particle within a volume element $\delta V = (dr)^3$ centered at position $\mathbf{r}$ at time t. We can then multiply Eq. (2.18) on both sides by $N/\delta V$ (N being the total number of particles) and interpret $Nf/\delta V = n$ as the particle density at position $\mathbf{r}$ and at time t. In this way,

$$\frac{\partial n}{\partial t} = D\nabla^2 n, \tag{2.19}$$

that is known as *diffusion equation*. The number of particles should be conserved over time, then the continuity equation,

$$\frac{\partial n}{\partial t} + \nabla \cdot J = 0, \tag{2.20}$$

must be valid, where J is the particle flux density. Comparing Eqs. (2.19) and (2.20) we find

$$J = -D\nabla n, \tag{2.21}$$

that is exactly the Fourrier-Fick's law in Eq. (2.8) [39, 40].

Coming back to Eq. (2.18), a possible solution with proper boundary conditions is

$$f(\mathbf{r}, t) = \frac{1}{(4\pi Dt)^{3/2}} \exp\left(-\frac{\mathbf{r}^2}{4Dt}\right). \tag{2.22}$$

It means that $f(\mathbf{r}, t)$ is Gaussian distribution with zero mean and variance $\langle \mathbf{r}^2 \rangle = 6Dt$ ($2Dt$ for each dimension). Applying Einstein's relation (2.9), we obtain

$$\langle \mathbf{r}^2 \rangle = 6\mu k_B T t = \frac{k_B T t}{\pi \eta a}, \tag{2.23}$$

and taking $k_B = R/N_A$, where N_A is Avogadro's number and R is the ideal gas constant, we get the following relation:

$$N_A = \frac{RT}{\pi\eta a}\frac{t}{\langle \mathbf{r}_t^2 \rangle}, \tag{2.24}$$

where $\mathbf{r}_t$ represents the position $\mathbf{r}$ of the Brownian particle measured at time t, given that the particle starts at the origin at time $t = 0$. Note that $\langle \mathbf{r}_t^2 \rangle$, the mean square displacement of the Brownian particle at time t, can be verified experimentally with the aid of a microscope; therefore, Eq. (2.24) represents a practical way to obtain Avogadro's number or, equivalently, the Boltzmann constant.

The main result of Einstein's 1905 paper on the theory of Brownian motion, Eq. (2.24), reveals an intrinsic connection between the microscopic and macroscopic properties of matter. This finding provided a solid foundation for establishing the atomic hypothesis in the early 20th century.

2.1.2 Langevin's Theory of Brownian Motion

In 1908, Langevin presented an alternative derivation of Brownian motion, inspired by Einstein's earlier work [41]. In his own words, this new demonstration is "infinitely more simple by means of a method that is entirely different". His approach, based on methods previously developed by Smoluchowski [42], recovers the same result obtained by Einstein, Eq. (2.24).

Langevin's analysis begins with the same fundamental assumption adopted by Einstein: the theorem of equipartition of the kinetic energy for a system in thermal equilibrium. Defining the one-dimensional velocity

$$v = \frac{dx}{dt},$$

of a Brownian particle of mass M, the equipartition theorem [36] implies that, for a large ensemble of identical particles,

$$Mv^2 = k_B T. \tag{2.25}$$

Assuming that the suspended particle is sufficiently large for Stokes' law [33] to remain valid, the viscous force acting on it when moving with velocity v relative to the surrounding fluid is given by $-6\pi\eta a v$, where a is the particle radius and η is the viscosity coefficient. However, this viscous force accounts only for the mean effect of the medium. The irregular molecular impacts must be represented by an additional fluctuating, or complementary, force $\xi(t)$. Therefore, the equation of motion in the x-direction reads

$$M\frac{d^2x}{dt^2} = -6\pi\eta a\frac{dx}{dt} + \xi, \tag{2.26}$$

where ξ is a rapidly fluctuating force, equally likely to be positive or negative, whose magnitude is such that it compensates the dissipative effect of the viscous resistance

and maintains the particle in a state of perpetual agitation. Any equation of the form of Eq. (2.26), i.e.,

$$\frac{dv(t)}{dt} = -\alpha v(t) + \sigma\xi(t), \tag{2.27}$$

namely a dynamical equation supplemented by a fluctuating term, is generically referred to as a *Langevin equation*.

Multiplying Eq. (2.26) by x, one obtains

$$\frac{M}{2}\frac{d^2x^2}{dt^2} - Mv^2 = -3\pi\eta a\frac{dx^2}{dt} + \xi x. \tag{2.28}$$

Considering a large number of particles and taking the ensemble average of Eq. (2.28), the term ξx vanishes due to the irregularity of the fluctuating force. Introducing

$$z \equiv \left\langle \frac{dx^2}{dt} \right\rangle,$$

we obtain the differential equation

$$\frac{M}{2}\frac{dz}{dt} + 3\pi\eta a z = k_B T, \tag{2.29}$$

whose general solution is

$$z = \frac{k_B T}{3\pi\eta a} + C\exp\left(-\frac{6\pi\eta a}{M}t\right), \tag{2.30}$$

where C is an integration constant. The exponential term decays over a characteristic relaxation time $M/6\pi\eta a$, which is of the order of 10^{-8} s for typical Brownian particles [41]. After this short transient, the system reaches a stationary regime and

$$\left\langle \frac{dx^2}{dt} \right\rangle = \frac{RT}{N_A}\frac{1}{3\pi\eta a}, \tag{2.31}$$

where we have used $k_B = R/N_A$. Integrating over a time interval t,

$$\langle x^2 \rangle - \langle x_0^2 \rangle = \frac{RT}{N_A}\frac{t}{3\pi\eta a}. \tag{2.32}$$

Setting $x_0 = 0$, the mean-squared one-dimensional displacement becomes

$$\langle x^2 \rangle = \frac{RT}{N_A}\frac{t}{3\pi\eta a}. \tag{2.33}$$

This is precisely the same result obtained by Einstein, Eq. (2.24), except that Einstein's original formula refers to the three-dimensional displacement of the Brownian particle.

2.2 STOCHASTIC CALCULUS

In this section, we introduce the main mathematical tools employed in the study of stochastic processes. For completeness, Appendices A and B present a concise review of the basic elements of probability theory and of the formalism underlying stochastic processes, respectively. The discussion developed here builds upon those definitions; however, a detailed reading of the appendices is not strictly necessary for understanding the material that follows. A detailed presentation of stochastic calculus can be found in Ref. [43].

A particularly important class of stochastic processes is the *Markov processes*. These are characterized by the property that the future evolution of the system depends solely on its present state and not on its previous history. This "memoryless" behavior implies that all relevant information about the system at a given time is fully encoded in its current state [37, 38, 44, 45].

For a Markov process represented by the stochastic variable $x(t)$, the probability density $p(x,t)$ satisfies the differential equation known as the *forward Fokker-Planck equation*:

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}[a_1(x)\,p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[a_2(x)\,p(x,t)]\,, \tag{2.34}$$

where $a_1(x)$ is the *drift coefficient* and $a_2(x)/2$ is the *diffusion coefficient* [44].

In addition to the evolution of the probability density, it is often necessary to consider the behavior of the *conditional probability* $p(x,t|z,s)$, which gives the probability of the system being at position x at time t, given that it occupied position z at an earlier time s. For Markov processes, this conditional probability satisfies the *Kolmogorov backward equation*, also referred to as the *backward Fokker-Planck equation*:

$$\frac{\partial}{\partial s}p(x,t|z,s) = -a_1(z)\,\frac{\partial}{\partial z}p(x,t|z,s) - \frac{1}{2}a_2(z)\,\frac{\partial^2}{\partial z^2}p(x,t|z,s), \tag{2.35}$$

in which the derivatives are taken with respect to the initial coordinates (z,s) [44]. The backward equation plays a central role in problems involving mean first-passage times, boundary-crossing probabilities, and other quantities that depend on the initial configuration of the system [38]. Together, these two equations provide a complete description of the time evolution of Markovian stochastic processes.

2.2.1 Wiener Process

As we have already discussed, Brownian motion can be characterized as the random motion of particles suspended in a medium, such as dust grains suspended in the air or pollen grains suspended in a liquid. In 1900, the French mathematician Louis Bachelier (1870-1946) showed the relationship between Brownian motion and the diffusion equation when he developed a model to describe asset prices in the financial market for his doctoral thesis [46]. Five years later, in 1905, Einstein published his famous work in

which he described the Brownian motion of pollen particles as the result of collisions with innumerable water molecules [25]. However, it was only in 1923 that a rigorous mathematical theory of Brownian motion was developed by the American mathematician Norbert Wiener (1894-1964) [47], after which, Brownian motion also became known as Wiener process [37, 44].

Definition 1 *The standard Brownian motion or Wiener process* $\{ W(t),\ t \geq 0 \}$ *is a stochastic process with the following properties* [2]*:*

- $W(0) = 0$*;*
- *The increments* $W(t) - W(s)$ *are stationary and independent;*
- *For* $t > s$, $W(t) - W(s)$ *has a normal (Gaussian) distribution* $\mathcal{N}(0, \sqrt{t-s})$*;*
- *The trajectories are continuous (i.e., it has "no jumps").*

The stationarity implies that the probability distribution function (pdf) of $W(t) - W(s)$, for $t > s$, depends only on the time difference $t - s$. From the properties defined above, it is easy to see that $W(t)$ is distributed according to $\mathcal{N}(0, \sqrt{t})$ for $t > 0$. We have $\mathbb{E}[W(t)] = 0$ for all $t \geq 0$. Now, since from the definition above $W(t) - W(s)$ has zero mean, we get $\mathbb{E}[(W(t) - W(s))^2] = \text{var}[W(t) - W(s)] = t - s$ for $t > s$, then

$$\begin{aligned} \mathbb{E}[(W(t) - W(s))^2] &= \mathbb{E}[W^2(t) - 2W(t)W(s) + W^2(s)] \\ &= \mathbb{E}[W^2(t)] - 2\mathbb{E}[W(t)W(s)] + \mathbb{E}[W^2(s)] \\ &= t + s - 2\mathbb{E}[W(t)W(s)] = t - s, \end{aligned} \tag{2.36}$$

leading to

$$\mathbb{E}[W(t)W(s)] = s, \quad \text{for} \quad t > s, \tag{2.37}$$

where $\mathbb{E}[W(t)W(s)]$ is the covariance of the Wiener process or Brownian motion. Since the Wiener process is Gaussian and a Gaussian process is fully characterized by its mean and covariance, the following alternative definition can be stated [37].

Definition 2 *The standard Brownian motion or Wiener process* $\{ W(t),\ t \geq 0 \}$ *is a Gaussian process with* $\mathbb{E}[W(t)] = 0$ *and* $\mathbb{E}[W(t)W(s)] = \min(s, t)$.

Consider now a partition $\{ t_i \}_{i=0}^{n}$ of the interval $[0, t]$, where $0 = t_0 < t_1 < \ldots < t_n = t$ and $t_i - t_{i-1} = \Delta t = \dfrac{t}{n}$. We define

$$Q_n = \sum_{i=0}^{n} \Delta W_i^2 \tag{2.38}$$

[2] In some references the Wiener process is represented by $B(t)$ in allusion to Brownian motion.

where $\Delta W_i = W(t_i) - W(t_{i-1})$. Since ΔW_i is distributed according to $\mathcal{N}(0, \sqrt{\Delta t})$, we have that $\mathbb{E}[\Delta W_i^2] = \Delta t$ and then

$$\mathbb{E}[Q_n] = t. \tag{2.39}$$

Furthermore, once ΔW_i are independent and using the property that the variance of the sum of independent random variables is the sum of the variances, we get

$$\begin{aligned} \text{var}[Q_n] &= \sum_{i=0}^{n} \text{var}[\Delta W_i^2] = \sum_{i=0}^{n} \left\{ \mathbb{E}[\Delta W_i^4] - (\mathbb{E}[\Delta W_i^2])^2 \right\} \\ &= \sum_{i=0}^{n} \left[3(\Delta t)^2 - (\Delta t)^2 \right] = \frac{2t^2}{n}, \end{aligned} \tag{2.40}$$

where we have applied the property in Eq. (A.35) for Gaussian distributions, since ΔW_i has distribution $\mathcal{N}(0, \sqrt{\Delta t})$. Thus

$$\text{var}[Q_n] \to 0, \quad \text{as} \quad n \to \infty. \tag{2.41}$$

On the other hand,

$$\text{var}[Q_n] = \mathbb{E}\left[(Q_n - \mathbb{E}[Q_n])^2 \right] = \mathbb{E}[(Q_n - t)^2], \tag{2.42}$$

where we have used (2.39). Comparing the results in (2.41) and (2.42) leads to

$$\lim_{n\to\infty} \mathbb{E}\left[(Q_n - t)^2 \right] = 0. \tag{2.43}$$

This result proves that Q_n converges to t in the mean square sense. Let us abandon the index i and write just ΔW for the Wiener increment, with $\mathbb{E}[\Delta W^2] = \Delta t$. Equation (2.43) suggests to us that ΔW^2 can be thought as being of the order of Δt and with $\Delta t \to 0$ ($n \to \infty$) the quantity ΔW^2 resembles more and more the deterministic quantity Δt. Consequently, we can write this relation using differentials [45]:

$$(dW)^2 = dt. \tag{2.44}$$

It is thus said that $W(t)$ has a *quadratic bounded variation*. Naturally, we can say that dW is of order $\sqrt{dt}$.

The Wiener process $W(t)$ has an important property called *self-similarity* or *self-affinity*, such that

$$W(at) \overset{\text{d}}{=} \sqrt{a}\, W(t), \tag{2.45}$$

for all $a > 0$. In other words, the two processes $W(at)$ and $\sqrt{a}\, W(t)$ have exactly the same finite dimensional distribution $p(x_1, t_1; \ldots; x_n, t_n)$ for any choice of t_i, $i = 1, \ldots, n$ and $n \geq 1$. Moreover, the process

$$X(t) = \frac{1}{a} W(a^2 t) \tag{2.46}$$

is also a Wiener process. This property means that any finite portion of a Wiener process, when properly rescaled, is statistically indistinguishable from the whole path. Essentially, zooming-in in any region of the time axis, no matter how small, of a Wiener process path by a factor of a and multiplying the vertical axes by a factor of $\sqrt{a}$, we get a path similar to the original in the statistical sense [3].

Furthermore, the Wiener process is nowhere differentiable. We can see this property considering that ΔW is of order $\sqrt{\Delta t}$, thus

$$\frac{\Delta W}{\Delta t} = \mathcal{O}\left(\frac{1}{\sqrt{t}}\right), \tag{2.47}$$

then $dW/dt \to \infty$ as $\Delta t \to 0$. A rigorous proof of this fact is given in Ref. [49], where the self-similarity property is used to show that the probability of

$$\limsup_{h\to 0} \frac{|W(t_0+h) - W(t_0)|}{h} \leq \infty$$

is zero.

Theorem 1 *Almost surely, the standard Brownian motion or Wiener process is nowhere differentiable. Furthermore, almost surely, for all t, either*

$$\limsup_{h\to 0} \frac{W(t+h) - W(t)}{h} = \infty$$

or

$$\liminf_{h\to 0} \frac{W(t+h) - W(t)}{h} = -\infty$$

or both.

2.2.2 Langevin Equation

In physics, the evolution equation of a system is usually described by differential equations. When we have processes depending on random interactions, like a particle suffering an uncountable number of collisions due to its medium background, we can model such a process by an equation of the type of the Langevin equation presented in Sec. 2.1.2,

$$\frac{dx(t)}{dt} = a(x(t)) + b(x(t))\xi(t). \tag{2.48}$$

We are supposing that the real functions a and b are stationary, i.e., they do not depend explicitly on time. The first term represents the deterministic effects, while the second term describes the fluctuations, where $\xi(t) \equiv \xi(t,\omega)$ with $\omega \in \Omega$, the set of random outcomes

[3] In the language of fractals, we can say that the Wiener process trajectory is a fractal curve with fractal dimension $D = 2$ [48].

(see Appendix A), is formally defined by a random function known as Gaussian white noise satisfying the following properties [44]:

$$\begin{aligned}
&\langle \xi(t) \rangle = 0 \quad \forall t, \\
&\langle \xi(t)\xi(t') \rangle = \delta(t - t'), \\
&\langle \xi^n(t) \rangle = 0, \quad n \geq 3, \\
&\langle \xi(t) a(x(t')) \rangle = \langle \xi(t) \rangle \langle a(x(t')) \rangle = 0, \quad t' \leq t, \\
&\langle \xi(t) b(x(t')) \rangle = \langle \xi(t) \rangle \langle b(x(t')) \rangle = 0, \quad t' \leq t.
\end{aligned} \tag{2.49}$$

The properties above indicate that the noise $\xi(t)$ corresponds to random variables with a Gaussian probability distribution and that a given noise at time t is uncorrelated with past values of $x(t')$; that is, the past of the variable x does not depend on future fluctuations. Furthermore, Eq. (2.48) can be written in its integral representation as [44]:

$$x(t) = x_0 + \int_0^t dt' \; a(x(t')) + \int_0^t dt' \; b(x(t'))\xi(t'). \tag{2.50}$$

As $x(t)$ has a random term and, consequently, is a stochastic process, we can identify $x(t)$ as a random variable $X(t)$. Making $x(t = 0) \equiv x_0 = 0$ and taking the mean over the random realizations of the noise, we have

$$\begin{aligned}
\langle x(t) \rangle &= \int_0^t dt' \langle a(x(t')) \rangle + \int_0^t dt' \langle b(x(t')) \rangle \langle \xi(t') \rangle \\
&\overset{t \to 0}{=} a(0)t + \mathcal{O}(t).
\end{aligned} \tag{2.51}$$

Similarly,

$$\begin{aligned}
\langle x^2(t) \rangle &= \int_0^t dt' \int_0^{t'} dt'' \langle a(x(t''))a(x(t')) \rangle + 2 \int_0^t dt' \int_0^{t'} dt'' \langle a(x(t''))b(x(t'))\xi(t') \rangle \\
&\quad + \int_0^t dt' \int_0^{t'} dt'' \langle b(x(t'))b(x(t''))\xi(t')\xi(t'') \rangle \\
&\overset{t \to 0}{=} b^2(0) \int_0^t dt' \int_0^{t'} dt'' \delta(t' - t'') = b^2(0)t + \mathcal{O}(t),
\end{aligned} \tag{2.52}$$

and for the remaining moments it is easy to see that

$$\langle x^n(t) \rangle = \mathcal{O}(t). \tag{2.53}$$

Therefore, by comparing the above results for the moments calculated from the Langevin equation with the corresponding results calculated using the Fokker-Planck equation (see Eqs. (B.46), (B.48), and (B.49) in Appendix B), we can establish a correspondence between these two equations. Whereas the Langevin equation describes the time evolution of the trajectories of a certain stochastic process, the Fokker-Planck equation describes the time evolution of the probability density [37, 38, 45]. Hence, the relation between the coefficients of these two equations are $a_1(x) = a(x)$ and $a_2(x) = b^2(x)$, where $a_1(x)$, $a_2(x)$ are the coefficients in the Fokker-Planck equation (2.34) and $a(x)$, $b(x)$ are the coefficients

in the Langevin equation (2.48). Later, it will be presented in a more explicit form the connection between these coefficients.

The quantity $\xi(t)$ does not have, however, a precise mathematical definition. To see that, consider the case where $a(x(t)) = 0$ and $b(x(t)) = 1$, so only the random noise is present, i.e.,

$$\dot{x}(t) = \xi(t) \tag{2.54}$$

and in integral form

$$x(t) = \int_{t_0}^{t} \xi(t')dt', \tag{2.55}$$

where $x(t_0) = 0$. As we have concluded just above, the probability distribution of this process satisfies the Fokker-Planck equation with $a_1(x) = 0$ and $a_2(x) = 1$, this is

$$\frac{\partial}{\partial t}p(x,t) = \frac{1}{2}\frac{\partial^2}{\partial t^2}p(x,t). \tag{2.56}$$

The solution for this equation with initial condition $p(x,t_0) = \delta(x)$ and boundary conditions $p(x \to \pm\infty, t) = 0$ is

$$p(x,t) = \frac{1}{\sqrt{2\pi(t-t_0)}} \exp\left[-\frac{x^2}{2(t-t_0)}\right] = \mathcal{N}(0, \sqrt{t-t_0}). \tag{2.57}$$

Nevertheless, we have seen in the previous section that a process with such a probability distribution is the Wiener process increment $W(t) - W(t_0)$. Thus, we can write

$$W(t) - W(t_0) = \int_{t_0}^{t} \xi(t')dt', \tag{2.58}$$

and if we consider the Fundamental Principle of Calculus, then $\xi(t)$ can be understood as the time derivative of $W(t)$:

$$\frac{dW(t)}{dt} \coloneqq \xi(t). \tag{2.59}$$

But, the Theorem 1 states that the Wiener process is nowhere differentiable, so $\xi(t)$ is not a proper function, although it can be identified as a generalized process. Even though $\xi(t)$ is not a proper function, the differential quantity $\xi(t)dt = dW(t)$ is mathematically well defined. From Eq. (2.58), the Wiener process can be given as

$$W(t) \coloneqq \int_{0}^{t} dW(t). \tag{2.60}$$

It follows from this that the Langevin equation can be put on a well defined mathematical ground as

$$dX(t) = a(X(t))dt + b(X(t))dW(t). \tag{2.61}$$

Equations of the form of (2.61) are known as *Stochastic Differential Equations* [38, 45]. Before proceeding to integrate this equation, we need to define the stochastic integral precisely.

2.2.3 Stochastic Integral

We need to define a stochastic integral of the form

$$\int_a^b g(t)dW(t) \tag{2.62}$$

as the limit of partial sums,

$$S_n = \sum_{i=1}^{n} g(t_i^*)\Delta W_i = \sum_{i=1}^{n} g(t_i^*)[W(t_i) - W(t_{i-1})], \tag{2.63}$$

where $a = t_0 < t_1 < \ldots < t_n = b$ is a partition of $[a, b]$ and $t_i^* \in [t_{i-1} - t_i]$ is an intermediate point.

Let us suppose, first, that $g(t)$ is a deterministic function, then

$$\mathbb{E}[S_n] = \mathbb{E}\left[\sum_{i=1}^{n} g(t_i^*)\Delta W_i\right] = \sum_{i=1}^{n} g(t_i^*)\mathbb{E}[\Delta W_i] = 0 \tag{2.64}$$

independent of t_i^*. Additionally

$$\begin{aligned}\mathbb{E}[S_n^2] &= \mathbb{E}\left[\sum_{i=1}^{n}\sum_{j=1}^{n} g(t_i^*)g(t_j^*)\Delta W_i\Delta W_j\right] \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n} g(t_i^*)g(t_j^*)\mathbb{E}[\Delta W_i\Delta W_j] \\ &= \sum_{i=1}^{n} g^2(t_i^*)\Delta t,\end{aligned} \tag{2.65}$$

where we used the fact that $\langle \Delta W_i \Delta W_j \rangle = \delta_{ij}\Delta t$, with $\Delta t = t_i - t_{i-1}$, which can be deduced straightforwardly from the definition of the Wiener process. Taking the limit $n \to \infty$ gives

$$\lim_{n\to\infty} \mathbb{E}[S_n^2] = \int_a^b [g(t)]^2 dt, \tag{2.66}$$

independently of the choice of intermediate times t_i^*.

Now, suppose that $g(t)$ is a stochastic process. For example, taking $g(t) = W(t)$ leads us to

$$\begin{aligned}\mathbb{E}[S_n] &= \mathbb{E}\left[\sum_{i=1}^{n} W(t_i^*)[W(t_i) - W(t_{i-1})]\right] \\ &= \sum_{i=1}^{n} \{\mathbb{E}[W(t_i^*)W(t_i)] - \mathbb{E}[W(t_i^*)W(t_{i-1})]\} \\ &= \sum_{i=1}^{n} [\min(t_i^*, t_i) - \min(t_i^*, t_{i-1})] \\ &= \sum_{i=1}^{n} (t_i^* - t_{i-1}).\end{aligned} \tag{2.67}$$

This implies, for example, $\mathbb{E}[S_n] = 0$ if $t_i^* = t_{i-1}$, whereas $\mathbb{E}[S_n] = b - a$ if $t_i^* = t_i$. So, the mean value of the integral

$$\int_a^b W(t)dW(t) \tag{2.68}$$

can be anything between zero and $b-a$. From this case, we can conclude that the stochastic integral of a stochastic process $g(t)$ depends on the choice of intermediate times t_i^* [37].

Let us now introduce the convergence criteria for stochastic integrals. Before, we need the definition of mean square limit [44].

Definition 3 *The mean square limit of a function X_n as $n \to \infty$, denoted by*

$$\underset{n\to\infty}{\text{ms-lim}}\ X_n,$$

converges to X if

$$\lim_{n\to\infty} \langle (X_n - X)^2 \rangle = 0.$$

Then, the stochastic integral of a function $g(t)$ can be defined by

$$\int_a^b g(t)dW(t) = \underset{n\to\infty}{\text{ms-lim}} \sum_{i=1}^{n} g(t_i^*)[W(t_i) - W(t_{i-1})]. \tag{2.69}$$

The convergence in the mean square sense is a weaker requirement than the point-wise convergence used in Riemannian integrals [44]. Equation (2.69) defines the stochastic integral upon the choice of the intermediate time $t_i^* \in [t_{i-1}, t_i]$. The two most important choices for t_i^* are:

i. $t_i^* = t_{i-1}$, defining the *Itô stochastic integral*;

ii. $t_i^* = \dfrac{t_{i-1} + t_i}{2}$, defining the *Stratonovich stochastic integral*.

Before proceeding further, some additional definitions are necessary.

2.2.3.1 Filtration or Information Flow

First, let us define the notion of "information" generated by a stochastic process.

Definition 4 *Let $\{ X_t \}_{t\geq 0}$ be a stochastic process on some probability space $(\Omega, \mathcal{F}, P)$. The σ-algebra $\mathcal{F}_t^X \subset \mathcal{F}$ generated by the process X_t is defined to be the σ-algebra generated by the random variables X_s, $s \leq t$ fixed. In other words, $\mathcal{F}_t^X$ is the smallest σ-algebra containing all sets of the form*

$$\{ \omega \mid X_{t_1}(\omega) \in B_1, \ldots, X_{t_n}(\omega) \in B_n \}$$

where $t_j \leq t$ and $B_j \subset \mathbb{R}$ are Borel sets [4], for $j \leq n = 1, 2, \ldots$.

[4] For a definition of Borel sets, see Appendix A

It is difficult to visualize the set $\mathcal{F}_t^X$, but in synthesis it is the σ-algebra that contains all possible trajectories of X_t in the time interval $[0, t]$: this is a collection of all these trajectories as well as union, intersection and complement of such trajectories. We can think $\mathcal{F}_t^X$ as the "history of X_t up to time t" or, alternatively, as the "information contained in the trajectories of X_t up to time t". As time progresses, we get a succession of such σ-algebras $\mathcal{F}_t^X \subset \mathcal{F}_s^X$, $t < s$, which represents an *information flow*, or, more technically, a *filtration* [37, 50].

Definition 5 *A filtration or information flow on a probability space $(\Omega, \mathcal{F}, P)$ is a collection $\{ \mathcal{F}_t \}_{t \geq 0}$ of σ-algebras $\mathcal{F}_t \subset \mathcal{F}$ such that*

$$\mathcal{F}_s \subset \mathcal{F}_t, \quad \textit{for} \quad 0 \leq s \leq t.$$

Remark 1 *A probability space together with a filtration is called a filtered probability space.*

It is important to note that the definition above makes no reference to any stochastic process. If we have a stochastic process X_t and its values can be completely determined by the information obtained from $\mathcal{F}_t$, for all $t \geq 0$, then we say X_t is adapted to the filtration $\{ \mathcal{F}_t \}_{t \geq 0}$ [37].

Definition 6 *A stochastic process $\{ X_t \}_{t \geq 0}$ defined on a filtered probability space with filtration $\{ \mathcal{F}_t \}_{t \geq 0}$ is called adapted to the filtration if $X_t(\omega)$ is $\mathcal{F}_t$-measurable for all $t \geq 0$.*

As defined above, a stochastic process $\{ X_t \}$ naturally generates a filtration $\{ \mathcal{F}_t^X \}$. A process $\{ X_t \}$ is obviously adapted to its natural filtration. If a process $g(t)$ is adapted to the filtration generated by the Wiener process $W(t)$, we shall say that $g(t)$ is *adapted to the Wiener process*. This means that to know the values of $g(t)$ it suffices to know the trajectories of $W(t)$ up to time t. In other words, the value of $g(t)$ is a functional of the trajectories of the Wiener process on the interval $[0, t]$. For this reason a process $g(t)$ adapted to the Wiener process is sometimes called a *non-anticipating function*, since the present value of $g(t)$ is independent of the future increments $W(s) - W(t)$, $t < s$, of the Wiener process [37, 45].

Definition 7 *A function $g(t)$ is called a non-anticipating function of t when $g(t)$ is statistically independent of $W(s) - W(t)$ for all s, t with $t < s$.*

This is, in some sense, a causality requirement, where we do not want $g(t)$ to anticipate what will be the future values of the process $W(t)$ [44].

2.2.3.2 Itô Stochastic Integral

Now, we will formalize the definition of stochastic integral based on the work of the Japanese mathematician Kiyoshi Itô (1915-2008). Let us start by defining the general class of processes to which this integration applies [37, 50].

Definition 8 *Consider $g(t)$ a stochastic process. It is said that g belongs to the class $\mathcal{L}^2[a,b]$ if the two following properties holds:*

- *g does not grow explosively, i.e.,*
$$\int_a^b \mathbb{E}[g^2(t)]dt < \infty;$$
- *g is adapted to the Wiener process.*

It said that g belongs to the class $\mathcal{L}^2$ if $g \in \mathcal{L}^2[0,t]\ \forall\, t$.

Let us define below what is meant by *simple stochastic process*.

Definition 9 *The stochastic process $g(t)$ with $t \in [a,b]$ is called simple if exists a partition of the interval $[a,b]$*
$$a = t_0 < t_1 < \ldots < t_n = b$$
and a sequence of random variables Z_i, $i = 1, 2, \ldots, n$, such that
$$g(t) = Z_i \quad for \quad t_{i-1} \leq t < t_i, \quad i = 1, \ldots, n,$$
and the sequence Z_i is adapted to the filtration $\{\, \mathcal{F}^W_{t_{i-1}} \,\}_{i=1,\ldots,n}$.

Thus, a simple stochastic process has constant values in each sub-interval $[t_{i-1}, t_i]$ of the partition. In other words, the trajectory is constant by parts. The adaptation of Z_i to the filtration $\{\, \mathcal{F}^W_{t_{i-1}} \,\}$ means that the value of $g(t)$ in each sub-interval $[t_{i-1}, t_i]$ only depends on the Wiener process up to the beginning of this sub-interval. This leads to important properties of the Itô stochastic integral. Even though simple stochastic processes are not commonly found in real phenomena, this concept is very useful because non-simple stochastic processes of the class $\mathcal{L}^2$ can always be approximated by simple stochastic processes [37, 50].

Based on the definition above, we can precisely define the Itô stochastic integral [44, 45, 50, 51].

Definition 10 *The Itô stochastic integral of a simple stochastic process g in $[a,b]$ is defined by the formula*
$$\int_a^b g(t)dW(t) = \sum_{i=1}^{n} g(t_{i-1})[W(t_i) - W(t_{i-1})].$$

If the process g is not simple, however, if it is of class $\mathcal{L}^2$, then it can always be approximated by a sequence of simple processes g_n such that

$$\lim_{n\to\infty}\int_a^b \mathbb{E}\Big[\Big(g(t)-g_n(t)\Big)^2\Big]dt = 0, \tag{2.70}$$

it means that g_n converges in quadratic mean to the process g. Then, the Itô stochastic integral for a non-simple process $g(t)$ is defined by

$$\int_a^b g(t)dW(t) = \lim_{n\to\infty}\int g_n(t)dW(t). \tag{2.71}$$

Based on that, the Itô integral of any stochastic process $g(t)\in\mathcal{L}^2$ is given by

$$\mathcal{I} = \int_a^b g(t)dW(t) = \lim_{n\to\infty}\sum_{i=1}^{n} g(t_{i-1})[W(t_i)-W(t_{i-1})]. \tag{2.72}$$

Note that this integral is not a number but a random variable. For each realization of $W(t)$, the integral $\mathcal{I}$ will return a different value. Particularly, if we have

$$\mathcal{I}(t) = \int_0^t g(t)dW(t), \tag{2.73}$$

for $t>0$, then $\mathcal{I}(t)$ is a stochastic process. Below, some properties of the Itô integral are presented [50].

Proposition 1 *Consider a stochastic process g of class $\mathcal{L}^2$. Then the Itô stochastic integral satisfies the following properties:*

1. $\mathbb{E}\left[\int_a^b g(t)dW(t)\right] = 0$;
2. $\mathbb{E}\left[\left(\int_a^b g(t)dW(t)\right)^2\right] = \int_a^b \mathbb{E}[g^2(t)]dt$ *(isometry property);*
3. $\int_a^b g(t)dW(t)$ *is $\mathcal{F}_b^W$-measurable;*
4. $\int_0^t g(t)dW(t)$ *has continuous trajectories.*

A proof for the properties 1 and 2 above follows from Eqs.(2.64) and (2.65), taking $t_i^* = t_{i-1}$ and $g(t)$ as a stochastic function in $\mathcal{L}^2$. The proofs for the properties 3 and 4 follow straightforwardly from the definitions of the Itô integral and the Wiener process. An important remark is that, from the isometry property of the Itô integral (property 2), it is possible to write

$$\langle dW(t')dW(t'')\rangle = \delta(t'-t'')dt'dt''. \tag{2.74}$$

It is worth noting that the Itô stochastic integral does not follow the same rules of the conventional calculus as would the Stratonovich integral [50]. However, the Itô integral

is preferred when working with stochastic processes, one reason for this is that a function defined as

$$X(t) = \int_0^t g(s)dW(s) \tag{2.75}$$

is a martingale (see Appendix B), meaning that its current value represents the best possible estimate of its future value. In fact, for $t \geq t'$ holds

$$\begin{aligned}
\mathbb{E}[X(t) \,|\, X(t')] &= \mathbb{E}\left[\int_0^t g(s)dW(s) \,\middle|\, X(t')\right] \\
&= \mathbb{E}\left[\int_0^{t'} g(s)dW(s) + \int_{t'}^t g(s)dW(s) \,\middle|\, X(t')\right] \\
&= \mathbb{E}[X(t')|X(t')] + \mathbb{E}\left[\int_{t'}^t g(s)dW(s) \,\middle|\, X(t')\right] \\
&= X(t') + \mathbb{E}\left[\int_{t'}^t g(s)dW(s)\right] \\
&= X(t'),
\end{aligned} \tag{2.76}$$

where $X(t')$ is $\mathcal{F}_{t'}$-measurable, meaning that it is independent of the future in $s > t'$ [44].

2.2.4 Stochastic Differential Equations (SDEs)

Now that we have defined the Itô stochastic integral, we can properly define the differential equation (2.61), derived from the Langevin equation [44].

Definition 11 *A stochastic process $X(t)$ obeys an Itô Stochastic Differential Equation (SDE), written as*

$$dX(t) = a(X,t)dt + b(X,t)dW(t),$$

$$X(t_0) = X_0,$$

when for all t we have

$$X(t) = X_0 + \int_{t_0}^t a(X,t')dt' + \int_{t_0}^t b(X,t')dW(t'),$$

where X_0 is some random variable independent of the Wiener process $W(t)$.

It is important to note that the differential form is just a short-hand notation for the integral form that is defined taking the Itô stochastic integral. The coefficient $a(X,t)$ is called *drift coefficient* and $b(X,t)$ is called *fluctuation coefficient* or *noise amplitude*. Furthermore, the following theorem states the conditions for the existence and uniqueness of a solution of the SDE [44, 50].

Theorem 2 *For a given SDE, there exists a unique non-anticipating solution $X(t')$ in $[t_0, t]$ if and only if the following two conditions are fulfilled:*

- *Lipschitz condition:*

$$\exists k > 0 : \quad |a(x,t') - a(y,t')| + |b(x,t') - b(y,t')| \leq k|x-y|,$$

$\forall$ x, y *and* $t' \in [t_0, t]$;

- *growth condition:*

$$\exists k > 0 : \quad |a(x,t')|^2 + |b(x,t')|^2 \leq k(1+|x|^2),$$

$\forall$ $t' \in [t_0, t]$.

The solution $X(t')$ *is a Markov process.*

2.2.5 Itô's Formula

Suppose a functional $f(X,t)$ of the stochastic process

$$dX(t) = a(X,t)dt + b(X,t)dW(t). \tag{2.77}$$

We can expand $f(x,t)$ in a Taylor series, then

$$\begin{aligned} df = &\frac{\partial f}{\partial t}dt + \frac{\partial^2 f}{\partial t^2}(dt)^2 + \frac{\partial f}{\partial x}dX + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(dX)^2 \\ &+ \frac{1}{2}\frac{\partial^2 f}{\partial t \partial x}dtdX + \ldots \end{aligned} \tag{2.78}$$

where we have considered dx as the stochastic process dX in (2.77). Note that

$$\begin{aligned} (dX^2) &= a^2(dt)^2 + b^2(dW)^2 + 2ab\,dtdW \\ &= b^2 dt + \mathcal{O}(dt^{3/2}), \end{aligned} \tag{2.79}$$

where we have used the correspondence $dW^2 \to dt$ and $dW \to (dt)^{1/2}$. Substituting Eq. (2.79) in (2.78) and retaining only terms up to order dt, we get

$$df = \left[\frac{\partial f}{\partial t} + \frac{1}{2}b^2\frac{\partial^2 f}{\partial x^2}\right]dt + \frac{\partial f}{\partial x}dX, \tag{2.80}$$

and substituting dX in Eq. (2.77) we obtain *Itô's formula* [38, 44, 45]:

$$\begin{aligned} df(X,t) = &\left[\frac{\partial}{\partial t}f(x,t) + a(x,t)\frac{\partial}{\partial x}f(x,t) + \frac{1}{2}b^2(x,t)\frac{\partial^2}{\partial x^2}f(x,t)\right]_{x=X(t)}dt \\ &+ \left[b(x,t)\frac{\partial}{\partial x}f(x,t)\right]_{x=X(t)}dW(t). \end{aligned} \tag{2.81}$$

The result in (2.81) is a new SDE for the stochastic process $f(X,t)$ that is a functional of the stochastic process $X(t)$ in (2.77). Note that the fluctuation coefficient of $X(t)$ now also contributes to the drift coefficient of $f(X,t)$. Itô's formula will be especially important in the next chapter.

2.2.6 Relation between Fokker-Planck Equation and SDE

If a stochastic process follows an SDE of the type in Eq. (2.77), then its probability density satisfies a Fokker-Planck equation. To show this, let us first consider a function $f(X(t))$, where $X(t)$ is a stochastic process described by the SDE [44, 45]

$$dX(t) = a(X,t)dt + b(X,t)dW(t). \tag{2.82}$$

Differentiating $X(t)$ and applying Itô's formula yields

$$df(X(t)) = \left[a(x,t)\frac{d}{dx}f(x) + \frac{1}{2}b^2(x,t)\frac{d^2}{dx^2}f(x)\right]dt + \left[b(x,t)\frac{d}{dx}f(x)\right]dW(t). \tag{2.83}$$

If we take the mean of the expression above, the last term vanishes since X is adapted to the Wiener process. Then

$$\begin{aligned}\langle df(X(t))\rangle &= \left\langle \left[a(x,t)\frac{d}{dx}f(x) + \frac{1}{2}b^2(x,t)\frac{d^2}{dx^2}f(x)\right]dt \right\rangle \\ &= \int_{\mathbb{R}} \left[a(x,t)\frac{d}{dx}f(x) + \frac{1}{2}b^2(x,t)\frac{d^2}{dx^2}f(x)\right]p(x,t)dx\ dt,\end{aligned} \tag{2.84}$$

and integrating by parts,

$$\frac{d}{dt}\langle f(X(t))\rangle = \int_{\mathbb{R}} \left[-\frac{\partial}{\partial x}[a(x,t)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[b^2(x,t)p(x,t)]\right] f(x)dx, \tag{2.85}$$

where we have considered that the boundary terms vanish. To calculate the time derivative of the expected value is straightforward and yields

$$\int_{\mathbb{R}} \left[\frac{\partial}{\partial t}p(x,t)\right] f(x)dx = \int_{\mathbb{R}} \left[-\frac{\partial}{\partial x}[a(x,t)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[b^2(x,t)p(x,t)]\right] f(x)dx. \tag{2.86}$$

Since this result should be valid for any function $f(x)$, the terms inside the brackets in (2.86) must be equal, then

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}[a(x,t)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[b^2(x,t)p(x,t)], \tag{2.87}$$

which is the forward Fokker-Planck equation in (B.38) with $a_1 = a(x,t)$ and $a_2 = b^2(x,t)$. We can conclude that every stochastic process with its trajectory described by the SDE (2.82) has a forward (and consequently also a backward) Fokker-Planck equation (2.87) associated, describing the evolution of its probability density.

The Fokker-Planck equation (2.87) with $a(x,t) = 0$ is the diffusion equation in (2.19) with diffusion coefficient $D = b^2/2$ constant. Due to this connection, sometimes the stochastic process (2.82) is said to be a process with diffusive behavior.

2.3 BROWNIAN MOTION REVISITED

It is possible to provide a more modern and rigorous development for the problem of Brownian motion presented in Sec. 2.1, using the mathematical tools introduced in the previous sections. The development in this section is based on the references [37, 44, 45].

First, the fluid particles are much lighter than the Brownian particle. Due to the mass difference, the fluid particles move much faster, exerting a vast number of relatively weak collisions on the Brownian particle. However, as a result of the summed effect of all these collisions, a random force acts on the Brownian particle, in addition to the viscous drag force characteristic of the fluid. We can model these effects as follows.

Let us assume that the particle's velocity is small enough for Stokes' law to be valid. In this way, the viscous drag force will be proportional to the relative velocity between the Brownian particle and the fluid. Assuming the fluid is at rest, the viscous drag force is given by

$$\mathbf{F}_{\text{drag}} = -\gamma \mathbf{v}, \tag{2.88}$$

where γ is the friction coefficient of the Brownian particle.

Considering the above, we will approximate the collisions between the Brownian particle and the fluid particles as occurring instantaneously and causing a random change in the Brownian particle's velocity. Furthermore, we will assume that all these collisions are uncorrelated with each other. Thus, we can model the force acting on the Brownian particle due to stochastic collisions as a three-dimensional Gaussian white noise with intensity Γ (where each direction is an independent Gaussian white noise, with the properties in (2.49), and intensity Γ). Therefore, the evolution equation for the Brownian particle can be given by the Langevin equation, see Eq. 2.27,

$$M\frac{d\mathbf{v}}{dt} = \mathbf{F}_{\text{drag}} + \Gamma\xi(t), \tag{2.89}$$

where M is the mass of the Brownian particle. This Langevin equation can be rewritten as the following system of SDEs:

$$\begin{aligned} d\mathbf{v} &= -\frac{\gamma}{M}\mathbf{v}dt + \frac{\Gamma}{M}d\mathbf{W}(t) = -\alpha\mathbf{v}dt + \sigma d\mathbf{W}(t), \\ d\mathbf{x} &= \mathbf{v}dt, \end{aligned} \tag{2.90}$$

where we made the substitution $\alpha \equiv \gamma/M$ and $\sigma \equiv \Gamma/M$.

Note that the two differential equations in (2.90) are decoupled. Consequently, they may be treated independently: one first solves the stochastic differential equation governing the particle's velocity, and only afterwards integrates it to obtain the corresponding position process. We will now detail the two processes involved in this problem: the *velocity process* and the *position process*.

2.3.1 Velocity Process

Without loss of generality, we will treat this problem in one dimension. Thus, the stochastic differential equation for the velocity of the Brownian particle is given by

$$dv = -\alpha v\, dt + \sigma\, dW(t). \tag{2.91}$$

The stochastic process defined by the equation (2.91) is known as *Ornstein-Uhlenbeck process*, after the Dutch physicists Leonard Ornstein (1880-1941) and George Uhlenbeck (1900-1988) [52]. Calculating the expected value of Eq. (2.91), we obtain

$$\frac{d\langle v(t)\rangle}{\langle v(t)\rangle} = -\alpha dt, \tag{2.92}$$

which results in

$$\langle v(t)\rangle = \langle v_0\rangle e^{-\alpha t}. \tag{2.93}$$

The expected value is calculated for an ensemble of Brownian particles or realizations of the Ornstein-Uhlenbeck process. We can solve (2.91) explicitly by making the change of variable

$$Z = f(v,t) = e^{\alpha t} v. \tag{2.94}$$

Using Itô's formula, we have

$$\begin{aligned} dZ &= \left[\frac{\partial f}{\partial t} - \alpha v\frac{\partial f}{\partial v} + \frac{1}{2}\sigma^2\frac{\partial^2 f}{\partial v^2}\right] dt + \sigma\frac{\partial f}{\partial v} dW(t) \\ &= e^{\alpha t}\alpha v\, dt + e^{\alpha t}\left(-\alpha v\, dt + \sigma dW\right) \\ &= \sigma e^{\alpha t} dW. \end{aligned} \tag{2.95}$$

Integrating this equation leads us to

$$Z(t) = Z_0 + \sigma\int_0^t e^{\alpha t'} dW(t'). \tag{2.96}$$

Returning to the original variable $v = e^{-\alpha t}Z$, we obtain an explicit solution for the Ornstein-Uhlenbeck process given by

$$v(t) = v_0 e^{-\alpha t} + \sigma\int_0^t e^{-\alpha(t-t')} dW(t'). \tag{2.97}$$

With this solution, we can now calculate the mean square velocity of the Brownian particle, that is

$$\begin{aligned} \langle v^2(t)\rangle &= \langle v_0^2\rangle e^{-2\alpha t} + 2\langle v_0\rangle\sigma e^{-2\alpha t}\int_0^t e^{\alpha t'}\langle dW(t')\rangle \\ &\quad + \sigma^2 e^{-2\alpha t}\int_0^t\int_0^t e^{\alpha(t'+t'')}\langle dW(t')dW(t'')\rangle \\ &= \langle v_0^2\rangle e^{-2\alpha t} + \sigma^2 e^{-2\alpha t}\int_0^t e^{2\alpha t'} dt', \end{aligned} \tag{2.98}$$

where we made use of the result (2.74). Calculating the straightforward integral in the last term, we get

$$\langle v^2(t)\rangle = \frac{\sigma^2}{2\alpha} + \left(\langle v_0^2\rangle - \frac{\sigma^2}{2\alpha}\right) e^{-2\alpha t}. \tag{2.99}$$

The steady-state value occurs for long times, i.e., as $t \to \infty$, consequently

$$\langle v^2\rangle_{t\to\infty} = \frac{\sigma^2}{2\alpha}. \tag{2.100}$$

This value must be equal to the mean thermal velocity of the Brownian particle, which is in thermal equilibrium with the fluid through collisions with the fluid particles. If the fluid is kept at a temperature T, we have the following value for the mean kinetic energy of the Brownian particle, using the equipartition theorem of energy [36]:

$$\frac{M}{2}\langle v^2\rangle_{t\to\infty} = \frac{1}{2}k_B T. \tag{2.101}$$

Comparing Eq. (2.100) with Eq. (2.101), we can conclude that

$$\sigma^2 = \frac{2\alpha k_B T}{M} \Longrightarrow \Gamma^2 = 2\gamma k_B T. \tag{2.102}$$

Therefore, if relation (2.102) is satisfied, Eq. (2.91) correctly describes the behavior of the Brownian particle after the initial effects have died out and the motion is a consequence only of the particle's contact with the fluid at thermal equilibrium. Equation (2.102), which relates the coefficients of Eq. (2.91), is a version of the *fluctuation-dissipation theorem* [36], which relates the fluctuations at equilibrium (Γ) to the magnitude of the dissipation (γ).

The velocity autocorrelation can also be calculated explicitly:

$$\begin{aligned}\langle v(t)v(s)\rangle &= \langle v_0^2\rangle e^{-\alpha(t+s)} \\ &\quad + \frac{2\alpha k_B T}{M} e^{-\alpha(t+s)} \int_0^t \int_0^s e^{\alpha(t'+t'')} \langle dW(t')dW(t'')\rangle \\ &= \langle v_0^2\rangle e^{-\alpha(t+s)} + \frac{2\alpha k_B T}{M} e^{-\alpha(t+s)} \int_0^{\min(t,s)} e^{2\alpha t'} dt',\end{aligned} \tag{2.103}$$

where we have used again the result in (2.74). Then, we obtain

$$\langle v(t)v(s)\rangle = \left(\langle v_0^2\rangle - \frac{k_B T}{M}\right) e^{-\alpha(t+s)} + \frac{k_B T}{M} e^{-\alpha|t-s|}. \tag{2.104}$$

At equilibrium, as $t,\ s \to \infty$ with $|t-s|$ held fixed, we have the stationary case

$$\langle v(t)v(s)\rangle_{s,t\to\infty} = \frac{k_B T}{M} e^{-\alpha|t-s|}. \tag{2.105}$$

In the stationary limit, the velocity autocorrelation depends only on the time interval over which the velocities are taken. The mean square velocity ($t = s$) is constant and has the value $\langle v^2(t)\rangle = v_T^2$, with $v_T^2 = k_B T/M$ being the thermal velocity in accordance with (2.101). In Fig. 2, we can observe some curves of the velocity autocorrelation function for

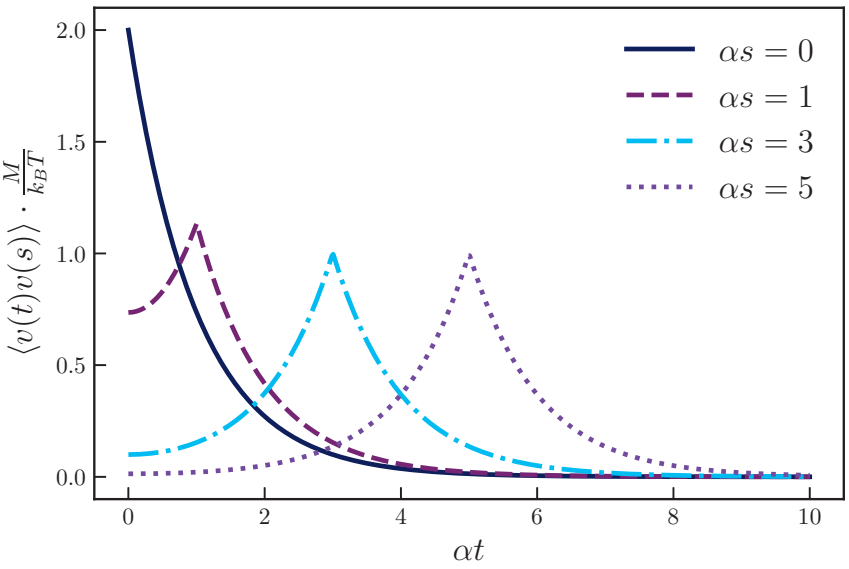


FIGURE 2 – Velocity autocorrelation for a Brownian particle, Eq. (2.104), with $\langle v_0^2\rangle = 2k_BT/M$, in function of the dimensionless unit αt for four different values of the reference time s.

a Brownian particle with $\langle v_0^2\rangle = 2v_T^2$. The velocity correlation curve is exponential with a cusp at $t = s$. Notice that the cusp becomes more symmetric and its maximum value approaches one as the reference time s increases.

Now, let us calculate the distribution of the difference between the velocity of the Brownian particle and its mean value, that is

$$u(t) \coloneqq v(t) - \langle v(t)\rangle = \sqrt{\frac{2\alpha k_BT}{M}} e^{-\alpha t} \int_0^t e^{\alpha t'} dW(t'), \tag{2.106}$$

where we have retained v_0 fixed in order that $\langle v_0\rangle = v_0$. We can conclude that $u(t)$ is a sum of Gaussian distributed random values $(dW(t))$, then $u(t)$ is itself a Gaussian distributed random value due to the stability property of Gaussian distributions. Calculating the mean and the variance of $u(t)$, we get

$$\langle u(t)\rangle = 0, \quad \langle u^2(t)\rangle = \frac{k_BT}{M}(1 - e^{-2\alpha t}). \tag{2.107}$$

Calculating the Gaussian distribution for $u(t)$ and rewritten in terms of $v(t)$ leads us to

$$p(v, t|v_0, 0) = \sqrt{\frac{M}{2\pi k_BT(1 - e^{-2\alpha t})}} \exp\left[-\frac{M}{2k_BT}\frac{(v - v_0e^{-\alpha t})^2}{1 - e^{-2\alpha t}}\right]. \tag{2.108}$$

The expression (2.108) is the solution for the Fokker-Planck equation associated with the process (2.91) with the initial condition $\delta(v - v_0)$ and the boundary condition $p(v \to \pm\infty, t|v_0, 0) = 0$. Solution (2.108) is known as the Green's function for this Fokker-Planck equation or as the Green's propagator between $(v_0, 0)$ and (v, t). We can express the probability of finding a velocity v at a time t by

$$p(v, t) = \int_{-\infty}^{+\infty} p(v, t|v', 0)p(v', 0)dv'. \tag{2.109}$$

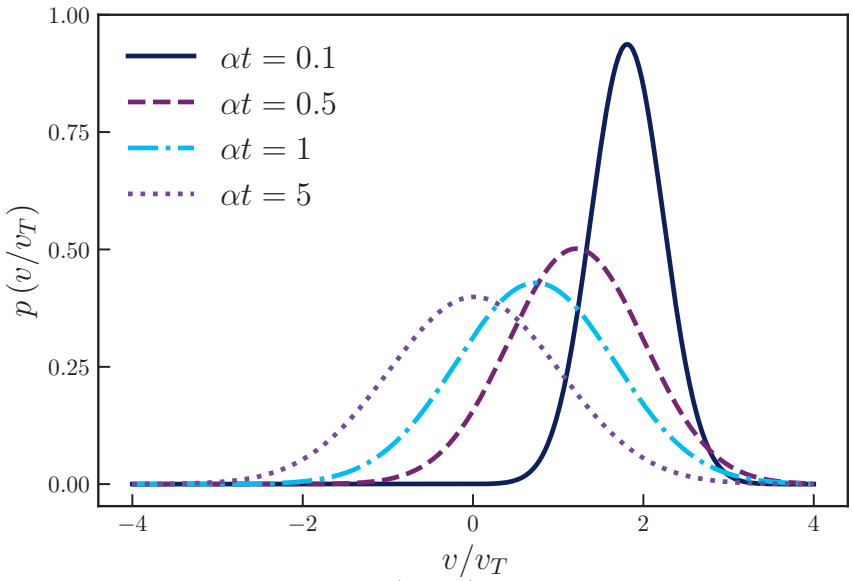


FIGURE 3 – Velocity distribution, Eq. (2.108), for a Brownian particle with $v_0 = 2v_T = 2\sqrt{k_BT/M}$ for four different values of time t.

In the stationary limit ($t \to \infty$), distribution (2.108) tends to the *Maxwell-Boltzmann velocity distribution* [36]:

$$p(v,t|v_0,0) \underset{t\to\infty}{\longrightarrow} p_{eq}(v) = \sqrt{\frac{M}{2\pi k_B T}} \exp\left[-\frac{Mv^2}{2k_BT}\right]. \tag{2.110}$$

We can conclude that the Ornstein-Uhlenbeck process is stationary, Gaussian, and Markovian. From a more detailed analysis, it can be concluded that the Ornstein-Uhlenbeck process is the only stochastic process with these properties [44, 53].

In Fig. 3, one can see several velocity distributions for a Brownian particle at different times with the initial condition $v_0 = 2v_T$. Note that for short times, the distribution is narrow and centered around v_0. As time increases, the distribution becomes more dispersed and centered at zero, approaching the equilibrium distribution.

2.3.2 Position Process

The position of the Brownian particle can be calculated by a direct integration of the equation

$$dx(t) = v(t)dt \implies x(t) = \int_0^t v(t')dt', \tag{2.111}$$

where we are considering $x(t=0) = 0$. Substituting the equation for $v(t)$ in (2.97), we obtain

$$x(t) = \frac{v_0}{\alpha}(1 - e^{-\alpha t}) + \sqrt{\frac{2\alpha k_B T}{M}} \int_0^t dt' e^{-\alpha t'} \int_0^{t'} e^{\alpha t''} dW(t''). \tag{2.112}$$

The expected position of the Brownian particle is

$$\langle x(t)\rangle = \frac{\langle v_0\rangle}{\alpha}(1 - e^{-\alpha t}). \tag{2.113}$$

Note that for short times, the mean value of the position behaves as $\langle x(t)\rangle = v_0 t$ and approaches v_0/α as $t \to \infty$, which is the asymptotic displacement of the particle, starting from $x = 0$, under the influence of the viscous force.

It can be noted that the double integral in the last term of Eq. (2.112) has the triangular domain $0 \leq t' \leq t$, $0 \leq t'' \leq t'$, which can be rewritten as $0 \leq t'' \leq t$, $t'' \leq t' \leq t$. Hence, the double integral is transformed into

$$\int_0^t dW(t'') \int_{t''}^t dt' e^{-\alpha(t'-t'')} = \int_0^t \frac{1 - e^{-\alpha(t-t'')}}{\alpha} dW(t''), \tag{2.114}$$

which gives a more suitable expression for $x(t)$,

$$x(t) = \frac{v_0}{\alpha}(1 - e^{-\alpha t}) + \sqrt{\frac{2k_B T}{M\alpha}} \int_0^t \left(1 - e^{-\alpha(t-t')}\right) dW(t'). \tag{2.115}$$

The mean square position can be calculated as

$$\langle x^2(t)\rangle = \frac{\langle v_0^2\rangle}{\alpha^2}(1 - e^{-\alpha t})^2 + \frac{2k_B T}{M\alpha} \int_0^t \left(1 - e^{-\alpha(t-t')}\right)^2 dt', \tag{2.116}$$

and after performing the integral we get

$$\begin{aligned} \langle x^2(t)\rangle &= \left[\langle v_0^2\rangle - \frac{k_B T}{M}\right] \left(\frac{1 - e^{-\alpha t}}{\alpha}\right)^2 + \frac{2k_B T}{M\alpha} \left[t - \frac{1 - e^{-\alpha t}}{\alpha}\right] \\ &= \frac{2k_B T}{M\alpha} t + \frac{\langle v_0^2\rangle}{\alpha^2}(1 - e^{-\alpha t})^2 - \frac{k_B T}{M\alpha^2}(3 - 4e^{-\alpha t} + e^{-2\alpha t}). \end{aligned} \tag{2.117}$$

Asymptotically, i.e., as $t \to \infty$, we recover the diffusive behavior

$$\langle x^2(t)\rangle \underset{t\to\infty}{\propto} 2Dt, \tag{2.118}$$

where $D \equiv k_B T/M\alpha = k_B T/\gamma$ is the diffusion coefficient. Comparing with the result obtained in Sec. 2.1.1, it is noted that this result for D is nothing more than the Einstein relation, Eq. (2.9), for the motion of the Brownian particle. For short periods of time, it is easy to show, by expanding the exponentials in Taylor series up to the first order, that the Ornstein-Uhlenbeck process approaches the ballistic behavior of the particle, that is:

$$\langle x(t)\rangle = \langle v_0\rangle t \quad \text{and} \quad \langle x^2(t)\rangle = \langle v_0^2\rangle t^2. \tag{2.119}$$

Let us consider the stationary regime ($t \to \infty$), in this case the Brownian particle has reached the equilibrium and then its velocity does not depend on time, thus $\langle v_0^2\rangle = \langle v^2\rangle = k_B T/M$. Inserting this in (2.117), yields

$$\langle x^2(t)\rangle = \frac{2k_B T}{M\alpha} \left[t - \frac{1 - e^{-\alpha t}}{\alpha}\right]. \tag{2.120}$$

This is the mean square position if we start to observe the position of the Brownian particle after a time long enough for its velocity to have reached the equilibrium.

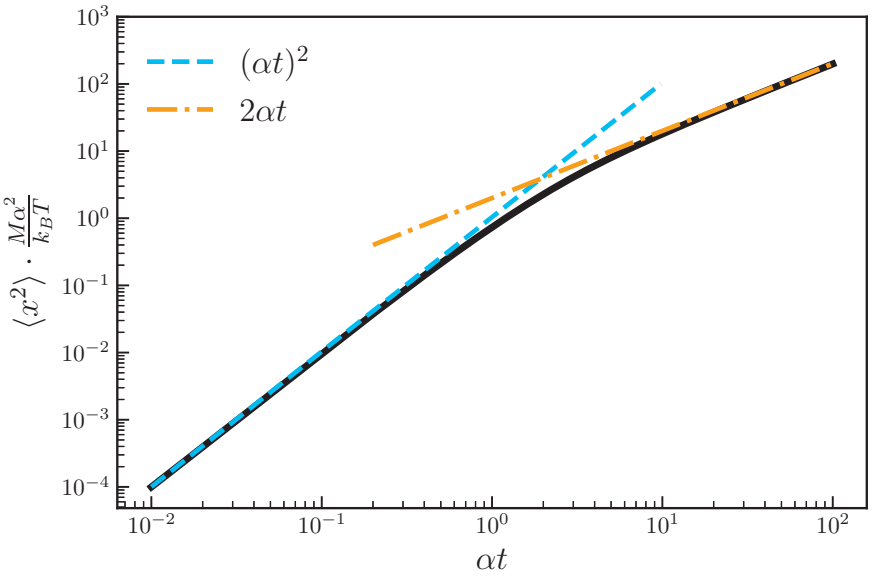


FIGURE 4 – Transition of a Brownian particle in thermal equilibrium, i.e., $\langle v_0^2\rangle = k_BT/M$, from the ballistic regime, $\langle x^2\rangle \propto t^2$, to the diffusive regime, $\langle x^2\rangle \propto t$.

Figure 4 shows the behavior of the function (2.120). Note that for short times ($\alpha t < 1$), the mean square displacement follows a t^2 law as a consequence of the particle's ballistic behavior. At $\alpha t \sim 1$, we can see a transition to diffusive behavior, where we have a linear relationship with t, as predicted by Einstein for the behavior of a Brownian particle.

Furthermore, let us analyze the distribution function for the position of the Brownian particle. Let us define the deviation from the mean

$$u(t) := x(t) - \langle x(t)\rangle = x(t) - \frac{v_0}{\alpha}(1-e^{-\alpha t}) = \sqrt{\frac{2\alpha k_BT}{M}}\int_0^t dt' e^{-\alpha t'}\int_0^{t'} e^{\alpha t''}dW(t''), \quad (2.121)$$

where we are taking $\langle v_0\rangle = v_0$ fixed. We find the following for the mean and the variance:

$$\begin{aligned} &\langle u(t)\rangle = 0 \\ &\sigma_x^2(t) := \langle u(t)^2\rangle = \frac{2v_0^2}{\alpha}t - \frac{v_0^2}{\alpha^2}(3 - 4e^{-\alpha t} + e^{-2\alpha t}), \end{aligned} \quad (2.122)$$

where we have used the result in Eq. (2.117). Since the sum of Gaussian distributions is also a Gaussian distribution, these values completely determine the conditional probability $p(x,t|x_0,0)$. Taking $p(x_0,0) = \delta(x_0)$, yields

$$p(x,t) = \frac{1}{\sqrt{2\pi\sigma_x^2(t)}}\exp\left\{-\frac{\left[x - \frac{v_0}{\alpha}(1-e^{-\alpha t})\right]^2}{2\sigma_x^2(t)}\right\}. \quad (2.123)$$

Taking the asymptotic limit $t \to \infty$ and considering $v_0 = \sqrt{k_BT/M} \equiv v_T$, we find the equilibrium position distribution

$$p(x,t) \underset{t\to\infty}{=} \frac{1}{\sqrt{4\pi Dt}}\exp\left[-\frac{\left(x - \frac{v_TM}{\gamma}\right)^2}{4Dt}\right], \quad (2.124)$$

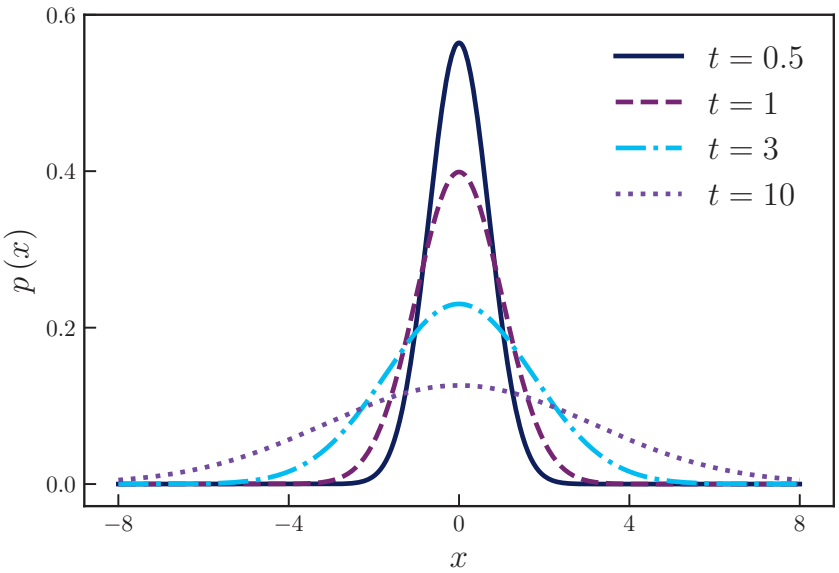


FIGURE 5 – Equilibrium position distribution, Eq. (2.124), for the case when $\gamma \to \infty$ and $D = 1/2$ for four different values of time t. This distribution corresponds to the distribution of the Wiener process $W(t)$.

where $D = k_B T/\gamma$ is the diffusion coefficient, as shown before. From (2.124), we can see that the position process is not stationary as $t \to \infty$, unlike the velocity process. It can also be noted that in the limit $\gamma \to \infty$ while keeping $D = k_B T/\gamma$ fixed, the distribution becomes a Wiener process $W(\tilde{t})$ with standard deviation $\sigma = \sqrt{\tilde{t}} = \sqrt{2Dt}$ and, as we have seen from the self-similarity property, $W(\tilde{t}) = \sqrt{2D}\, W(t)$. Keeping D fixed implies that we need to increase the temperature so that the thermal energy counterbalances the decrease in the Brownian particle's velocity due to the increase in the viscosity coefficient γ.

In Fig. 5, we can see the equilibrium position distribution with $\gamma \to \infty$ and $D = 1/2$ for some different values of time, which corresponds exactly to the distribution for the Wiener process $W(t)$.

3 QUANTUM MECHANICS AS STOCHASTIC PROCESS

This section describes the formulation of non-relativistic quantum mechanics as a stochastic process. The central concept, introduced by the Hungarian physicist Imre Fényes in 1952 [3] and further developed by the American mathematician Edward Nelson in 1966 [4], posits that every particle is subject to a random background perturbation modeled as a Wiener process.

Typically, a physical problem is understood to have three components: the system of interest, the environment in which it exists, and the interactions between the two. In most physical models, the interactions between a system and its environment are disregarded. This simplification is based on the often-implicit assumption that these interactions are insignificant. Under this assumption, the dynamics of the system alone determine the solution to the problem. However, the core argument of Nelson's 1966 work is that this conventional approach is inadequate for quantum phenomena [4, 44]. The foundation of this alternative view is that for quantum particles, environmental perturbations, unavoidably present due to background fluctuations, are not negligible. On the contrary, they must be considered fundamental to the description of quantum behavior. Because these perturbations cannot be known in detail, their statistical properties must be analyzed in a manner analogous to the treatment of Brownian motion [4, 54, 55].

Following this initial hypothesis, quantum mechanics can be formulated through a forward SDE for the particle's position, expressed by

$$d\mathbf{x}(t) = \mathbf{v}_+(\mathbf{x}, t)dt + \sigma d\mathbf{W}(t), \tag{3.1}$$

where $\mathbf{v}_+$ is the forward velocity and $d\mathbf{W}(t)$ is an increment of the forward Wiener process that was discussed in the last chapter. The process $\mathbf{W}(t)$ is independent of all $\mathbf{x}(s)$ with $t > s$. The factor σ is a constant amplitude of the fluctuation term. Additionally, another SDE must be introduced in order to recover the time symmetry of quantum mechanics:

$$d\mathbf{x}(t) = \mathbf{v}_-(\mathbf{x}, t)dt + \sigma d\mathbf{W}_*(t), \tag{3.2}$$

where $\mathbf{v}_-$ is the backward velocity and $d\mathbf{W}_*(t)$ is an increment of the backward Wiener process $\mathbf{W}_*(t)$. The process $\mathbf{W}_*(t)$ has the same properties of the Wiener process but reversed in time, such that $\mathbf{W}_*(t)$ is independent of all $\mathbf{x}(s)$ with $t < s$.

Equations (3.1) and (3.2) are shorthand representations of the stochastic processes defined as

$$\begin{aligned} \mathbf{x}(t) &= \mathbf{x}(0) + \int_0^t \mathbf{v}_+(\mathbf{x}, t')\, dt' + \sigma \mathbf{W}(t), \\ \mathbf{x}(0) &= \mathbf{x}_0 \in \mathbb{R}^d, \end{aligned} \tag{3.3}$$

for the forward process. Recall that $\mathbf{W}(0) = 0$ from the definition of the Wiener process. We say that the forward Wiener process $\mathbf{W}(t)$ is adapted to the filtration $\{\,\mathcal{F}_t^-\,\}_{t\geq 0}$, where $\mathcal{F}_t^-$ is the σ-algebra induced by the past history of the particle: $\{\,\mathbf{x}(s);\ 0 \leq s \leq t\,\}$. We can think that the process $\mathbf{W}(t)$ only has information about the past of the trajectory. The backward process is analogously given by

$$\begin{aligned} \mathbf{x}(t) &= \mathbf{x}(T) - \int_t^T \mathbf{v}_-(\mathbf{x}, t')\, dt' + \sigma[\mathbf{W}_*(t) - \mathbf{W}_*(T)], \\ \mathbf{x}(T) &= \mathbf{x}_T(\omega) \in \mathbb{R}^d, \end{aligned} \tag{3.4}$$

where the terminal condition $\mathbf{x}_T$ is the final point of the forward trajectory, with its value being subjected to randomness indicated by the dependence on ω. The backward Wiener process $\mathbf{W}_*(t)$ is adapted to the filtration $\{\,\mathcal{F}_t^+\,\}_{t\leq T}$, where $\mathcal{F}_t^+$ is the σ-algebra induced by the future of the particle: $\{\,\mathbf{x}(s);\ t \leq s \leq T\,\}$. The process $\mathbf{W}_*(t)$ can be thought as only having information about the future, or the past of the time-reversed trajectory.

Note that the process $\mathbf{x}(t)$ should be the same in both processes defined in Eqs. (3.1) and (3.2). Consequently, the following relation holds [56].

Corollary 1 *Suppose the process* $\mathbf{x}(t)$ *is the solution of Eqs.* (3.1) *and* (3.2)*, then*

$$\mathbf{W}_*(t_1) - \mathbf{W}_*(t_0) = \frac{1}{\sigma}\int_{t_0}^{t_1} \Big[\mathbf{v}_+\Big(\mathbf{x}(t), t\Big) - \mathbf{v}_-\Big(\mathbf{x}(t), t\Big)\Big] dt + \mathbf{W}(t_1) - \mathbf{W}(t_0)$$

is fulfilled for $t_1 \geq t_0 \geq 0$.

Now, let us introduce the hydrodynamical formalism for quantum mechanics, also known as *Conservative Diffusion Process*, proposed by Edward Nelson [4, 5].

3.1 STOCHASTIC QUANTUM DYNAMICS

First, we introduce the notion of the forward and backward mean derivatives. As established in the previous chapter, stochastic processes are continuous yet nowhere differentiable (Theorem 1). Although a conventional derivative cannot be defined for such processes, it is possible to introduce a generalized notion of differentiation appropriate for stochastic dynamics. The issue of non-differentiable trajectories in quantum mechanics was already noted by Heisenberg in 1927 [57], who pointed out that the indeterminacy inherent in quantum phenomena prevents the definition of sharply defined particle paths.

Let $\mathbf{x}(t)$ be a Markov stochastic process governed by an SDE like the one in (3.1). The mean forward time derivative of a function $f(\mathbf{x}(t), t)$ is defined as

$$D_+ f(\mathbf{x}, t) = \lim_{\Delta t \to 0} \mathbb{E}\left[\frac{f\Big(\mathbf{x}(t+\Delta t), t+\Delta t\Big) - f\Big(\mathbf{x}(t), t\Big)}{\Delta t}\,\middle|\, \mathbf{x}(t)\right], \tag{3.5}$$

where the average is conditional on the known position $\mathbf{x}(t)$. Similarly, the mean backward time derivative takes the form

$$D_- f(\mathbf{x},t) = \lim_{\Delta t\to 0} \mathbb{E}\left[\frac{f\Big(\mathbf{x}(t),t\Big) - f\Big(\mathbf{x}(t-\Delta t),t-\Delta t\Big)}{\Delta t}\middle|\mathbf{x}(t)\right]. \tag{3.6}$$

As Nelson showed, these derivatives satisfy a theorem analogous to the product rule for conventional derivatives [54].

Theorem 3 (Nelson) *Let X_t, $-\infty < t < \infty$, be a stochastic process with continuous mean forward and backward derivatives. Let f and g be real valued functions defined on such that $X_t, D_+f(X_t,t)$ and $D_-g(X_t,t)$ belong to $L^2(\Omega,\mathcal{B},P)$ (the space of functions of X_t with finite second moment), and the mappings $t \mapsto X_t, D_+f(X_t,t)$ and $D_-g(X_t,t)$ are continuous. Then we have*

$$\frac{d}{dt}\mathbb{E}\{f(X_t,t)g(X_t,t)\} = \mathbb{E}\{[D_+f(X_t,t)]g(X_t,t) + f(X_t,t)D_-g(X_t,t)\}.$$

Using Itô's formula (2.81), together with the forward SDE (3.1), the mean forward derivative can be expressed as

$$D_+ f(\mathbf{x},t) = \left(\frac{\partial}{\partial t} + \mathbf{v}_+\cdot\nabla + \frac{\sigma^2}{2}\nabla^2\right) f(\mathbf{x},t). \tag{3.7}$$

Applying again Itô's formula, but now together with the backward SDE (3.2), the mean backward derivative can be written as

$$D_- f(\mathbf{x},t) = \left(\frac{\partial}{\partial t} + \mathbf{v}_-\cdot\nabla - \frac{\sigma^2}{2}\nabla^2\right) f(\mathbf{x},t). \tag{3.8}$$

where we used $(d\mathbf{W}_*)^2 \to -dt$, since in the backward trajectory $dt < 0$ and we shall require that $\mathrm{var}[d\mathbf{W}_*(t)] > 0$.

From Theorem 3 with $f = f(\mathbf{x})$ and $g = 1$, we obtain

$$\frac{d}{dt}\mathbb{E}[f(\mathbf{x})] = \mathbb{E}[D_+f(\mathbf{x})] = \mathbb{E}\left[\left(\mathbf{v}_+\cdot\nabla + \frac{\sigma^2}{2}\nabla^2\right) f(\mathbf{x})\right]. \tag{3.9}$$

Now, making the substitution $f = 1$ and $g = g(\mathbf{x})$, we get

$$\frac{d}{dt}\mathbb{E}[g(\mathbf{x})] = \mathbb{E}[D_-g(\mathbf{x})] = \mathbb{E}\left[\left(\mathbf{v}_-\cdot\nabla - \frac{\sigma^2}{2}\nabla^2\right) g(\mathbf{x})\right]. \tag{3.10}$$

The average can be explicitly expressed in Eqs. (3.9) and (3.10) to obtain

$$\begin{aligned}\frac{d}{dt}\int f(\mathbf{x})p(\mathbf{x},t)d\mathbf{x} &= \int\left[\left(\mathbf{v}_+\cdot\nabla + \frac{\sigma^2}{2}\nabla^2\right) f(\mathbf{x})\right] p(\mathbf{x},t)d\mathbf{x} \\ &= \int f(\mathbf{x})\left\{-\nabla\cdot[\mathbf{v}_+p(\mathbf{x},t)] + \frac{\sigma^2}{2}\nabla^2 p(\mathbf{x},t)\right\}d\mathbf{x}\end{aligned} \tag{3.11}$$

and

$$\begin{aligned}\frac{d}{dt}\int g(\mathbf{x})p(\mathbf{x},t)d\mathbf{x} &= \int\left[\left(\mathbf{v}_-\cdot\nabla-\frac{\sigma^2}{2}\nabla^2\right)g(\mathbf{x})\right]p(\mathbf{x},t)d\mathbf{x}\\ &= \int g(\mathbf{x})\left\{-\nabla\cdot[\mathbf{v}_-p(\mathbf{x},t)]-\frac{\sigma^2}{2}\nabla^2p(\mathbf{x},t)\right\}d\mathbf{x},\end{aligned} \tag{3.12}$$

where we have applied integration by parts with vanishing boundary terms. Since f and g are arbitrary functions, the following relations hold:

$$\frac{\partial p}{\partial t} = -\nabla\cdot(\mathbf{v}_+p)+\frac{\sigma^2}{2}\nabla^2p, \tag{3.13}$$

$$\frac{\partial p}{\partial t} = -\nabla\cdot(\mathbf{v}_-p)-\frac{\sigma^2}{2}\nabla^2p, \tag{3.14}$$

where we have omitted the dependence on $\mathbf{x}$ and t of the probability distribution p. Equation (3.13) is precisely the forward Fokker–Planck equation associated with the forward process (3.1); while Eq. (3.14) corresponds to the Fokker–Planck equation associated with the backward process (3.2), referred to as the backward Fokker–Planck equation [58]. It is essential to note, however, that this is not equivalent to the Kolmogorov backward equation (2.35) (derived in Appendix B), also referred to as the backward Fokker-Planck equation. The latter describes the conditional probability of the forward process, with derivatives taken with respect to the conditional variables.[1]

We can easily verify that $D_+\mathbf{x}(t)=\mathbf{v}_+(\mathbf{x},t)$ and $D_-\mathbf{x}(t)=\mathbf{v}_-(\mathbf{x},t)$. Then, it is possible to define the *mean* or *current velocity* of the particle by

$$\mathbf{v}(\mathbf{x},t)=\frac{D_+\mathbf{x}(t)+D_-\mathbf{x}(t)}{2}=\frac{\mathbf{v}_+(\mathbf{x},t)+\mathbf{v}_-(\mathbf{x},t)}{2}. \tag{3.15}$$

Since the probability distributions of the forward and backward equations are the same, as they describe the same stochastic time-reversible trajectory, we can sum Eqs. (3.13) and (3.14), yielding

$$\frac{\partial p}{\partial t}+\nabla\cdot(\mathbf{v}p)=0. \tag{3.16}$$

This corresponds to the *continuity equation* for the probability with probability current density given by $\mathbf{j}=\mathbf{v}p$. We can further introduce an additional velocity field–called *osmotic velocity*–defined by

$$\mathbf{u}(\mathbf{x},t)=\frac{D_+\mathbf{x}(t)-D_-\mathbf{x}(t)}{2}=\frac{\mathbf{v}_+(\mathbf{x},t)-\mathbf{v}_-(\mathbf{x},t)}{2}. \tag{3.17}$$

Therefore, subtracting Eq. (3.14) from (3.13), we find

$$\nabla\cdot\left[\mathbf{u}p-\frac{\sigma^2}{2}\nabla p\right]=0. \tag{3.18}$$

[1] To avoid ambiguity: the equation denoted as the backward Fokker–Planck equation (3.14) is associated with the dynamics of the backward stochastic process, while Eq. (2.35) is derived from the forward process and involves differentiation with respect to the z, s variables of the conditional probability density $p(x,t|z,s)$.

This leads to the following expression for $\mathbf{u}$,

$$\mathbf{u}(\mathbf{x},t) = \frac{\sigma^2}{2}\nabla \ln p(\mathbf{x},t). \tag{3.19}$$

Note that the average of the osmotic velocity $\mathbf{u}(\mathbf{x},t)$ vanishes, namely,

$$\mathbb{E}[\mathbf{u}(\mathbf{x},t)] = \frac{\sigma^2}{2}\int p(\mathbf{x},t)\,\nabla \ln p(\mathbf{x},t)\,d\mathbf{x} = \frac{\sigma^2}{2}\int \nabla p(\mathbf{x},t)\,d\mathbf{x} = 0, \tag{3.20}$$

where the last equality follows from the fact that the probability density vanishes as $|\mathbf{x}| \to \infty$. This result expresses a fundamental property of the osmotic velocity: although it locally describes the diffusive motion of particles due to spatial variations in the probability density, its global average is zero. In other words, the osmotic component represents a purely dispersive contribution, without producing any net drift in the ensemble. This behavior contrasts with the current velocity, $\mathbf{v}(\mathbf{x},t)$, whose average reflects the net flux of particles.

The continuity equation (3.16) can be written in terms of the velocity fields $\mathbf{v}$ and $\mathbf{u}$. First, from Eq. (3.16) it follows that

$$\begin{aligned} \frac{\partial p}{\partial t} = -\nabla\cdot(p\mathbf{v}) \implies \frac{\partial}{\partial t}\ln p &= -\frac{1}{p}\nabla\cdot(p\mathbf{v}) \\ &= -\mathbf{v}\cdot\nabla \ln p - \nabla\cdot\mathbf{v}. \end{aligned} \tag{3.21}$$

By applying the gradient on both sides, we obtain

$$\frac{2}{\sigma^2}\frac{\partial \mathbf{u}}{\partial t} = \nabla\left(-\frac{2}{\sigma^2}\mathbf{v}\cdot\mathbf{u} - \nabla\cdot\mathbf{v}\right), \tag{3.22}$$

which results in

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla(\mathbf{v}\cdot\mathbf{u}) + \frac{\sigma^2}{2}\nabla(\nabla\cdot\mathbf{v}) = 0. \tag{3.23}$$

We can also define two mean accelerations, the first is called *advective acceleration* and is defined as

$$\mathbf{a}_{\text{adv}} = \frac{1}{2}\left[D_+D_- + D_-D_+\right]\mathbf{x}(t) = \frac{D_+\mathbf{v}_- + D_-\mathbf{v}_+}{2}. \tag{3.24}$$

The second is called *diffusive acceleration* and is defined as

$$\mathbf{a}_{\text{diff}} = \frac{1}{2}\left[D_+D_+ - D_-D_-\right]\mathbf{x}(t) = \frac{D_+\mathbf{v}_+ - D_-\mathbf{v}_-}{2}. \tag{3.25}$$

From Eqs. (3.7) and (3.8), we find

$$\mathbf{a}_{\text{adv}} = \frac{\partial \mathbf{v}}{\partial t} + \frac{1}{2}\mathbf{v}_+\cdot\nabla\mathbf{v}_- + \frac{1}{2}\mathbf{v}_-\cdot\nabla\mathbf{v}_+ - \frac{\sigma^2}{2}\nabla^2\mathbf{u}. \tag{3.26}$$

Expanding the drift terms, $\mathbf{v}_\pm = \mathbf{v} \pm \mathbf{u}$, yields

$$\mathbf{v}_+\cdot\nabla\mathbf{v}_- = (\mathbf{v}+\mathbf{u})\cdot\nabla(\mathbf{v}-\mathbf{u}) = \mathbf{v}\cdot\nabla\mathbf{v} - \mathbf{v}\cdot\nabla\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{v} - \mathbf{u}\cdot\nabla\mathbf{u}, \tag{3.27}$$

$$\mathbf{v}_-\cdot\nabla\mathbf{v}_+ = (\mathbf{v}-\mathbf{u})\cdot\nabla(\mathbf{v}+\mathbf{u}) = \mathbf{v}\cdot\nabla\mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{u} - \mathbf{u}\cdot\nabla\mathbf{v} - \mathbf{u}\cdot\nabla\mathbf{u}. \tag{3.28}$$

Summing these two equations leads to

$$\frac{1}{2}(\mathbf{v}_+ \cdot \nabla \mathbf{v}_- + \mathbf{v}_- \cdot \nabla \mathbf{v}_+) = \mathbf{v} \cdot \nabla \mathbf{v} - \mathbf{u} \cdot \nabla \mathbf{u}, \tag{3.29}$$

so that the advective acceleration can be written as

$$\mathbf{a}_{\text{adv}} = \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} - \mathbf{u} \cdot \nabla \mathbf{u} - \frac{\sigma^2}{2} \nabla^2 \mathbf{u}. \tag{3.30}$$

Similarly, for the diffusive acceleration, we obtain

$$\mathbf{a}_{\text{diff}} = \frac{\partial \mathbf{u}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{v} + \frac{\sigma^2}{2} \nabla^2 \mathbf{v}. \tag{3.31}$$

Since $p(\mathbf{x}, t)$ is invariant under time reversal, it follows from (3.16) and (3.19) that, under the transformation $t \to -t$, the velocity fields transform as $\mathbf{v} \to -\mathbf{v}$ and $\mathbf{u} \to \mathbf{u}$. This indicates that $\mathbf{v}$ represents a true velocity field, whereas $\mathbf{u}$ behaves as a pseudo-velocity field. Similarly, under time reversal, the accelerations transform as $\mathbf{a}_{\text{adv}} \to \mathbf{a}_{\text{adv}}$ and $\mathbf{a}_{\text{diff}} \to -\mathbf{a}_{\text{diff}}$. Hence, $\mathbf{a}_{\text{adv}}$ exhibits the expected behavior of a true acceleration, while $\mathbf{a}_{\text{diff}}$ is a sort of pseudo-acceleration. To ensure a time-reversible dynamics, we thus require that

$$\mathbf{a}_{\text{diff}} = 0. \tag{3.32}$$

Consequently, from Eqs. (3.31) and (3.32), we obtain our first dynamical equation:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{v} + \frac{\sigma^2}{2} \nabla^2 \mathbf{v} = 0. \tag{3.33}$$

Now, considering the following identity

$$\nabla(\mathbf{m} \cdot \mathbf{n}) = \mathbf{m} \cdot \nabla \mathbf{n} + \mathbf{n} \cdot \nabla \mathbf{m} + \mathbf{m} \times (\nabla \times \mathbf{n}) + \mathbf{n} \times (\nabla \times \mathbf{m}), \tag{3.34}$$

noting that $\mathbf{u}$ is irrotational, see Eq. (3.19), and from the comparison of Eqs. (3.23) and (3.33) we see that in order for both these equations to be verified, we must have: $\nabla \times \mathbf{v} = 0$. Then, Eq. (3.33) can be written as

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla(\mathbf{u} \cdot \mathbf{v}) + \frac{\sigma^2}{2} \nabla^2 \mathbf{v} = 0. \tag{3.35}$$

Consequently, from the irrotationality of $\mathbf{v}$, we can express

$$\mathbf{v} \propto \nabla S(\mathbf{x}, t), \tag{3.36}$$

which can be interpreted as a direct consequence of time-reversibility [59]. A related discussion is given in Ref. [60], where it is shown that postulating that $\mathbf{v}$ is irrotational leads to Eq. (3.32). In contrast, here we have argued on physical grounds (from time-reversal symmetry) that Eq. (3.32) must hold, which in turn implies that $\mathbf{v}$ is irrotational.

Our next step is to take the curl of Eq. (3.30). Noting that both $\mathbf{u}$ and $\mathbf{v}$ are curl-free, we obtain

$$\nabla \times \mathbf{a}_{\text{adv}} = 0 \tag{3.37}$$

which implies that

$$\mathbf{a}_{\text{adv}} = \nabla\varphi(\mathbf{x}) \tag{3.38}$$

where $\varphi(\mathbf{x})$ is an arbitrary function. Thus, combining Eqs. (3.30) and (3.38), we obtain our second dynamical equation:

$$\frac{\partial \mathbf{v}}{\partial t} + \frac{1}{2}\nabla\mathbf{v}^2 - \frac{1}{2}\nabla\mathbf{u}^2 - \frac{\sigma^2}{2}\nabla^2\mathbf{u} = \nabla\varphi. \tag{3.39}$$

So far, we have obtained two dynamical equations governing the motion of a particle described by the stochastic trajectories, namely Eqs. (3.1) and (3.2). We are now in a position to establish the link between these stochastic equations and the standard formulation of quantum mechanics.

3.1.1 Hydrodynamic Equations

Recall that the two dynamical equations governing the conservative Brownian motion that preserves time-reversal symmetry, as derived above, are

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} &= -\frac{\sigma^2}{2}\nabla^2\mathbf{v} - \nabla\left(\mathbf{v}\cdot\mathbf{u}\right), \\ \frac{\partial \mathbf{v}}{\partial t} &= -\frac{1}{2}\nabla\mathbf{v}^2 + \frac{1}{2}\nabla\mathbf{u}^2 + \frac{\sigma^2}{2}\nabla^2\mathbf{u} + \nabla\varphi. \end{aligned} \tag{3.40}$$

Since both $\mathbf{u}$ and $\mathbf{v}$ are irrotational, then they can be expressed as the gradient of scalar functions,

$$\mathbf{u}(\mathbf{x},t) = \sigma^2\nabla R(\mathbf{x},t), \tag{3.41}$$

$$\mathbf{v}(\mathbf{x},t) = \frac{1}{m}\nabla S(\mathbf{x},t), \tag{3.42}$$

where m is the mass of the particle performing the Brownian motion. Note that this new definition for $\mathbf{u}$ is equivalent to setting $p = \exp(2R)$ in Eq. (3.19). Inserting these definitions for $\mathbf{u}$ and $\mathbf{v}$ into Eqs. (3.40) and rearranging the terms, we obtain

$$\begin{aligned} \sigma^2\nabla\left(\frac{\partial R}{\partial t} + \frac{1}{2m}\nabla^2 S + \frac{1}{m}\nabla R\cdot\nabla S\right) &= 0, \\ \frac{1}{m}\nabla\left(\frac{\partial S}{\partial t} - m\varphi + \frac{1}{2m}(\nabla S)^2 - \frac{m\sigma^4}{2}\left[(\nabla R)^2 + \nabla^2 R\right]\right) &= 0, \end{aligned} \tag{3.43}$$

that results in

$$\frac{\partial R}{\partial t} + \frac{1}{2m}\nabla^2 S + \frac{1}{m}\nabla R\cdot\nabla S = 0, \tag{3.44}$$

$$\frac{\partial S}{\partial t} - m\varphi + \frac{1}{2m}(\nabla S)^2 - \frac{m\sigma^4}{2}\left[(\nabla R)^2 + \nabla^2 R\right] = 0. \tag{3.45}$$

Equations (3.44) and (3.45) determine R and S up to a position-independent phase $\phi(t)$ in the scalar field S, once R is fixed through the normalization of the probability p. These equations represent the stochastic counterpart of the hydrodynamic formulation of Newtonian mechanics [44]. Notice that, for $\sigma = 0$ and $\varphi = -V/m$, Eq. (3.45) reduces to the classical Hamilton–Jacobi equation [61], while Eq. (3.44) corresponds precisely to the continuity equation for probability conservation (3.16), expressed in terms of the functions R and S.

3.1.2 Madelung Equations

If we start with the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)\Psi(\mathbf{x},t) \tag{3.46}$$

and write the wave function Ψ in the polar form

$$\Psi(\mathbf{x},t) = \exp\!\left(R(\mathbf{x},t) + \frac{i}{\hbar}S(\mathbf{x},t)\right), \tag{3.47}$$

where $R(\mathbf{x},t)$ and $S(\mathbf{x},t)$ are real functions related respectively to the probability density and to the phase of the particle, then we get

$$\begin{aligned}\left(i\hbar\frac{\partial R}{\partial t} - \frac{\partial S}{\partial t}\right)\Psi = \\ -\frac{\hbar^2}{2m}\left(\nabla^2 R + \frac{i}{\hbar}\nabla^2 S + (\nabla R)^2 + \frac{2i}{\hbar}\nabla R\cdot\nabla S - \frac{1}{\hbar^2}(\nabla S)^2\right)\Psi + V\Psi.\end{aligned} \tag{3.48}$$

Dividing both sides of the above expression by Ψ and separating the real and imaginary parts, yields

$$\frac{\partial R}{\partial t} = -\frac{1}{2m}\nabla^2 S - \frac{1}{m}\nabla R\cdot\nabla S, \tag{3.49}$$

$$\frac{\partial S}{\partial t} = \frac{\hbar^2}{2m}\left[\nabla^2 R + (\nabla R)^2\right] - \frac{1}{2m}(\nabla S)^2 - V. \tag{3.50}$$

Equations (3.49) and (3.50) constitute the Madelung flow equations, originally derived by Erwin Madelung (1881-1972) in 1926 [62]. Solving these two coupled, nonlinear, second-order partial differential equations is equivalent to solving the Schrödinger equation (3.46) for the ground state of stationary problems, i.e., node-free wavefunctions. The excited states of the bound spectrum are obtained iteratively through a supersymmetric procedure, as illustrated later in Sec. 3.5, where it is possible to transform the excited states into nodeless ground states by iteratively changing the potential.

From the Madelung equations, the function $S(x,t)$ (the phase of the wave function) cannot be completely determined. This issue was first pointed out by Wallstrom [6, 63]. It leads to multi-valued wave functions and therefore requires the imposition of an *ad hoc*

quantization condition on the current velocity $\mathbf{v}$ in order to recover the correct single-valued solution of the Schrödinger equation. Therefore, the Madelung formulation admits a wider range of possible solutions [6] and, as discussed in [18, 63, 64], the Schrödinger equation can be viewed as a particular simplification of the more general Madelung equations. However, there are several suggested answers to the Wallstrom criticism, as this problem is known, one of them is the *Zitterbewegung Hypothesis* [65], which assumes that a spinless particle undergoes a steady-state oscillation at the Compton frequency ($\omega_c = mc^2/\hbar$) in its instantaneous rest frame, naturally leading to the quantization of the phase S and the single-valued wave function. Other analyses have argued that appropriate regularity, topological, or variational considerations remove the spurious solutions; see, e.g., Ref. [66].

Comparing Eq. (3.44) with (3.49), we see that they are identical. Similarly, comparing Eq. (3.45) with (3.50), we find that they coincide provided we define

$$\sigma^2 = \frac{\hbar}{m}, \tag{3.51}$$

and

$$\varphi(\mathbf{x}) = -\frac{V(\mathbf{x})}{m}. \tag{3.52}$$

Therefore, we can conclude that the two SDEs in (3.1) and (3.2), together with the definition of the mean derivatives $D_\pm$, and the conditions $\mathbf{a}_{\text{diff}} = 0$ and $\mathbf{a}_{\text{adv}} = \nabla\varphi = -\nabla V/m$, reproduce the quantum dynamics, where the probability distribution is obtained from the wave function via the Schrödinger equation using the Born rule, $p = |\Psi|^2$.

Since $\mathbf{v}_\pm = \mathbf{v} \pm \mathbf{u}$, and employing Eqs. (3.19) and (3.42) for $\mathbf{u}$ and $\mathbf{v}$, the forward and backward SDEs describing the dynamics of the quantum particle can be written as

$$\begin{aligned} d\mathbf{x}(t) &= \left(\frac{\nabla S(\mathbf{x},t)}{m} + \frac{\hbar}{2m}\nabla \ln p(\mathbf{x},t)\right) dt + \sqrt{\frac{\hbar}{m}} d\mathbf{W}(t), \\ d\mathbf{x}(t) &= \left(\frac{\nabla S(\mathbf{x},t)}{m} - \frac{\hbar}{2m}\nabla \ln p(\mathbf{x},t)\right) dt + \sqrt{\frac{\hbar}{m}} d\mathbf{W}_*(t), \end{aligned} \tag{3.53}$$

where S and p can be obtained direct from the wave function written in the form $\Psi(\mathbf{x},t) = \sqrt{p(\mathbf{x},t)}\exp\left(\frac{i}{\hbar}S(\mathbf{x},t)\right)$. This constitutes Nelson's stochastic quantization.

The description of quantum particle trajectories through forward and backward SDEs is the core of the first hypothesis in Nelson's formalism, which he referred to as *the Hypothesis of Universal Brownian Motion* [4]. The second hypothesis in Nelson's formalism is the generalization of Newton's second law, referred to as the *Newton–Nelson law*. This law states that the mean acceleration, $\mathbf{a} = \mathbf{a}_{\text{adv}}$ (recall that the diffusive acceleration vanishes, leaving only the advective component), defined by

$$\mathbf{a} = \frac{1}{2}\left[D_+D_- + D_-D_+\right]\mathbf{x}(t), \tag{3.54}$$

is related to the potential acting on the particle in the same manner as in Newton's second law, i.e.,

$$\mathbf{a} = -\frac{\nabla V(\mathbf{x})}{m}. \tag{3.55}$$

Note that, in the limit $\hbar/m \to 0$, the classical deterministic equations are immediately recovered.

These two hypotheses are sufficient to formulate non-relativistic spinless quantum mechanics. In Nelson's formulation, the wave function does not occupy the central role it holds in conventional quantum mechanics [67]. Instead, the wave function appears merely as a mathematical construct, and the Schrödinger equation can be interpreted as a compact complex representation of two coupled nonlinear real equations.

To conclude this section, it is worth emphasizing that Nelson's formulation of quantum mechanics can be seen as more than just an alternative interpretation. This formalism provides a fundamentally different way of conceptualizing and computing quantum phenomena. It is not opposed to conventional quantum mechanics but rather complementary, as both formalisms are supposed to yield identical results for problems accessible to either approach. Moreover, Nelson's framework can extend beyond the reach of the conventional formalism, perhaps offering insights into problems where standard methods encounter difficulties.

Within Nelson's formulation, it is also possible to construct a variational principle for quantum mechanics, analogous to the classical Hamilton principle. This topic is addressed in the next section.

3.2 VARIATIONAL PRINCIPLE

Hamilton's principle, the cornerstone of classical mechanics, asserts that the actual trajectory of a system extremizes the action functional. Extending this principle to quantum mechanics has motivated numerous approaches, among which Nelson's stochastic mechanics [4] offers a particularly transparent picture, as we have seen. Pavon's works [15, 68] have shown that the osmotic and current velocities, present in Nelson's formalism, can be derived from a variational method.

The derivation of Pavon's variational principle proceeds by defining appropriate stochastic action and entropy production functionals, introducing Lagrange multipliers that enforce Nelson's stochastic dynamics as a constraint, and solving the resulting saddle-point problems [15]. First, let us state the Lagrange Lemma, which will be useful in the next derivations [15].

Lemma 1 (Lagrange) *Let Y be an arbitrary set. Suppose that $C \subset Y$ is a non-empty subset, and let $I : Y \to \mathbb{R}$ be a function. Consider also a functional $\Lambda : Y \to \mathbb{R}$, and let*

$y_0 \in Y$ be a global minimum of $I + \Lambda$ over Y. Assume that $\Lambda(y_0)$ is finite and constant for all $y \in C$. Then, if $y_0 \in C$, it follows that y_0 minimizes I over C.

Proof: For any $y \in C$, we have

$$I(y_0) + \Lambda(y_0) \leq I(y) + \Lambda(y) = I(y) + \Lambda(y_0).$$

Hence,

$$I(y_0) \leq I(y),$$

which proves the claim.

A functional Λ that is constant and finite over C is called a *Lagrange functional*.

Along the following calculations, we shall assume that the so-called *finite energy conditions* are satisfied, namely,

$$\mathbb{E}\left\{\int_{t_0}^{t_1} |\mathbf{v}(\mathbf{x},t)|^2 dt\right\} < \infty, \tag{3.56}$$

$$\mathbb{E}\left\{\int_{t_0}^{t_1} |\mathbf{u}(\mathbf{x},t)|^2 dt\right\} < \infty. \tag{3.57}$$

These conditions ensure that the stochastic process $\mathbf{x}(t)$, with its associated current velocity $\mathbf{v}$ and osmotic velocity $\mathbf{u}$, possesses finite second moments. This guarantees that the subsequent manipulations of expectations and variational principles are mathematically well defined.

3.2.1 Saddle-Point Action Principle

Let $\mathbf{x} = \mathbf{x}(t)$ be a stochastic process, with $\mathbf{v} = \mathbf{v}(\mathbf{x}(t), t)$ denoting its current velocity and $\mathbf{u} = \mathbf{u}(\mathbf{x}(t), t)$ its osmotic velocity. We define the stochastic action over the interval $[t_1, t_2]$ as

$$I(\mathbf{x}, \mathbf{v}, \mathbf{u}) = \mathbb{E}\left\{\int_{t_1}^{t_2} \left[\frac{1}{2}m\mathbf{v}^2 - \frac{1}{2}m\mathbf{u}^2 - V(\mathbf{x})\right] dt + S(\mathbf{x}(t_1), t_1)\right\}, \tag{3.58}$$

where V is the potential and S is a continuous function related with the initial condition at t_1. This action coincides with the action that was introduced by Guerra and Morato [69]. Let us consider the following stochastic control problem:

$$\min_{\mathbf{v}} \max_{\mathbf{u}} \; I(\mathbf{x}, \mathbf{v}, \mathbf{u}) \tag{3.59}$$

subjected to the dynamical constraints

$$\begin{aligned} d\mathbf{x}(t) &= (\mathbf{v} + \mathbf{u})dt + \sigma d\mathbf{W}(t), \\ d\mathbf{x}(t) &= (\mathbf{v} - \mathbf{u})dt + \sigma d\mathbf{W}_*(t). \end{aligned} \tag{3.60}$$

That is, a triplet $(\mathbf{x}, \mathbf{v}, \mathbf{u})$ satisfies the constraints (3.60) if and only if $\mathbf{v}$ and $\mathbf{u}$ correspond to the current and osmotic velocities, respectively, of the process $\mathbf{x}$.

The equilibrium solution corresponding to the saddle point $(\mathbf{x}^*, \mathbf{v}^*, \mathbf{u}^*)$ satisfies the following property:

$$I(\mathbf{x}_1, \mathbf{v}^*, \mathbf{u}_1) \;\leq\; I(\mathbf{x}^*, \mathbf{v}^*, \mathbf{u}^*) \;\leq\; I(\mathbf{x}_2, \mathbf{v}_2, \mathbf{u}^*). \tag{3.61}$$

We now proceed to generalize the Lagrange Lemma to the context of saddle-point problems. The validity of this generalization can be readily established by employing the same arguments used in the proof of the extremization problem.

Let us introduce a class of Lagrangian functionals suitable for our problem. Let $F, G : \mathbb{R}^n \times [t_1, t_2] \to \mathbb{R}$ be two arbitrary functions, continuous and at least twice differentiable. We define

$$\begin{aligned}\Lambda^{F,G}(\mathbf{x}, \mathbf{v}, \mathbf{u}) = \mathbb{E}\Bigg\{ \int_{t_1}^{t_2} \left[m\sigma^2 \mathbf{u} \cdot \nabla F + \frac{m\sigma^4}{2} \nabla^2 F - \frac{\partial G}{\partial t} - \mathbf{v} \cdot \nabla G \right] (\mathbf{x}(t), t) dt \\ + G(\mathbf{x}(t_2), t_2) - G(\mathbf{x}(t_1), t_1) \Bigg\},\end{aligned} \tag{3.62}$$

as the Lagrange functional for our problem. The terms involving F in the Lagrange functional yield

$$\begin{aligned}&\mathbb{E}\left\{ \int_{t_1}^{t_2} \left[m\sigma^2 \mathbf{u} \cdot \nabla F + \frac{m\sigma^4}{2} \nabla^2 F \right] (\mathbf{x}(t), t) dt \right\} \\ &\qquad = \int_{t_1}^{t_2} \int_{\mathbb{R}^n} \left[m\sigma^2 \mathbf{u} \cdot \nabla F + \frac{m\sigma^4}{2} \nabla^2 F \right] p(\mathbf{x}, t) d\mathbf{x} dt \\ &\qquad = \int_{t_1}^{t_2} \int_{\mathbb{R}^n} F \left[-m\sigma^2 \nabla \cdot (p\mathbf{u}) + \frac{m\sigma^4}{2} \nabla^2 p \right] d\mathbf{x} dt,\end{aligned} \tag{3.63}$$

where we have applied integration by parts, assuming that the boundary terms vanish due to the condition $p(\mathbf{x}, t) \to 0$ as $|\mathbf{x}| \to \infty$. Moreover, the terms between the square brackets vanish once we apply the dynamical relation $\mathbf{u} = \frac{\sigma^2}{2} \nabla \ln p$ which was derived in the previous section as a fundamental consequence of the constraints (3.60). Otherwise, the terms in the Lagrange functional involving G yield

$$\begin{aligned}&\mathbb{E}\left\{ \int_{t_1}^{t_2} \left[-\frac{\partial G}{\partial t} - \mathbf{v} \cdot \nabla G \right] (\mathbf{x}(t), t) dt + G(\mathbf{x}(t_2), t_2) - G(\mathbf{x}(t_1), t_1) \right\} \\ &\qquad = \int_{t_1}^{t_2} \int_{\mathbb{R}^n} \left[-\frac{\partial G}{\partial t} - \mathbf{v} \cdot \nabla G \right] p(\mathbf{x}, t) d\mathbf{x} dt \\ &\qquad + \int_{\mathbb{R}^n} G(\mathbf{x}(t_2), t_2) p(\mathbf{x}, t_2) d\mathbf{x} - \int_{\mathbb{R}^n} G(\mathbf{x}(t_1), t_1) p(\mathbf{x}, t_1) d\mathbf{x} \\ &\qquad = \int_{t_1}^{t_2} \int_{\mathbb{R}^n} G \frac{\partial p}{\partial t} d\mathbf{x} dt - \int_{t_1}^{t_2} \int_{\mathbb{R}^n} (\mathbf{v} \cdot \nabla G) p \; d\mathbf{x} dt,\end{aligned} \tag{3.64}$$

where we have applied integration by parts in time to the term involving the partial derivative of G with respect to time. Next, if we perform integration by parts in space on the last term, we obtain

$$\int_{t_1}^{t_2} \int_{\mathbb{R}^n} G \left[\frac{\partial p}{\partial t} + \nabla \cdot (\mathbf{v} p) \right] d\mathbf{x} dt. \tag{3.65}$$

The term inside the square brackets vanishes by virtue of the continuity equation. Consequently, the Lagrange functional $\Lambda^{F,G}$ is constant and equal to zero for any choice of the functions F and G, provided that the constraints (3.60) are satisfied. Therefore, $\Lambda^{F,G}$ constitutes a valid Lagrange functional for our problem.

Now, the saddle-point action principle can be stated as the optimization problem

$$\min_{\mathbf{x}} \min_{\mathbf{v}} \max_{\mathbf{u}} (I + \Lambda^{F,G})(\mathbf{x}, \mathbf{v}, \mathbf{u}), \tag{3.66}$$

without constraints. The minimization with respect to $\mathbf{x}$ is merely formal and can be replaced by a maximization without altering the solution. For each $\mathbf{x}$, we seek to determine $\mathbf{v}^*$ and $\mathbf{u}^*$ by minimizing and maximizing, respectively, the integrand of $I + \Lambda^{F,G}$. In this way, we arrive at the following problem:

$$\begin{aligned} \min_{\mathbf{v}\in\mathbb{R}^n} \max_{\mathbf{u}\in\mathbb{R}^n} \Bigg\{ & \frac{1}{2}m\mathbf{v}^2 - \frac{1}{2}m\mathbf{u}^2 - V(\mathbf{x}(t)) + m\sigma^2\mathbf{u}\cdot\nabla F(\mathbf{x}(t),t) \\ & + \frac{m\sigma^4}{2}\nabla^2 F(\mathbf{x}(t),t) - \frac{\partial G}{\partial s}(\mathbf{x}(t),t) - \mathbf{v}\cdot\nabla G(\mathbf{x}(t),t) \Bigg\}. \end{aligned} \tag{3.67}$$

Then, we get

$$\mathbf{v}^*(t) = \frac{1}{m}\nabla G(\mathbf{x}(t),t), \tag{3.68}$$

and

$$\mathbf{u}^*(t) = \sigma^2\nabla F(\mathbf{x}(t),t). \tag{3.69}$$

We can conclude that if $G(\mathbf{x}(t),t) = S(\mathbf{x}(t),t)$ and $F(\mathbf{x}(t),t) = R(\mathbf{x}(t),t)$, with R and S satisfying the second Madelung equation with $\sigma^2 = \hbar/m$, i.e.,

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V(\mathbf{x}) - \frac{m\sigma^4}{2}[\nabla R\cdot\nabla R + \nabla^2 R] = 0, \tag{3.70}$$

then the functional

$$\Gamma^{R,S}(\mathbf{x}) = (I + \Lambda^{R,S})(\mathbf{x}, \mathbf{v}^*, \mathbf{u}^*) \tag{3.71}$$

is constant and solves the extremization problem with respect to $\mathbf{x}$. A straightforward calculation gives

$$\begin{aligned} \Gamma^{R,S}\left(\mathbf{x}, \frac{1}{m}\nabla S, \sigma^2\nabla R\right) &= \mathbb{E}\{S(\mathbf{x}(t_1),t_1) + S(\mathbf{x}(t_2),t_2) - S(\mathbf{x}(t_1),t_1)\} \\ &= \mathbb{E}\{S(\mathbf{x}(t_2),t_2)\}. \end{aligned} \tag{3.72}$$

Therefore, the equilibrium solution for the saddle-point problem (3.59) is

$$\left(\mathbf{x}(t), \frac{1}{m}\nabla S(\mathbf{x}(t),t), \sigma^2\nabla R(\mathbf{x}(t),t)\right) \tag{3.73}$$

with $\mathbf{x}$ subjected to the constraints (3.60) and the functions R and S satisfying the second Madelung equation (3.70).

If we set $F = 0$ (or equivalently $R = 0$) in the Lagrange functional, we obtain a functional analogous to the classical case. Solving the saddle-point problem for this new functional Λ^G, we find $\mathbf{u}^* = 0$, which, according to the constraints, is only possible if $\sigma = 0$. In this case, we also obtain $\mathbf{v}_+ = \mathbf{v}_- = \mathbf{v}^* = \frac{1}{m}\nabla S$, thereby recovering classical mechanics [61]. Thus, the saddle-point principle of action can be regarded as an extension of the classical principle of least action. Conversely, when $\sigma \neq 0$, the osmotic velocity is non-zero, and the stochastic terms in the dynamics reproduce the full quantum behavior, as encoded in Nelson's stochastic mechanics. Hence, the formalism naturally interpolates between the classical and quantum regimes, depending on whether σ vanishes or not.

We can also note that making $G = 0$ (or equivalently $S = 0$), then the saddle-point action principle yields $\mathbf{v}^* = 0$ and $\mathbf{u}^* = \mathbf{v}_+ = (\hbar/m)\nabla R$, with probability density given by $p = \exp(2R)$. If R satisfies the equation

$$V(\mathbf{x}) - E - \frac{m\sigma^4}{2}\left[(\nabla R)^2 + \nabla^2 R\right] = 0, \tag{3.74}$$

where E is a constant, than the functional $\Gamma^R(\mathbf{x}) = (I + \Lambda^R)(\mathbf{x}, 0, \sigma^2\nabla R) = -E(t_2 - t_1)$ is constant with respect to $\mathbf{x}$ and the triple $(\mathbf{x}, 0, \sigma^2\nabla R(\mathbf{x}(t), t)$ solves the saddle-point action problem. Furthermore, the constant E has dimension of energy and (3.74) is equivalent to the time-independent Schrödinger equation

$$\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi, \tag{3.75}$$

where $\psi(\mathbf{x}) = \exp R(\mathbf{x})$ and $\sigma^2 = \hbar/m$. This derivation is very similar to the original variational derivation presented by Erwin Schrödinger in 1926 [70].

3.2.2 Saddle-Point Entropy Production Principle

Again, let $\mathbf{x}$ be a stochastic process, with $\mathbf{v}$ and $\mathbf{u}$ denoting its current and osmotic velocities, respectively. For this process, we define the following functional:

$$J(\mathbf{x}, \mathbf{v}, \mathbf{u}) = \mathbb{E}\left\{\int_{t_1}^{t_2}\left[\frac{1}{\sigma^2}\mathbf{v}(t)\cdot\mathbf{u}(t)\right]dt + R(\mathbf{x}(t_1), t_1)\right\} \tag{3.76}$$

where R is a continuous function related to the initial condition at t_1. Moreover, a new stochastic control problem is defined by

$$\max_{\mathbf{v}}\min_{\mathbf{u}}\ J(\mathbf{x}, \mathbf{v}, \mathbf{u}), \tag{3.77}$$

with the dynamical constraints

$$\begin{aligned} d\mathbf{x}(t) &= (\mathbf{v} + \mathbf{u})dt + \sigma d\mathbf{W}(t), \\ d\mathbf{x}(t) &= (\mathbf{v} - \mathbf{u})dt + \sigma d\mathbf{W}_*(t). \end{aligned} \tag{3.78}$$

Before proceeding, we first examine the meaning of the functional (3.76). Let $\mathbf{x}$ be a Markov diffusion process, and let $p(\mathbf{x}, t)$ denote its probability density at time t. We

define the configurational entropy, $\mathcal{S}(t)$, of $\mathbf{x}$ at time t using the Shanon entropy function for continuous systems or differential entropy [71], i.e.,

$$\mathcal{S}(t) = -\int_{\mathbb{R}^n} p(\mathbf{x},t)\ln p(\mathbf{x},t)d\mathbf{x}. \tag{3.79}$$

Now, we calculate the entropy time variation:

$$\begin{aligned}\frac{d\mathcal{S}}{dt} &= \int_{\mathbb{R}^n}\left[-\frac{\partial p}{\partial t}(\ln p+1)\right]d\mathbf{x} = \int_{\mathbb{R}^n}[\nabla\cdot(\mathbf{v}p)(\ln p+1)]d\mathbf{x}\\ &= -\int_{\mathbb{R}^n}\mathbf{v}\cdot\nabla(\ln p)p\ d\mathbf{x} = -\int_{\mathbb{R}^n}\frac{2}{\sigma^2}(\mathbf{v}\cdot\mathbf{u})p\ d\mathbf{x}\\ &= -\mathbb{E}\left[\frac{2}{\sigma^2}\mathbf{v}\cdot\mathbf{u}\right],\end{aligned} \tag{3.80}$$

where we have performed an integration by parts with vanishing boundary terms, and we have used the dynamical relations:

$$\frac{\partial p}{\partial t} = -\nabla\cdot(\mathbf{v}p) \tag{3.81}$$

and

$$\mathbf{u}(\mathbf{x},t) = \frac{\sigma^2}{2}\nabla\ln p(\mathbf{x},t). \tag{3.82}$$

Therefore, for a conservative diffusion process, we have

$$\mathbb{E}\left\{\int_{t_1}^{t_2}\frac{1}{\sigma^2}\mathbf{v}(t)\cdot\mathbf{u}(t)dt\right\} = \frac{1}{2}[\mathcal{S}(t_1)-\mathcal{S}(t_2)] = -\frac{\Delta\mathcal{S}}{2}. \tag{3.83}$$

Setting $R(\mathbf{x}(t_1),t_1)=0$ in (3.76), the problem (3.77) can be interpreted as follows: the current velocity $\mathbf{v}$ seeks to minimize the configurational entropy production, while the osmotic velocity $\mathbf{u}$ seeks to maximize the configurational entropy production over the interval $[t_1,t_2]$.

We now solve the problem (3.77) using Lagrange functionals in the same manner as done previously for the stochastic action principle. Let $F,G:\mathbb{R}\times[t_1,t_2]\to\mathbb{R}$ be two arbitrary functions, continuous and differentiable. We define

$$\begin{aligned}\Phi^{F,G}(\mathbf{x},\mathbf{v},\mathbf{u}) = \mathbb{E}\Bigg\{&\int_{t_1}^{t_2}\left[-\frac{1}{m\sigma^2}\mathbf{u}\cdot\nabla G-\frac{1}{2m}\nabla^2 G-\frac{\partial F}{\partial t}-\mathbf{v}\cdot\nabla F\right]dt\\ &+F(\mathbf{x}(t_2),t_2)-F(\mathbf{x}(t_1),t_1)\Bigg\},\end{aligned} \tag{3.84}$$

as the Lagrange functional for our saddle-point problem. With $\mathbf{u}$ and $\mathbf{v}$ satisfying the dynamical equations (3.81) and (3.82), the functional $\Phi^{F,G}$ is constant and equal to zero. A proof follows from an analogous calculation as done for the functional $\Lambda^{F,G}$ previously. Therefore, $\Phi^{F,G}$ is a valid Lagrange functional for our problem.

We are now faced with the following unconstrained optimization problem:

$$\min_{\mathbf{x}}\max_{\mathbf{v}}\min_{\mathbf{u}}\ (J+\Phi^{F,G})(\mathbf{x},\mathbf{v},\mathbf{u}). \tag{3.85}$$

Again, the minimization with respect to $\mathbf{x}$ is merely formal and can be replaced by a maximization. For each $\mathbf{x}$, we have the problem

$$\max_{\mathbf{v}\in\mathbb{R}^n}\min_{\mathbf{u}\in\mathbb{R}^n}\left\{\frac{1}{\sigma^2}\mathbf{v}\cdot\mathbf{u}-\frac{1}{m\sigma^2}\mathbf{u}\cdot\nabla G(\mathbf{x}(t),t)-\frac{1}{2m}\nabla^2 G(\mathbf{x}(t),t)\right.$$
$$\left.-\frac{\partial F}{\partial t}(\mathbf{x}(t),t)-\mathbf{v}\cdot\nabla F(\mathbf{x}(t),t)\right\}. \tag{3.86}$$

From this, we see that the minimum with respect to $\mathbf{u}$ is $-\infty$ unless

$$\mathbf{v}^*(t)=\frac{1}{m}\nabla G(\mathbf{x}(t),t), \tag{3.87}$$

and, similarly, the maximum with respect to $\mathbf{v}$ is $+\infty$ unless

$$\mathbf{u}^*(t)=\sigma^2\nabla F(\mathbf{x}(t),t). \tag{3.88}$$

These conditions ensure that the saddle-point of the functional is finite, providing well-defined equilibrium values for the current and osmotic velocities. It follows then, that if $F(\mathbf{x}(t),t)=R(\mathbf{x}(t),t)$ and $G(\mathbf{x}(t),t)=S(\mathbf{x}(t),t)$ satisfy the first Madelung equation

$$\frac{\partial R}{\partial t}+\frac{1}{m}\nabla R\cdot\nabla S+\frac{1}{2m}\nabla^2 S=0, \tag{3.89}$$

then the functional

$$\Xi^{F,G}(\mathbf{x})=(J+\Phi^{F,G})(\mathbf{x},\mathbf{v}^*,\mathbf{u}^*) \tag{3.90}$$

in the position space is constant and, furthermore, it solves the extremization problem with respect to $\mathbf{x}$. A simple calculation yields

$$\begin{aligned}\Xi^{R,S}\left(\mathbf{x},\frac{1}{m}\nabla S,\sigma^2\nabla R\right)&=\mathbb{E}\{R(\mathbf{x}(t_1),t_1)+R(\mathbf{x}(t_2),t_2)-R(\mathbf{x}(t_1),t_1)\}\\&=\mathbb{E}\{R(\mathbf{x}(t_2),t_2)\}.\end{aligned} \tag{3.91}$$

Therefore, the equilibrium solution for the saddle-point problem (3.77) is

$$\left(\mathbf{x}(t),\frac{1}{m}\nabla S(\mathbf{x}(t),t),\sigma^2\nabla R(\mathbf{x}(t),t)\right) \tag{3.92}$$

with $\mathbf{x}$ subjected to the constraints (3.78) and the functions R and S satisfying the first Madelung equation (3.89).

As we have already seen in the previous section, if R and S satisfy both Madelung equations with the identification $\sigma^2=\hbar/m$, then the function $\Psi=\exp\left(R+\frac{i}{\hbar}S\right)$ is the wave function satisfying the time-dependent Schrödinger equation.

Note that the irrotationality of $\mathbf{v}$, which was justified as a consequence of time-reversibility, also emerges naturally as a result of both variational principles.

3.2.3 Quantum Hamilton Principle

Now, following the work of Pavon [15], we can combine the two saddle-point principles discussed previously into a single extremization problem. In particular, we have established, within the framework of the action principle, that

$$(I + \Lambda^{R,S})(\mathbf{x}^*, \mathbf{v}^*, \mathbf{u}^*) = \mathbb{E}\{S(\mathbf{x}^*(t_2), t_2)\}, \tag{3.93}$$

where $(\mathbf{x}^*, \mathbf{v}^*, \mathbf{u}^*)$ are the equilibrium solution satisfying the dynamical constraints. However, remember that $\Lambda^{R,S}$ is zero if the constraints are satisfied, then we have

$$I(\mathbf{x}^*, \mathbf{v}^*, \mathbf{u}^*) = \mathbb{E}\{S(\mathbf{x}^*(t_2), t_2)\}, \tag{3.94}$$

and similarly for the entropy production principle,

$$J(\mathbf{x}^*, \mathbf{v}^*, \mathbf{u}^*) = \mathbb{E}\{R(\mathbf{x}^*(t_2), t_2)\}. \tag{3.95}$$

Putting Eqs. (3.94) and (3.95) together and writing the wave function in the polar form (3.47), we have

$$\mathbb{E}\{(\hbar/i)\ln\Psi(\mathbf{x}^*(t_2), t_2)\} = [(\hbar/i)J + I](\mathbf{x}^*, \mathbf{v}^*, \mathbf{u}^*), \tag{3.96}$$

and from the expressions for the functionals I in Eq. (3.58) and J in Eq. (3.76), we can write

$$\begin{aligned}\mathbb{E}\{(\hbar/i)\ln\Psi(\mathbf{x}^*(t_2), t_2)\} = \mathbb{E}\Bigg\{ \int_{t_1}^{t_2} \left[\frac{1}{2}m(\mathbf{v}^* - i\mathbf{u}^*)\cdot(\mathbf{v}^* - i\mathbf{u}^*) - V(\mathbf{x}^*)\right] dt \\ + \frac{\hbar}{i}\ln\Psi(\mathbf{x}(t_1), t_1)\Bigg\}.\end{aligned} \tag{3.97}$$

Therefore, let us define the Lagrangian $\mathcal{L}_1$ of the functional I as

$$\mathcal{L}_1(\mathbf{x}, \mathbf{v}, \mathbf{u}) = \frac{1}{2}m\mathbf{v}^2 - \frac{1}{2}m\mathbf{u}^2 - V(\mathbf{x}) \tag{3.98}$$

and, in addition, define the Lagrangian $\mathcal{L}_2$ of the functional J by

$$\mathcal{L}_2(\mathbf{x}, \mathbf{v}, \mathbf{u}) = \frac{1}{\sigma^2}\mathbf{v}\cdot\mathbf{u}. \tag{3.99}$$

With these definitions, one finds the remarkable relation:

$$\mathcal{L}_1(\mathbf{x}, \mathbf{v}, \mathbf{u}) - i\hbar\mathcal{L}_2(\mathbf{x}, \mathbf{v}, \mathbf{u}) = \mathcal{L}(\mathbf{x}, \mathbf{v} - i\mathbf{u}), \tag{3.100}$$

where $\mathcal{L} = \mathcal{L}(\mathbf{x}, \dot{\mathbf{x}})$ denotes the canonical classical Lagrangian, i.e., $\mathcal{L} = T - V$. This naturally suggests the introduction of a complex velocity field,

$$\mathbf{v}_q(t) \coloneqq \mathbf{v}(t) - i\mathbf{u}(t), \tag{3.101}$$

which we shall refer to as the *quantum velocity*.

Next, based on the definition of the complex velocity field $\mathbf{v}_q$, we can combine the two dynamical constraints given in Eqs. (3.78). Multiplying the first equation in (3.78) by $(1-i)/2$ and the second equation by $(1+i)/2$, and then summing the results, we obtain

$$d\mathbf{x}(t) = \mathbf{v}_q(t)dt + d\mathbf{W}_q(t), \tag{3.102}$$

where the stochastic increment

$$d\mathbf{W}_q(t) \coloneqq \frac{\sigma}{2}[(1-i)d\mathbf{W}(t) + (1+i)d\mathbf{W}_*(t)], \tag{3.103}$$

is referred to as the *quantum noise*. This process satisfies the correlation property

$$\mathbb{E}\{d\mathbf{W}_q(t)d\mathbf{W}_q(s)\} = \delta(t-s)\frac{\sigma}{i}dt + \mathcal{O}(dt). \tag{3.104}$$

As mentioned by Pavon [68], at each time t, $\mathbf{v}_q$ and the pair $(\mathbf{v}(t), \mathbf{u}(t))$ contain exactly the same information, but it is only the choice of $\mathbf{v}_q$ as kinematical variable that allows the full development of the Lagrangian and Hamiltonian formulation of stochastic mechanics in a form that naturally extends the classical one, as we will see bellow.

The quantum noise has a distinct nature: $\mathbf{W}_q(t)$ is not a forward nor a backward process. Even though the position process $\mathbf{x}(t)$ is Markovian, the quantum noise $\mathbf{W}_q(t)$ is not Markovian and is adapted both to the increasing filtration of the past and the decreasing filtration of the future [72].

Using Eq. (3.102), Itô's formula can be reformulated in the complex framework as follows:

$$d[f(\mathbf{x}(t),t)] = \left[\frac{\partial}{\partial t} + \mathbf{v}_q(t)\cdot\nabla - i\frac{\sigma}{2}\nabla^2\right] f(\mathbf{x}(t),t)dt + \nabla f(\mathbf{x}(t),t)\cdot d\mathbf{W}_q(t). \tag{3.105}$$

Finally, the Hamiltonian principle can be formulated in the context of stochastic processes as follows.

Let X_μ denote the family of all finite-energy diffusion processes defined on $[t_1, t_2]$, taking values in $\mathbb{R}^n$, with the same probability density $p(\mathbf{x}, t)$ and with the same diffusion coefficient σ^2. Let V_c be the set of complex finite-energy stochastic processes $\mathbf{z}(t)$ defined on the time interval $[t_1, t_2]$, such that

$$\mathbb{E}\left\{\int_{t_1}^{t_2} |\mathbf{z}(t)|^2\, dt\right\} < \infty. \tag{3.106}$$

For $(\mathbf{x}, \mathbf{v}_q) \in X_\mu \times V_c$, we define the *quantum action functional* as

$$I_Q(\mathbf{x}, \mathbf{v}_q) = \mathbb{E}\left\{\int_{t_1}^{t_2} \left[\frac{1}{2}m\mathbf{v}_q^2(t) - V(\mathbf{x}(t))\right] dt + \phi(\mathbf{x}(t_1), t_1)\right\}. \tag{3.107}$$

The dynamical equations of motion are obtained extremizing the functional $I_Q(\mathbf{x}, \mathbf{v}_q)$, i.e.,

$$\delta I_Q = 0, \tag{3.108}$$

subjected to the constraint

$$d\mathbf{x}(t) = \mathbf{v}_q(t)dt + d\mathbf{W}_q(t). \tag{3.109}$$

This is the *quantum Hamilton principle*. In Appendix C it is shown how the time-dependent Schrödinger equation can be obtained directly from the variational problem (3.108). Consequently, the following theorem can be stated [15].

Theorem 4 (Pavon) *In problem* (3.108)*, let* $p(\mathbf{x},t) = |\Psi(\mathbf{x},t)|^2$*, where* Ψ *is the solution of the Schrödinger equation with initial condition* $\Psi(\mathbf{x},t_1) = \exp[(i/\hbar)\phi(\mathbf{x},t_1)]$*. If* $\phi(\mathbf{x},t) = -i\hbar \ln \Psi(\mathbf{x},t)$ *satisfies*

$$\mathbb{E}\left\{\int_{t_1}^{t_2} |\nabla\phi(\mathbf{x}(t),t)|^2 dt\right\} < \infty,$$

then the unique solution of the problem is the Nelson process (3.109) *with its quantum drift*

$$\mathbf{v}_q(t) = \frac{1}{m}\nabla\phi(\mathbf{x}(t),t).$$

The formulation of the quantum Hamilton principle demonstrates how the classical variational approach can be consistently extended to the stochastic domain. By introducing the complex velocity $\mathbf{v}_q$ and the corresponding notion of quantum noise, the two stochastic constraints merge into a unified dynamical prescription. This variational framework not only recovers the familiar structure of classical mechanics in the deterministic limit, but also encodes the intrinsic fluctuations that underlie quantum phenomena. In this sense, the quantum Hamilton principle provides a natural foundation for deriving quantum dynamics from a variational viewpoint.

To conclude this section, let us connect the stochastic formalism with the conventional quantum mechanical framework. Consider the wave function written in polar form as $\Psi(\mathbf{x},t) = \exp[R(\mathbf{x},t) + (i/\hbar)S(\mathbf{x},t)]$. Using the standard quantum mechanical momentum operator $P = (\hbar/i)\nabla$, the expectation value of momentum reads

$$\langle\Psi|P|\Psi\rangle = \int \Psi^*(\mathbf{x},t)\, P\, \Psi(\mathbf{x},t)\, d\mathbf{x} = \mathbb{E}\left[m\mathbf{v}_q(\mathbf{x},t)\right]. \tag{3.110}$$

This shows that

$$\mathbf{p} = m\mathbf{v}_q = m(\mathbf{v} - i\mathbf{u}) \tag{3.111}$$

can be interpreted as the instantaneous (complex) momentum of the quantum particle. Its real part corresponds to the mean local momentum, while its imaginary component encodes the osmotic contribution associated with quantum diffusion.

Similarly, if we compute the expectation value of the Hamiltonian operator $H = -(\hbar^2/2m)\nabla^2 + V(\mathbf{x})$, we find

$$\langle\Psi|H|\Psi\rangle = \int \rho(\mathbf{x},t)\left[\frac{1}{2}m\left(\mathbf{v}^2 + \mathbf{u}^2\right) + V(\mathbf{x},t)\right] d\mathbf{x} = \mathbb{E}\left[\frac{1}{2m}\mathbf{p}\bar{\mathbf{p}} + V(\mathbf{x})\right], \tag{3.112}$$

where $\rho = e^{2R}$ is the probability density and the bar denotes complex conjugation. This expression reveals that the total mean energy is composed of two distinct contributions besides the potential energy: the kinetic energy associated with the current motion (through $\mathbf{v}$), and the internal or diffusive kinetic energy related to the osmotic velocity $\mathbf{u}$.

However, Pavon [15] notes that the distribution of $\mathbf{p}$ differs from that of P, sharing only the same mean value and variance. Nevertheless, $\mathbf{p}$ provides a simple stochastic interpretation of a fundamental result of the uncertainty principle [15], demonstrating the full consistency between the stochastic dynamics and the Hilbert space formulation of quantum mechanics.

In his 1985 work [5], Nelson argued that the instantaneous energy of a system consisting of a particle interacting with a scalar potential,

$$E(\mathbf{x},t) = \frac{1}{2}m\left[\mathbf{v}^2(\mathbf{x},t) + \mathbf{u}^2(\mathbf{x},t)\right] + V(\mathbf{x}), \tag{3.113}$$

is conserved along the stochastic flow according to

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) E(\mathbf{x},t) = 0. \tag{3.114}$$

However, in a later work published in 1988 [56], Nelson corrected this claim. He concluded that Eq. (3.114) is in general false even for free diffusions. The origin of this inconsistency lies in the fact that Eq. (3.114) results in a third-order differential equation for R and S that must be satisfied at each time. But this can not be true, since the initial value can be chosen arbitrarily, subjected only to the normalization condition of the probability density $\rho(\mathbf{x},t)$.

It is worth mentioning that the uncertainty relation between position and momentum can be readily obtained from the stochastic formulation of quantum mechanics [68]. Consider the random vectors $x_0(t) = x(t) - \mathbb{E}[x(t)]$ and $p_0(t) = p(t) - \mathbb{E}[p(t)]$, using the Cauchy-Schwarz inequality and Eq. (3.111), we obtain

$$\begin{aligned}\mathbb{E}\{x_0(t)^2\}\mathbb{E}\{|p_0(t)|^2\} &\geq |\mathbb{E}\{x_0(t)p_0(t)\}|^2 \\ &= |m\mathbb{E}\{x_0(t)v_0(t)\} - im\mathbb{E}\{x_0(t)u_0(t)\}|^2 \\ &= |m\mathbb{E}\{x_0(t)v_0(t)\}|^2 + |m\mathbb{E}\{x_0(t)u(t)\}|^2,\end{aligned} \tag{3.115}$$

since $\mathbb{E}[u(t)] = 0$. Furthermore,

$$\begin{aligned}|m\mathbb{E}\{x_0(t)u(t)\}|^2 &= |m\mathbb{E}\{x(t)u(t)\}|^2 \\ &= \left|\frac{\hbar}{2}\int x\frac{\partial}{\partial x}\rho(x,t)\,dx\right|^2 \\ &= \left|-\frac{\hbar}{2}\int \rho(x,t)\,dx\right|^2 = \frac{\hbar^2}{4},\end{aligned} \tag{3.116}$$

where we have applied integration by parts. Substituting this result into (3.115), yields

$$\operatorname{var}[x(t)]\operatorname{var}[p(t)] \geq |m\mathbb{E}\{x_0(t)v_0(t)\}|^2 + \frac{\hbar^2}{4} \tag{3.117}$$

with $v_0(t) = v(t) - \mathbb{E}[v(t)]$, which is equivalent to the general uncertainty relation of Robertson-Schrödinger [73, 74]. Note that this relation encompasses Heisenberg's uncertainty principle. A detailed discussion about the generalization of the uncertainty relation for quantum and stochastic systems can be found in [75].

3.3 STOCHASTIC OPTIMAL CONTROL THEORY

Making use of the stochastic optimal control theory applied to the Lagrangian formalism introduced in the last section, it is possible to derive a stochastic Hamiltonian formalism for quantum mechanics [76]. First, a brief introduction to the stochastic optimal control theory is given.

3.3.1 General (Non-zero) Stochastic Differential Games

Here, we present the maximum principle for stochastic differential games by forward-backward in time stochastic differential equations (FBSDEs) according to Ref. [77]. A stochastic differential game is an optimization problem involving two or more decision-making agents, referred to as *players*, who act within a dynamical system driven by stochastic differential equations. Each player seeks to optimize an expected payoff functional. To this end, each player adjusts a variable known as a *control*, which influences the evolution of the underlying stochastic process. The central objective of the game is to determine equilibrium strategies in which no player can improve their expected payoff by unilaterally modifying their control [78].

Let $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t\geq 0}, P)$ be a filtered probability space and consider the controlled forward stochastic differential equation

$$\begin{aligned} &dX(t) = b(t, X(t), u(t), \omega)dt + \sigma(t, X(t), u(t), \omega)dW(t), \quad 0 \leq t \leq T, \\ &X(0) = x \in \mathbb{R}, \end{aligned} \tag{3.118}$$

where $W(t)$ is a standard Wiener process and $u = (u_1, u_2)$ denotes the control pair, with $u_i(t)$ being the control of player i, for $i = 1, 2$.

We assume that each player i has access to a subfiltration

$$\mathcal{E}_t^{(i)} \subseteq \mathcal{F}_t, \quad t \in [0, T], \tag{3.119}$$

representing the information available to that player at time t. Let $\mathcal{A}_i$ denote the set of admissible control processes for player i, consisting of $\mathcal{E}_t^{(i)}$-predictable processes taking values in a control set $A_i \subset \mathbb{R}^d$. We define $\mathbb{U} := A_1 \times A_2$ and assume that, for every

$x \in \mathbb{R}$ and $u \in \mathbb{U}$, the functions $b(t,x,u,\omega)$ and $\sigma(t,x,u,\omega)$ are given predictable processes such that (3.118) admits a unique solution for each admissible control u. The explicit dependence of the functions on ω indicates a possible dependence on the underlying randomness of the system.

Associated with (3.118), we consider the controlled backward SDEs for $\Big(Y_i(t), Z_i(t)\Big)$ given by

$$\begin{aligned} dY_i(t) &= -g_i\Big(t, X(t), Y_i(t), Z_i(t), u(t), \omega\Big)dt + Z_i(t)dW(t), \quad 0 \le t \le T, \\ Y_i(T) &= h_i\Big(X(T), \omega\Big), \quad i = 1, 2, \end{aligned} \tag{3.120}$$

where $g_i(t,x,y,z,u,\omega)$ are given predictable process and $h_i(x,\omega)$ are $\mathcal{F}_T$-measurable terminal conditions. We assume that for each $u \in \mathbb{U}$, the FBSDE system (3.118)-(3.120) admits a unique adapted solution. This system of FBSDEs is called state process.

Next, let $f_i(t,x,u) : [0,T] \times \mathbb{R} \times \mathbb{U} \to \mathbb{R}$, $\varphi_i(x) : \mathbb{R} \to \mathbb{R}$ and $\psi_i : \mathbb{R} \to \mathbb{R}$. We introduce the performance or cost functional of player i by

$$J_i(u) \coloneqq \mathbb{E}\left[\int_0^T f_i\Big(t, X^u(t), u(t), \omega\Big)dt + \varphi_i\Big(X^u(T), \omega\Big) + \psi_i\Big(Y_i^u(0)\Big)\right], \quad i = 1, 2, \tag{3.121}$$

where, the superscript u indicates dependence on the control process $u = (u_1, u_2)$. The functions f_i, φ_i, and ψ_i are assumed to be such that all integrals and expectation values in (3.121) are well-defined. In an economic interpretation, f_i represents the instantaneous profit (or running cost), while $\varphi_i(x,\omega)$ and $\psi_i(y)$ correspond to terminal and initial costs, respectively. In a physical interpretation, J_i plays the role of an action functional, and the integrand f_i corresponds to a Lagrangian.

Throughout, we assume that b, σ, g_i, h_i, f_i, φ_i and ψ_i are continuously differentiable (C^1) with respect to (x,y,z,u).

A pair of admissible controls $(\hat{u}_1, \hat{u}_2) \in \mathcal{A}_1 \times \mathcal{A}_2$ is said to constitute a *Nash equilibrium* for the system (3.118)–(3.121) if

$$J_1(u_1, \hat{u}_2) \le J_1(\hat{u}_1, \hat{u}_2) \qquad \forall\ u_1 \in \mathcal{A}_1, \tag{3.122}$$

$$J_2(\hat{u}_1, u_2) \le J_2(\hat{u}_1, \hat{u}_2) \qquad \forall\ u_2 \in \mathcal{A}_2. \tag{3.123}$$

This means that the player i has no incentive to deviate from the control $\hat{u}_i$, as long as player j ($j \neq i$) does not deviate from $\hat{u}_j$. Consequently, a Nash equilibrium represents a stable point of the game where both players' objectives are simultaneously optimized and, therefore, a Nash equilibrium can be interpreted as a likely outcome of a game.

Suppose now that there exists a Nash equilibrium $(\hat{u}_1, \hat{u}_2)$ for the FBSDEs above. Øksendal and Sulem have presented a method to find this equilibrium pair for a more sophisticated system of FBSDEs associated with a Lévy process [77]. Here, we present a simplified version of their method. Define the *Hamiltonian function* $\mathcal{H}_i(t,x,y,z,u_1,u_2,\lambda,p,q)$:

$[0,T]\times\mathbb{R}^3\times\mathbb{U}\times\mathbb{R}^3\to\mathbb{R}$ for each player i, as follows:

$$\begin{aligned}\mathcal{H}_i(t,x,y,z,u_1,u_2,\lambda,p,q) \coloneqq\ & f_i(t,x,u_1,u_2)+\lambda_i g_i(t,x,y,z,u_1,u_2)\\ &+p_i b(t,x,u_1,u_2)+q_i\sigma(t,x,u_1,u_2),\qquad i=1,2,\end{aligned}\tag{3.124}$$

where $\Big(\lambda_i(t),p_i(t),q_i(t)\Big)$ are called *adjoint processes*.

Although the controls (u_1,u_2) as well as the adjoint processes depend implicitly on the controlled processes $\Big(X(t),\,Y_i(t),\,Z_i(t)\Big)$, they are treated as independent variables in the Hamiltonian formalism. The maximum principle, as demonstrated by Øksendal and Sulem [77], states that the cost functionals and the associated Hamiltonian functionals have their Nash equilibrium at the same optimal control $(\hat{u}_1,\hat{u}_2)$. In other words, the mathematical problem of finding the controls u_i that extremize the cost functionals J_i can be equivalently formulated as the problem of maximizing the corresponding Hamiltonians $\mathcal{H}_i$. This equivalence provides a powerful tool for characterizing equilibrium strategies in stochastic differential games involving coupled forward–backward dynamics.

For simplicity, we shall adopt the following shortened notation for the partial derivatives of the Hamiltonians:

$$\frac{\partial\mathcal{H}_i}{\partial x}(t)=\left.\frac{\partial\mathcal{H}_i}{\partial x}\right|_{x=X(t)}\Big(t,x,Y_i(t),Z_i(t),u_1(t),u_2(t),\lambda_i(t),p_i(t),q_i(t)\Big),\tag{3.125}$$

and similarly for partial derivatives of $\mathcal{H}_i$ with respect to the other variables.

Associated with these Hamiltonians, we have a system of FBSDEs for the adjoint processes $\lambda_i(t)$, $p_i(t)$, and $q_i(t)$.The adjoint process $\lambda_i(t)$, corresponding to the backward controlled equation for $Y_i(t)$, satisfies the forward SDE

$$\begin{aligned}d\lambda_i(t)&=\frac{\partial\mathcal{H}_i}{\partial y}(t)\,dt+\frac{\partial\mathcal{H}_i}{\partial z}(t)\,dW(t)\\ &=\lambda_i(t)\left[\frac{\partial g_i}{\partial y}(t)\,dt+\frac{\partial g_i}{\partial z}(t)\,dW(t)\right],\qquad t\in[0,T],\\ \lambda_i(0)&=\psi_i'\Big(Y_i(0)\Big),\end{aligned}\tag{3.126}$$

where the prime denotes differentiation with respect to the argument. The adjoint processes $p_i(t)$ and $q_i(t)$, associated with the forward process $X(t)$ and the backward component $Z_i(t)$, satisfy the backward SDE

$$\begin{aligned}dp_i(t)&=-\frac{\partial\mathcal{H}_i}{\partial x}(t)\,dt+q_i(t)\,dW(t),\qquad t\in[0,T],\\ p_i(T)&=\varphi_i'\Big(X(T)\Big)+h_i'\Big(X(T)\Big)\,\lambda_i(T).\end{aligned}\tag{3.127}$$

Starting from the maximization of the Hamiltonians, one obtains the stochastic differential equations governing the optimal controls $\hat{u}_1(t)$ and $\hat{u}_2(t)$ in terms of the state and adjoint processes. These optimality conditions characterize the Nash equilibrium of the

forward–backward stochastic differential game. The theorems establishing the necessary and sufficient maximum principles for stochastic differential games, detailed discussions, and complete proofs are provided in the literature [77, 79, 80].

3.3.2 Controlled Backward Doubly Stochastic Differential Equations

The case under consideration here is that of the system governed by a controlled SDE of the form

$$\begin{aligned} -dy^v(t) &= b\Big(t, y^v(t), z^v(t), v(t)\Big)dt + \sigma\Big(t, y^v(t), z^v(t), v(t)\Big)dW_*(t) \\ &\quad - z^v(t)dW(t), \qquad 0 \le t \le T, \\ y^v(T) &= \xi \in \mathbb{R}^n, \end{aligned} \tag{3.128}$$

which is known as a backward doubly stochastic differential equation (BDSDE) [81]. Here, the superscript denotes the dependence on the control variable v; b and σ are given measurable maps; $W(t)$ and $W_*(t)$ denote two mutually independent standard forward and backward Wiener processes, respectively taking values in $\mathbb{R}^d$ and $\mathbb{R}^k$, and defined on a complete probability space $(\Omega, \mathcal{F}, P)$. The terminal time $T > 0$ is fixed and finite.

This type of SDE has important applications in mathematical finance. For instance, it may be used to model a scenario in which an investor known the past performance of the general stock market, represented by the forward Wiener process $W(t)$, but also has a partial anticipative information, a "tip-off", regarding the future path evolution of a specific company's stock price, represented by the backward process $W_*(t)$.

An admissible control variable $v = v(t)$ is a $\mathcal{G}_t$-adapted process with values in a convex set $U \subset \mathbb{R}^m$, where the filtration $\mathcal{G}_t$ is defined as

$$\mathcal{G}_t = \mathcal{F}_t^W \vee \mathcal{F}_T^{W_*}, \tag{3.129}$$

with the filtration $\mathcal{F}_t^W$ denoting the σ-algebra generated by the forward Wiener process up to time t, and the filtration $\mathcal{F}_T^{W_*}$ denoting the σ-algebra generated by the backward process over the entire time interval $[0, T]$. Intuitively, $\mathcal{F}_t^W$ encodes the information available from the past evolution of $W(t)$, while $\mathcal{F}_T^{W_*}$ contains information about the path of $W_*(t)$ over both the past and future of the time t. The symbol $\vee$ denotes the join, i.e., the smallest σ-algebra containing both filtrations.

We denote by $\mathcal{U}$ the set of all admissible controls. Furthermore, let $\mathcal{M}_{n\times d}(\mathbb{R})$ denote the space of real $n \times d$ matrices. The functions b and σ in (3.128) are such that

$$\begin{aligned} b &: [0, T] \times \mathbb{R}^n \times \mathcal{M}_{n\times d}(\mathbb{R}) \times U \longrightarrow \mathbb{R}^n, \\ \sigma &: [0, T] \times \mathbb{R}^n \times \mathcal{M}_{n\times d}(\mathbb{R}) \times U \longrightarrow \mathcal{M}_{n\times k}(\mathbb{R}). \end{aligned} \tag{3.130}$$

The objective of the control problem is to minimize, over the class $\mathcal{U}$ of admissible controls, the cost functional of the form

$$J(v) = \mathbb{E}\left[\int_0^T h\Big(t, y^v(t), z^v(t), v(t)\Big)dt + g\Big(y^v(0)\Big)\right], \tag{3.131}$$

where the functions

$$\begin{aligned} &g : \mathbb{R}^n \longrightarrow \mathbb{R}, \\ &h : [0,T] \times \mathbb{R}^n \times \mathcal{M}_{n\times d}(\mathbb{R}) \times U \longrightarrow \mathbb{R} \end{aligned} \tag{3.132}$$

are given. A control u is said to be optimal if it satisfies

$$J(u) = \min_{v \,\in\, \mathcal{U}} J(v). \tag{3.133}$$

Furthermore, we assume that $b(t,y,z,v)$, $\sigma(t,y,z,v)$, $h(t,y,z,v)$ and $g(y)$ are continuous and continuously differentiable with respect to (y,z,v).

Following the approach introduced by Bahlali and Gherbal [81], the Hamiltonian function

$$\mathcal{H} : [0,T] \times \mathbb{R}^n \times \mathcal{M}_{n\times d}(\mathbb{R}) \times U \times \mathbb{R}^n \times \mathcal{M}_{n\times k}(\mathbb{R}) \longrightarrow \mathbb{R}$$

associated to the BDSDE (3.128) and the cost functional (3.131) is defined as

$$\mathcal{H}(t,y,z,v,p,q) \coloneqq -h(t,y,z,v) - pb(t,y,z,v) + q\sigma(t,y,z,v), \tag{3.134}$$

with the corresponding adjoint process $\Big(p^u(t), q^u(t)\Big)$ satisfying

$$\begin{aligned} dp^u(t) &= -\frac{\partial \mathcal{H}}{\partial y}(t)\,dt + \frac{\partial \mathcal{H}}{\partial z}(t)\,dW(t) - q^u(t)\,dW_*(t), \\ p^u(0) &= g'\Big(y^u(0)\Big). \end{aligned} \tag{3.135}$$

Maximizing the Hamiltonian in (3.134) is therefore equivalent to solving the minimization problem for the cost functional (3.133).

The theorems providing the necessary and sufficient stochastic maximum principles for such backward doubly controlled systems, along with comprehensive discussions, technical conditions, and detailed proofs, can be found in the work of Bahlali and Gherbal [81], as well as in related literature, such as [82].

3.3.3 Quantum Hamilton Equations of Motion

We now discuss the application of stochastic optimal control theory, as presented in the last two subsections, to introduce a Hamiltonian formalism to quantum mechanics analogous to that employed in classical mechanics. It is important to emphasize that the stochastic optimal control Hamiltonians introduced below differ from the physical

Hamiltonian, which usually represents the total energy of the system. In the context of Nelson's stochastic quantization formalism, the physical Hamiltonian is defined as [17]

$$H = \frac{1}{2}m|(\mathbf{v} - i\mathbf{u})|^2 + V(\mathbf{x}). \tag{3.136}$$

where $\mathbf{v}$ and $\mathbf{u}$ denote the current and osmotic velocities, respectively, and $V(\mathbf{x})$ denotes the potential energy.

We begin by examining the stationary case, where the current velocity vanishes ($\mathbf{v} = 0$), and subsequently extend the discussion to non-stationary systems.

3.3.3.1 Stationary Systems

For clarity, we restrict the analysis to the one-dimensional case, although the results can be readily generalized to higher dimensions. In the stationary situation, where the current velocity $v(x,t)$ vanishes, the SDEs describing the kinematics of the particle take the form

$$\begin{aligned} dx(t) &= u(x)dt + \sigma dW(t), \qquad x(0) = x_0, \\ dx(t) &= -u(x)dt + \sigma dW_*(t), \qquad x(T) = x_T, \end{aligned} \tag{3.137}$$

where $\sigma^2 = \hbar/m$ and $t \in [0,T]$ with T fixed being a sufficiently large time duration. The corresponding stochastic optimal control problem consists of maximizing the expected action functional

$$I[\hat{u}] = \max_u \mathbb{E}\left\{\int_0^T \mathcal{L}(x,u)\,dt + S_0(x_0)\right\} \tag{3.138}$$

where the Lagrangian is given by

$$\mathcal{L}(x,u) = -\frac{1}{2}mu^2 - V(x). \tag{3.139}$$

Here, the control variable u corresponds to the osmotic velocity and acts on the coupled forward-backward stochastic system (3.137).

Following the approach developed for general stochastic differential games (see Sec. 3.3.1), the associated Hamiltonian $\mathcal{H}$ reads

$$\begin{aligned} \mathcal{H}(x,u,\lambda,p,q) &= \mathcal{L}(x,u) - \lambda u + pu + \sigma q \\ &= -\frac{1}{2}mu^2 - V(x) - \lambda u + pu + \sigma q. \end{aligned} \tag{3.140}$$

The corresponding adjoint process λ and p satisfy

$$d\lambda(t) = 0, \qquad \lambda(0) = 0, \tag{3.141}$$

$$dp(t) = \frac{dV(x)}{dx}dt + q(t)dW_*(t), \qquad p(T) = \lambda(T). \tag{3.142}$$

The adjoint process for λ equals zero. Applying the stochastic maximum principle to the Hamiltonian (3.140), yields

$$p(t) = mu(x(t)). \tag{3.143}$$

Substituting Eq. (3.143) into (3.142) gives

$$du(x) = \frac{1}{m}\frac{dV(x)}{dx}dt + \frac{q(t)}{m}dW_*(t). \tag{3.144}$$

Since the process $\lambda(t)$ vanishes identically, the backward SDE of the position process in (3.137) provides no further information about the optimal control problem and can thus be omitted [83].

Hence, the system is described by the coupled forward-backward stochastic differential equations (FBSDEs) of the form

$$dx(t) = u(x(t))dt + \sqrt{\frac{\hbar}{m}}dW(t), \qquad x(0) = x_0, \tag{3.145}$$

$$du(x(t)) = \frac{1}{m}\frac{dV(x(t))}{dx}dt + \frac{q(t)}{m}dW_*(t), \qquad u(x(T)) = 0. \tag{3.146}$$

The coupled system in (3.145) and (3.146) uniquely determines the dynamics of the quantum particle and can be solved independently of the Schrödinger equation [14]. In Appendix E, a numerical method is presented to solve this system and find the osmotic velocity u without any previous information about the wave function. An application of this method is also presented.

Making use of Itô's formula for the osmotic velocity $u(x(t))$, which does not depend explicitly on time, we get [83, 84]

$$\begin{aligned} du(x) &= \left(u(x)\frac{du(x)}{dx} + \frac{\sigma^2}{2}\frac{d^2u(x)}{dx^2}\right)dt + \sigma\frac{du(x)}{dx}dW_*(t) \\ &= \frac{1}{m}\frac{dV(x)}{dx}dt + \frac{q(t)}{m}dW_*(t). \end{aligned} \tag{3.147}$$

By identifying the deterministic and stochastic parts, we obtain a system of ordinary differential equations (ODEs):

$$0 = u(x)\frac{du(x)}{dx} + \frac{\hbar}{2m}\frac{d^2u(x)}{d^2x} - \frac{1}{m}\frac{dV(x)}{dx}, \tag{3.148}$$

$$q(x) = \sqrt{\hbar m}\frac{du(x)}{dx}. \tag{3.149}$$

Equation (3.148) represents the spatial derivative of a Ricatti-type equation. Remarkably, it coincides with the spatial gradient of the time-independent Schrödinger equation when one identifies $u(x) = \frac{\hbar}{m}\frac{d}{dx}\ln|\psi(x)|$. The nonlinear character of (3.148) implies that, in general, closed-form analytic solutions are not available.

Substituting the previously derived expressions for the adjoint processes into the Hamiltonian given in Eq. (3.140) yields

$$\mathcal{H}(x,u) = \frac{1}{2}mu^2 - V(x) + \hbar\frac{du}{dx}. \tag{3.150}$$

It is important to note that this Hamiltonian does not correspond to the physical Hamiltonian representing the total energy of the system, which, within Nelson's formalism, is defined as $H = (1/2)mu^2 + V(x)$. The fact that the Hamiltonian in classical mechanics coincides with the total energy of the system (in the majority of cases) is a fortuitous and particularly fruitful coincidence.

In the present context, the stochastic optimal control Hamiltonian serves as a mathematical construct designed to generate the dynamics through the corresponding stochastic maximum principle, rather than to represent a conserved physical quantity. Therefore, analogously to classical mechanics, quantum mechanics admits different but equivalent formalisms capable of describing the same physical phenomena. The choice of the most appropriate formalism depends on the nature of the problem under investigation. In this regard, Nelson's stochastic quantization offers a powerful and conceptually rich framework, providing new physical insights and mathematical tools to explore and solve quantum mechanical problems from a stochastic perspective.

The stationary formulation discussed above provides an insightful connection between stochastic control theory and quantum mechanics. However, most physical systems of interest are inherently non-stationary. Next, we develop the generalization of the quantum Hamilton equations for non-stationary systems.

3.3.3.2 Non-stationary Systems

For the non-stationary case, the dynamics of the stochastic process is governed by two control variables (or "players"): the osmotic velocity u and the current velocity v. We introduced two functionals associated with the saddle-point principles of action and entropy production, denoted respectively by I and J. In this game-theoretic setting, the player u seeks to maximize the functional I, while the player v seeks to maximize the functional J (or equivalently, u seeks to minimize J and v seeks to minimize I). This configuration defines a stochastic differential game whose solution corresponds to the Nash equilibrium, i.e., the optimal controls $(\hat{u}, \hat{v})$. To determine these optimal controls, we employ the framework of stochastic optimal control theory for general stochastic differential games, as introduced previously.

In the non-stationary situation, Nelson's forward and backward stochastic diffe-

rential equations of motion read

$$dx(t) = [v(x(t),t) + u(x(t),t)]\,dt + \sigma\,dW(t), \qquad x(0) = x_0, \tag{3.151}$$

$$dx(t) = [v(x(t),t) - u(x(t),t)]\,dt + \sigma\,dW_*(t), \qquad x(T) = x_T(\omega), \tag{3.152}$$

where the initial condition of the forward process is arbitrary, while the initial condition of the backward process must coincide with the final point of the forward process. Consequently, it is affected by the stochasticity of the trajectory; this dependence on randomness is represented by ω. In this regime, both velocities depend explicitly on position and time.

The current and osmotic velocities arise as the Nash equilibrium of two saddle-point variational principles:

$$I[\hat{u},\hat{v}] = \min_v \max_u \mathbb{E}\left\{\int_0^T \left[\frac{1}{2}m\Big(v^2(x,t) - u^2(x,t)\Big) - V(x,t)\right] dt + S_0(x_0)\right\}, \tag{3.153}$$

$$J[\hat{u},\hat{v}] = \max_v \min_u \mathbb{E}\left\{\int_0^T m\,v(x,t)\,u(x,t)\,dt + \hbar\,R_0(x_0)\right\}. \tag{3.154}$$

For a more detailed discussion on the maximum principle for saddle-point variational problems as a zero-sum game, see Refs. [77, 85]. Based on Sec. 3.3.1, the equilibrium conditions can be expressed as

$$I(u,\hat{v}) \le I(\hat{u},\hat{v}), \quad \forall\, u, \tag{3.155}$$

$$J(\hat{u},v) \le J(\hat{u},\hat{v}), \quad \forall\, v, \tag{3.156}$$

where $(\hat{u},\hat{v})$ denotes the Nash equilibrium pair.

Following the general strategy for finding Nash equilibria in stochastic differential games (see Sec. 3.3.1), we introduce two Hamiltonians associated with each saddle-point principle, i.e.,

$$\mathcal{H}_I(t,x,u,v) = \frac{1}{2}m(v^2-u^2) - V(x,t) + \lambda_I(u-v) + p_I(u+v) + \sqrt{\frac{\hbar}{m}}\,q_I, \tag{3.157}$$

$$\mathcal{H}_J(t,x,u,v) = m\,u\,v + \lambda_J(u-v) + p_J(u+v) + \sqrt{\frac{\hbar}{m}}\,q_J. \tag{3.158}$$

The corresponding adjoint processes satisfy the following stochastic differential equations:

$$d\lambda_I = 0, \qquad \lambda_I(0) = S'(x_0), \tag{3.159}$$

$$d\lambda_J = 0, \qquad \lambda_J(0) = R'(x_0), \tag{3.160}$$

$$dp_I(t) = \frac{\partial V(x,t)}{\partial x}\,dt + q_I(t)\,dW_*(t), \qquad p_I(T) = \lambda_I(T), \tag{3.161}$$

$$dp_J(t) = q_J(t)\,dW_*(t), \qquad p_J(T) = \lambda_J(T). \tag{3.162}$$

Applying the stochastic maximum principle to both Hamiltonians with respect to the control variables u and v, we obtain

$$m\,u(x,t) = \lambda_I + p_I, \qquad m\,u(x,t) = \lambda_J - p_J, \tag{3.163}$$

$$m\,v(x,t) = \lambda_I - p_I, \qquad m\,v(x,t) = -\lambda_J - p_J. \tag{3.164}$$

Substituting the adjoint processes into one of the two relations for each velocity yields

$$dv(x,t) = -\frac{1}{m}\frac{\partial V(x,t)}{\partial x}\,dt - \frac{q_I(t)}{m}\,dW_*(t) \tag{3.165}$$

$$du(x,t) = -\frac{q_J(t)}{m}\,dW_*(t) \tag{3.166}$$

Expanding $v(x,t)$ and $u(x,t)$ via Itô's formula, as in the stationary case, we find

$$q_I(t) = -\sqrt{\hbar m}\,\frac{\partial v(x,t)}{\partial x}, \tag{3.167}$$

$$q_J(t) = -\sqrt{\hbar m}\,\frac{\partial u(x,t)}{\partial x}. \tag{3.168}$$

Thus, the system of backward SDEs governing the two velocities is

$$dv(x,t) = -\frac{1}{m}\frac{\partial V(x,t)}{\partial x}\,dt + \sqrt{\frac{\hbar}{m}}\frac{\partial v(x,t)}{\partial x}\,dW_*(t), \tag{3.169}$$

$$du(x,t) = \sqrt{\frac{\hbar}{m}}\frac{\partial u(x,t)}{\partial x}\,dW_*(t). \tag{3.170}$$

A related derivation was presented by Köppe [83], where the equality between forward and backward processes for $x(t)$ was imposed as a constraint in the maximization of the Hamiltonians.

It is also possible to solve the optimal control problem for the non-stationary case via a complex formulation. Recall that Nelson's forward and backward stochastic trajectories can be combined into a single complex representation of the form

$$\begin{aligned} dx(t) &= v_q(x,t)\,dt + \frac{1}{2}\sqrt{\frac{\hbar}{m}}\Big[(1-i)\,dW(t) + (1+i)\,dW_*(t)\Big], \\ x(0) &= x_0, \end{aligned} \tag{3.171}$$

where $v_q(x,t) = v(x,t) - i\,u(x,t)$ is the quantum velocity. Equation (3.171) thus constitutes a particular instance of a backward doubly stochastic differential equation (BDSDE).

The stochastic optimal control problem can be formulated as the extremization of the expected cost functional, defining the quantum Hamilton principle, with respect to the complex control variable v_q. It is mathematically expressed as

$$I_Q[\hat{v}_q] = \max_{v_q}\,\mathbb{E}\left\{\int_0^T \mathcal{L}(x,v_q)\,dt + \phi_0(x_0)\right\}, \tag{3.172}$$

where the Lagrangian reads

$$\mathcal{L}(x, v_q) = \frac{1}{2} m v_q^2 - V(x,t). \tag{3.173}$$

Extending the BDSDE optimal control framework (see Sec. 3.3.2) to complex-valued functions, the associated Hamiltonian is given by

$$\begin{aligned} \mathcal{H}(x, v_q, p, q) &= -\mathcal{L}(x, v_q) + p\, v_q - q\sqrt{\frac{\hbar}{m}}\frac{(1+i)}{2} \\ &= -\frac{1}{2} m v_q^2 + V(x,t) + p\, v_q - q\sqrt{\frac{\hbar}{m}}\frac{(1+i)}{2}, \end{aligned} \tag{3.174}$$

where $p = p_1 + ip_2$ and $q = q_1 + iq_2$ are the adjoint processes satisfying

$$\begin{aligned} dp(t) &= -\frac{\partial V(x,t)}{\partial x}\, dt - q(t)\, dW_*(t), \\ p(0) &= \phi_0'(x_0). \end{aligned} \tag{3.175}$$

Applying the maximum principle to the Hamiltonian (3.174) setting $\dfrac{\partial \mathcal{H}}{\partial v_q} = 0$, yields

$$p = m v_q = m(v - iu), \tag{3.176}$$

which connects the adjoint process to the complex velocity. Note that p corresponds to our previous definition of quantum momentum in Eq. (3.111). Substituting Eq. (3.176) into the equation for the adjoint process (3.175) and separating real and imaginary parts gives

$$\begin{aligned} dv(x,t) &= -\frac{1}{m}\frac{\partial V(x,t)}{\partial x}\, dt - \frac{q_1(x,t)}{m}\, dW_*(t), \\ du(x,t) &= \frac{q_2(x,t)}{m}\, dW_*(t). \end{aligned} \tag{3.177}$$

Thus, we obtain two backward SDEs for the current and osmotic velocities. Since $x(t)$ is itself a stochastic process, we can expand the stochastic equations for u and v using Itô's formula and compare with Eqs. (3.177), yielding

$$\begin{aligned} q_1(x,t) &= -\sqrt{\hbar m}\frac{\partial v}{\partial x} \\ q_2(x,t) &= \sqrt{\hbar m}\frac{\partial u}{\partial x} \end{aligned} \tag{3.178}$$

Therefore, the resulting system of backward SDEs for the osmotic and current velocities reads

$$dv(x,t) = -\frac{1}{m}\frac{\partial V(x,t)}{\partial x}\, dt + \sqrt{\frac{\hbar}{m}}\frac{\partial v(x,t)}{\partial x}\, dW_*(t) \tag{3.179}$$

$$du(x,t) = \sqrt{\frac{\hbar}{m}}\frac{\partial u(x,t)}{\partial x}\, dW_*(t) \tag{3.180}$$

which are precisely the same as those obtained previously from the Nash equilibrium conditions.

To make the connection of the complex Hamiltonian formulation with the dynamical evolution of the system explicit, let us expand the adjoint process $p(t)$ using Itô's formula (3.105). Comparing the deterministic part of the resulting expression with Eq. (3.175), we obtain the following evolution equation:

$$\frac{\partial p}{\partial t} + v_q \frac{\partial p}{\partial x} - i \frac{\hbar}{2m} \frac{\partial^2 p}{\partial x^2} + \frac{\partial V}{\partial x} = 0. \tag{3.181}$$

Recalling that $p = m(v - iu)$, we can separate this complex equation into its real and imaginary components. This leads to two coupled partial differential equations:

$$\begin{aligned} \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} - u \frac{\partial u}{\partial x} - \frac{\hbar}{2m} \frac{\partial^2 u}{\partial x^2} + \frac{1}{m} \frac{\partial V}{\partial x} = 0, \\ \frac{\partial u}{\partial t} + v \frac{\partial u}{\partial x} + u \frac{\partial v}{\partial x} + \frac{\hbar}{2m} \frac{\partial^2 v}{\partial x^2} = 0. \end{aligned} \tag{3.182}$$

Equations (3.182) constitute the non-stationary system of partial differential equations (PDEs) governing the current and osmotic velocities in Nelson's stochastic mechanics. They coincide exactly with the equations derived by Köppe [17, 83], thereby confirming that the stochastic differential game formulation reproduces the dynamical structure of Nelson's theory. Moreover, Eqs. (3.182) are exactly Eqs. (3.40) from which one can recover the hydrodynamic (Madelung) representation of the Schrödinger equation. This means the dynamical SDEs (3.179) and (3.180) correspond to the Newton-Nelson law for the mean acceleration [18].

We can summarize the stochastic equations of the non-stationary case by the following system of coupled FBSDEs for the position and the controls u and v, in the three-dimensional case:

$$\begin{aligned} d\mathbf{x}(t) &= \Big[\mathbf{v}\Big(\mathbf{x}(t),t\Big) + \mathbf{u}\Big(\mathbf{x}(t),t\Big)\Big]dt + \sqrt{\frac{\hbar}{m}}\, d\mathbf{W}(t), \\ d\mathbf{x}(t) &= \Big[\mathbf{v}\Big(\mathbf{x}(t),t\Big) - \mathbf{u}\Big(\mathbf{x}(t),t\Big)\Big]dt + \sqrt{\frac{\hbar}{m}}\, d\mathbf{W}_*(t), \\ m\Big[d\mathbf{v}\Big(\mathbf{x}(t),t\Big) - d\mathbf{u}\Big(\mathbf{x}(t),t\Big)\Big] &= -\nabla V\Big(\mathbf{x}(t),t\Big)\, dt \\ &\quad + \sqrt{\hbar m}\, \nabla \cdot \Big[\mathbf{v}\Big(\mathbf{x}(t),t\Big) - \mathbf{u}\Big(\mathbf{x}(t),t\Big)\Big] d\mathbf{W}_*(t), \end{aligned} \tag{3.183}$$

called *quantum Hamilton equations of motion*. Here, the real and imaginary parts of the complex momentum $\mathbf{p} = m\mathbf{v}_q$ were used to form the real momentum $\tilde{\mathbf{p}} = m(\mathbf{v} - \mathbf{u})$. Unlike in [18], here we form the real momentum combining the real and imaginary parts of the complex momentum through subtraction of $\mathbf{u}$ from $\mathbf{v}$ in order to readily obtain the

stationary case ($\mathbf{v} = 0$). The quantum Hamilton equations above yield the stable ground-state solution, as they represent the unique critical point of the associated variational problem [18].

Additionally, if we take the limit $\hbar/m \to 0$, then the osmotic velocity $\mathbf{u}$ vanishes and the momentum is $\mathbf{p} = m\mathbf{v}$, this yields

$$\begin{cases} \dfrac{d\mathbf{x}}{dt} = \dfrac{\mathbf{p}}{m}, \\ \dfrac{d\mathbf{p}}{dt} = -\nabla V(\mathbf{x}, t), \end{cases} \tag{3.184}$$

that correspond to the classical Hamilton equations.

Finally, substituting the corresponding expressions for the adjoint processes, one can rewrite the stochastic Hamiltonian in (3.174) as

$$\mathcal{H}(x, v_q) = \frac{1}{2} m v_q^2 + V(x, t) + \frac{\hbar}{2}(1 + i)\frac{\partial v_q}{\partial x}. \tag{3.185}$$

The first two terms recall the structure of the physical Hamiltonian. However, it is important to note that the physical Hamiltonian, $H = (1/2)m|v_q|^2 + V(x)$, depends on the squared modulus of the complex velocity v_q, whereas the stochastic optimal control Hamiltonian $\mathcal{H}$ involves the complex quantity v_q^2.

If we now take the mean value of the stochastic differential equations (3.179) and (3.180) for the osmotic and current velocities, together with the stochastic equation for the position process (3.151), we obtain

$$\begin{aligned} \mathbb{E}[u] &= 0, \\ m\, d\,\mathbb{E}[v] &= -\,\mathbb{E}\left[\frac{\partial V(x,t)}{\partial x}\right] dt, \\ d\,\mathbb{E}[x] &= \mathbb{E}\Big[v\Big(x(t), t\Big)\Big]\, dt. \end{aligned} \tag{3.186}$$

These relations show that the expected values of the stochastic variables evolve according to the classical equations of motion. In particular, the vanishing of the mean osmotic velocity implies that diffusion effects cancel on average, and the mean current velocity follows Newton's second law in expectation. This result bears a close analogy with Ehrenfest's theorem [86], which states that the time evolution of the expectation values of the quantum mechanical position and momentum operators follows the classical dynamical laws. Hence, the stochastic mechanics formulation provides a bridge between quantum and classical dynamics, where the macroscopic (mean) motion obeys classical rules while microscopic fluctuations are governed by the underlying stochastic structure.

3.4 UNITARY EQUIVALENCE

While the hydrodynamical and Hamiltonian equivalence discussed in the previous sections establishes a clear correspondence between Nelson's stochastic quantization and

standard quantum mechanics, a deeper correspondence emerges when we turn to the operator formulation of the theory. This alternative viewpoint reveals that the stochastic and quantum evolutions are connected through a unitary transformation. In this framework, the stochastic dynamics governed by the forward and backward diffusions can be mapped into the standard formulation of quantum mechanics, showing that Nelson's approach is an exact reformulation of quantum mechanics.

As we have seen, the wave function can be represented by $\psi = \sqrt{\rho}\, e^{iS/\hbar}$ and defines the current and osmotic velocities, respectively, as

$$\mathbf{v}(\mathbf{x}, t) = \frac{1}{m}\nabla S(\mathbf{x}, t) \tag{3.187}$$

and

$$\mathbf{u}(\mathbf{x}, t) = \frac{\hbar}{2m}\nabla \ln \rho(\mathbf{x}, t) = \frac{\hbar}{m}\nabla \ln |\psi|. \tag{3.188}$$

The forward and backward drifts, denoted by $\mathbf{v}_\pm$ are given by $\mathbf{v}_\pm = \mathbf{v} \pm \mathbf{u}$ while the complex valued quantum velocity is defined as

$$\mathbf{v}_q(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}, t) - i\mathbf{u}(\mathbf{x}, t) = \frac{\hbar}{i\, m}\nabla \ln \psi(\mathbf{x}, t). \tag{3.189}$$

This complex drift encodes the essential quantum mechanical information, combining in a single complex field the current and osmotic velocities.

Let the forward and backward generators, acting on smooth (twice differentiable), compactly supported [2] test functions $f \in C_0^2 : \mathbb{R}^d \times [t_0, t_1] \longrightarrow \mathbb{C}$ be defined by

$$(L_\pm f)(\mathbf{x}, t) = \mathbf{v}_\pm(\mathbf{x}, t) \cdot \nabla f(\mathbf{x}, t) \pm \frac{\hbar}{2m}\nabla^2 f(\mathbf{x}, t). \tag{3.190}$$

These operators generate, respectively, the forward and backward diffusive evolutions associated with the stochastic processes $\mathbf{x}_\pm(t)$. By taking the complex linear combination

$$L_b = \frac{1 - i}{2} L_+ + \frac{1 + i}{2} L_-, \tag{3.191}$$

we define the *bi-directional generator*, which combines the forward and backward dynamics into a single complex operator. Its explicit form is

$$(L_b f)(\mathbf{x}, t) = \mathbf{v}_q(\mathbf{x}, t) \cdot \nabla f(\mathbf{x}, t) - \frac{i\hbar}{2m}\nabla^2 f(\mathbf{x}, t). \tag{3.192}$$

Note that the $L_\pm$ is present in the deterministic part of the forward/backward expansion of the function f via Itô's formula. Likewise, L_b is present on the deterministic part of the Itô-like expansion of a function f in the complex formulation of the stochastic process, see Eq. (3.105).

[2] A function with compact support is zero everywhere outside of a bounded region of space where it takes nonzero values.

Let $L^{2,1}$ denote the Hilbert space of complex-valued functions $g : \mathbb{R}^d \times [t_0, t_1] \longrightarrow \mathbb{C}$ satisfying

$$\int_{t_0}^{t_1} \int_{\mathbb{R}^d} |g(\mathbf{x}, t)|^2 \, d\mathbf{x} \, dt < \infty. \tag{3.193}$$

We can now state the central result establishing the operator equivalence between the stochastic and quantum mechanical descriptions as presented by Pavon [72].

Theorem 5 (Unitary Equivalence) *Let $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})$ defined in $L^{2,1}$ be the Hamiltonian operator and $\psi(\mathbf{x}, t)$ be a solution of the Schrödinger equation*

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi.$$

Assume that ψ is never vanishing on the time interval considered and satisfies the finite-action condition

$$\int \int |\nabla \psi|^2 \, d\mathbf{x} \, dt < \infty.$$

Let L_b denote the bi-directional generator of the associated Nelson process as defined in Eq. (3.192)*, and let $L^{2,1}(|\psi|^2)$ denote the Hilbert space of functions g such that $(g\,\psi) \in L^{2,1}$. Then, the stochastic evolution operator $\frac{\partial}{\partial t} + L_b$ defined in $L^{2,1}(|\psi|^2)$ is unitarily equivalent to the quantum evolution operator $\frac{\partial}{\partial t} + \frac{i}{\hbar}H$ via the conjugation relation*

$$\frac{\partial}{\partial t} + L_b = M_\psi^{-1} \left(\frac{\partial}{\partial t} + \frac{i}{\hbar} H \right) M_\psi, \tag{3.194}$$

where M_ψ is the multiplication operator defined by $(M_\psi\, g)(\mathbf{x}, t) = \psi(\mathbf{x}, t)\, g(\mathbf{x}, t)$. The operator M_ψ maps $L^{2,1}(|\psi|^2)$ isometrically onto $L^{2,1}$, and, under the never-vanishing assumption on ψ, it is invertible.

Equation (3.194) shows that Nelson's stochastic dynamics and the Schrödinger description of quantum mechanics are mathematically equivalent under a unitary transformation. The stochastic process described by the bi-directional generator L_b evolves in the Hilbert space weighted by $|\psi|^2$, while the corresponding wave dynamics governed by H evolves unitarily in $L^{2,1}$. The operator M_ψ thus provides the bridge between the probabilistic representation of motion in stochastic quantization and the Hilbert-space formulation of quantum mechanics. A detailed proof of this theorem is given in the Appendix D together with a proof for the following remark.

Remark 2 *Let ψ be a never–vanishing solution of the Schrödinger equation for the Hamiltonian H on a space of nodeless ground states. Consider $L_b(\psi)$ as the bi-directional generator with $\mathbf{v}_q$ calculated from ψ by $\mathbf{v}_q = \frac{\hbar}{im}\nabla \ln \psi$. Then the intertwining identity*

$$\frac{\partial}{\partial t} + L_b(\psi) = M_\psi^{-1} \left(\frac{\partial}{\partial t} + \frac{i}{\hbar} H \right) M_\psi$$

holds as an operator equality from $L^{2,1}(|\psi|^2)$ to $L^{2,1}$. Consequently, for every Schrödinger solution ϕ, the ratio $f = \phi/\psi$ satisfies the stochastic evolution equation $\left(\frac{\partial}{\partial t} + L_b(\psi)\right) f = 0$. In particular, if $H\phi_n = E_n\phi_n$ and $\psi(\mathbf{x}, t) = \psi_0(\mathbf{x})\, e^{-iE_0 t/\hbar}$ is a stationary and nodeless reference state, then

$$f_n(\mathbf{x}, t) = \frac{\phi_n(\mathbf{x})}{\psi_0(\mathbf{x})}\, e^{-i(E_n - E_0)t/\hbar}$$

is a solution of $(\partial_t + L_b(\psi))f_n = 0$. Thus, the spectral data of H are transported to the L_b–representation through the unitary map M_ψ, without the need for a state–dependent family of transformations.

Consequently, any quantum mechanical observable $\hat{A}$ corresponds to a stochastic observable $\tilde{A} = M_\psi^{-1}\hat{A}M_\psi$ such that at each fixed time t, the expectations are preserved, i.e.,

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle_{L^2} = \langle 1|\tilde{A}|1\rangle_{L^2(|\psi(t)|^2)}. \tag{3.195}$$

This correspondence, established through the unitary equivalence, reveals the full compatibility of Nelson's stochastic quantization with the quantum mechanical postulates. Such a framework opens promising avenues for computational implementations and conceptual developments in quantum theory. Note that ψ in (3.195) should be a ground-state (nodeless) wave function. Furthermore, we are able to incorporate the excited states as ground-state wave functions of a modified potential via a supersymmetric procedure introduced in the following.

3.5 EXCITED STATES

As we have seen, Nelson's stochastic formulation is restricted to the description of nodeless states, typically corresponding to the ground state of a quantum system. However, the formalism can be extended to include excited states; this is done by employing a supersymmetric (SUSY) procedure within the framework of bound states. This approach, inspired by supersymmetric quantum mechanics, establishes a hierarchy of Hamiltonians whose spectra are related through algebraic transformations, thereby allowing the construction of higher excited states from ground-state solutions [14].

Consider the quantum mechanical Hamiltonian

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x), \tag{3.196}$$

with eingenvalues E_n and eigenfunctions $\Psi_n(x)$ satisfying $\hat{H}_0\Psi_n(x) = E_n\Psi_n(x)$ for $n = 0, 1, 2, \ldots$. Following the SUSY formalism, this Hamiltonian can be factorized as

$$\hat{H}_0 = \hat{A}_0^+\hat{A}_0^- + E_0, \tag{3.197}$$

where the operators

$$\hat{A}_0^{\pm} \equiv \frac{\hbar}{\sqrt{2m}} \left(\mp \frac{d}{dx} - \frac{1}{\Psi_0(x)} \frac{d\Psi_0(x)}{dx} \right) = -\sqrt{\frac{m}{2}} \left(u_0(x) \pm \frac{\hbar}{m} \frac{d}{dx} \right) \tag{3.198}$$

are mutually Hermitian adjoints [87] and are referred to as *generalized ladder operators*. Here, $u_0(x)$ denotes the osmotic velocity associated with the ground state $\Psi_0(x)$.

The supersymmetric partner Hamiltonian is defined as

$$\hat{H}^1 = \hat{A}_0^- \hat{A}_0^+ + E_0, \tag{3.199}$$

which has the same energy spectrum of $\hat{H}_0$, except for the ground state energy E_0. Consequently, the ground state of $\hat{H}_1$ corresponds to the first excited state of the original Hamiltonian operator $\hat{H}_0$ [14, 83]. As demonstrated by [87], the first excited state wave function can be written as

$$\Psi_1(x) = \frac{1}{\sqrt{E_1 - E_0}} \hat{A}_0^+ \varphi_0^1(x) \tag{3.200}$$

where $\varphi_0^1(x)$ denotes the ground-state wave function of the supersymmetric partner Hamiltonian $\hat{H}_1$. The action of the ladder operators $\hat{A}_0^{\pm}$ establishes a correspondence between the eigenfunction spaces of the two superpartner Hamiltonians. In other words, applying $\hat{A}_0^+$ or $\hat{A}_0^-$ maps eigenfunctions of $\hat{H}_1$ to those of $\hat{H}_0$ and vice versa. This algebraic mechanism allows one to generate the excited states of the original Hamiltonian $\hat{H}_0$ recursively from the ground state of its successive SUSY partners.

The time-independent Shcrödinger equation for the ground state $\Psi_0 = e^{R_0(x)}$ yields

$$\left[-\frac{\hbar^2}{2m} R_0''(x) - \frac{\hbar}{2m} {R_0'}^2 + V(x) - E_0 \right] e^{R_0(x)} = 0, \tag{3.201}$$

where the prime denotes differentiation with respect to x. Inserting the expression for the osmotic velocity, $u_0(x) = \frac{\hbar}{m} R_0'(x)$, the potential $V(x)$ can be rewritten as

$$V(x) = E_0 + \frac{m}{2} u_0^2(x) + \frac{\hbar}{2} u_0'(x). \tag{3.202}$$

The superpartner Hamiltonian $\hat{H}_1$ can be expressed as

$$\begin{aligned} \hat{H}_1 &= \hat{A}_0^- \hat{A}_0^+ + E_0 \\ &= \frac{m}{2} \left(-u_0(x) + \frac{\hbar}{m} \frac{d}{dx} \right) \left(-u_0(x) - \frac{\hbar}{m} \frac{d}{dx} \right) + E_0 \\ &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m}{2} u_0^2(x) - \frac{\hbar}{2} \frac{du_0(x)}{dx} + E_0 \\ &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) - \hbar u_0'(x), \end{aligned} \tag{3.203}$$

where in the last step we have used the expression (3.202) for $V(x)$. Hence, the Hamiltonian $\hat{H}_1$ can be defined as

$$\hat{H}_1 \coloneqq -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x), \tag{3.204}$$

where the superpartner potential

$$V_1(x) = V(x) - \hbar u_0'(x) \tag{3.205}$$

is a modified potential readily obtained once the osmotic velocity $u_0(x)$ of the ground state of $\hat{H}_0$ is known.

Therefore, as suggested by Grigorenko [88], the stochastic quantization framework combined with optimal control theory can be employed to determine the ground-state wave function $\varphi_0^1(x)$ of $\hat{H}_1$. Once $\varphi_0^1(x)$ is obtained, it can be transformed into the first excited state of $\hat{H}_0$ through Eq. (3.200), namely,

$$\Psi_1(x) = -\sqrt{\frac{m}{2(E_1 - E_0)}} \left(u_0(x) + \frac{\hbar}{m} \frac{d}{dx} \right) \varphi_0^1(x). \tag{3.206}$$

Next, by factorizing the Hamiltonian $\hat{H}_1 = \hat{A}_1^+ \hat{A}_1^- + E_1$ in the same manner as for $\hat{H}_0$, the second excited state can be obtained by first determining the ground state $\varphi_0^2(x)$ of the superpartner Hamiltonian $\hat{H}_2 = \hat{A}_1^- \hat{A}_1^+ + E_1$ with potential $V_2 = V_1(x) - \hbar u_1'(x)$, where $u_1(x)$ is the osmotic velocity associated to the ground state $\varphi_0^1(x)$. This recursive procedure can be applied indefinitely to construct an arbitrary number of excited states. In general, the n-th excited-state wave function of the original Hamiltonian $\hat{H}_0$ is expressed as

$$\Psi_n(x) = \prod_{i=0}^{n-1} \left[\frac{\hat{A}_i^+}{\sqrt{E_n - E_i}} \right] \varphi_0^n(x), \tag{3.207}$$

where $\varphi_0^n(x)$ denotes the ground state wave function of the Hamiltonian operator associated with the n-fold modified potential

$$V_n(x) = V(x) - \hbar \sum_{i=0}^{n-1} u_i'(x), \tag{3.208}$$

where $u_i(x)$ denotes the osmotic velocity associated with the state $\varphi_0^i(x)$, $i < n$.

Once a numerical method is available to obtain the ground-state osmotic velocity by directly integrating the FBSDE system (3.183), the same approach can, through the SUSY procedure presented here, be extended to compute the ground-state osmotic velocity associated with each Hamiltonian $\hat{H}_n$. This allows the determination of all ground-state functions $\varphi_0^n(x)$ and, consequently, of the excited-state wave functions via Eq. (3.207).

As a direct consequence of relation (3.195), the corresponding eigenvalues can be computed from

$$E_n = \mathbb{E}\left[\frac{1}{2} m u_n^2(x) + V_n(x) \right] = \int_{-\infty}^{+\infty} \left[\frac{1}{2} m u_n^2(x) + V_n(x) \right] |\varphi_0^n(x)|^2 dx \tag{3.209}$$

where $u_n(x)$ denotes the osmotic velocity associated with the state $\varphi_0^n(x)$ of the operator $\hat{H}_n$. Therefore, a stationary quantum problem can be fully solved directly from the quantum

Hamilton equations of motion, combined with the SUSY formalism, without the need to explicitly solve the Schrödinger equation [14, 17].

In Ref. [14], examples are presented for the computation of all states of the quantum harmonic oscillator and several states of the quartic (double-well) potential. In Ref. [89], the Hydrogen atom is treated analogously. These works provide concrete demonstrations of the equivalence between Nelson's stochastic quantization and standard quantum mechanics.

3.6 REMARKS ABOUT STOCHASTIC QUANTIZATION

The formulation of quantum mechanics based on stochastic processes, presented in this chapter, combines the kinematic description of particle trajectories introduced by Nelson with the variational principles developed by Yasue [90] and Guerra and Morato [69], later refined by Pavon [15]. Altogether, these ideas are commonly referred to as *Nelson's Stochastic Quantization* or *Stochastic Mechanics*. As demonstrated here, this quantization scheme is unitarily equivalent to the standard formulation of quantum mechanics established by Schrödinger and Heisenberg. Furthermore, a direct correspondence between stochastic quantization and the Feynman path integral formulation can also be established, as shown in [72]. Moreover, the collapse of the wave function can also be reinterpreted in the light of Nelson's stochastic quantization [91]. A comprehensive and up-to-date presentation of stochastic mechanics can be found in Ref. [66].

The theoretical framework discussed here applies exclusively to non-relativistic, spinless, single-particle systems. The inclusion of the interaction with electromagnetic fields is also possible [54]. An extension of stochastic quantum formalism for multi-particle systems can be readily constructed [5, 92]. Extensions to include spin degrees of freedom have been developed [19, 93, 94, 95]. Furthermore, several works explore the generalization of stochastic quantization to differential manifolds, some of them aiming to construct a non-perturbative approach to quantum gravity [20, 21, 96, 97].

However, a conceptual difficulty can arise when the stochastic formulation is applied to entangled systems, as emphasized by Nelson [98]. In particular, he observed that the predictions of stochastic mechanics for certain multi-time correlation functions do not coincide with those of standard quantum mechanics. Since multi-time correlations are directly related to experimentally accessible measurement statistics, this discrepancy appeared to signal an inconsistency of the theory in the presence of entanglement. This issue was examined by Blanchard, Golin, and Serva [99]. They showed that the apparent disagreement was due to an incomplete treatment of the measurement process within the stochastic framework. In summary, once one properly accounts for measurement-induced state updating, the stochastic predictions for multi-time correlations are brought into agreement with those of standard quantum theory. More recent analyses have revisited

and clarified this point, further reinforcing the consistency of the approach [66, 92].

Nelson was also concerned about the explicitly nonlocal character of stochastic mechanics for entangled states, interpreting this feature as a potential failure of the theory [100]. From a contemporary standpoint, however, such nonlocality is not regarded as a defect but rather as an unavoidable structural aspect of any theory that reproduces quantum phenomena, for which nonlocal correlations are required to account for entanglement and the experimentally verified violations of Bell-type inequalities [66, 92, 101].

As Nelson pointed out [5], if the Schrödinger equation had been derived from stochastic principles before the advent of matrix mechanics, the history of modern physics might have taken a different course. According to him, "stochastic mechanics is more vulnerable than quantum mechanics, because it is more ambitious: it attempts to provide a realistic, objective description of physical events in classical terms. Stochastic mechanics is quantum mechanics made difficult" [5]. In a later reflection, Nelson suggested that stochastic mechanics should be regarded as an approximation to a correct, yet unknown, emergent theory of quantum mechanics [98].

In this sense, Nelson's stochastic quantization provides a conceptually distinct and mathematically rigorous formulation of quantum mechanics for single spinless particles. It not only reproduces predictions of the standard formalism for individual spinless non-relativistic particles but also offers new tools, which can be helpful to explore problems that are difficult to treat by conventional methods. One such long-standing problem is the determination of tunneling times. The question: "How long does a quantum particle take to traverse a potential barrier?" has remained open since the earliest days of quantum theory. The following chapters will address this problem within the framework of Nelson's stochastic quantization, providing new insights into the temporal aspects of quantum tunneling.

4 MEAN FIRST PASSAGE TIME

This chapter presents the mean first passage time theory, a key result in stochastic processes that will be essential in the fifth and sixth chapters of this thesis. The problem of the mean first passage time of a particle through a certain point is equivalent to asking how much time a particle spends in a certain region of x. So, using the theory of stochastic process, we are going to calculate the mean exit time from a region delimited by a and b [38, 44, 45].

We consider a particle whose position follows a stochastic process described by the SDE

$$dx(t) = a(x)dt + b(x)dW(t). \tag{4.1}$$

We will also consider two boundaries, one at $x = a$ and the other at $x = b$. At $t = 0$, the particle is in the position $a \leq x \leq b$. The probability that at time t the particle is still in this interval is given by

$$G(x,t) = \int_a^b dx' p(x',t|x,0), \tag{4.2}$$

where $p(x',t|x,0)$ denotes the conditional probability density for the particle to be found at position x' at time t, given that it was located at x at time $t = 0$. Let us define τ as the time when the particle leaves the region $[a,b]$. Therefore, $G(x,t)$ is the probability that $\tau \geq t$, because in this case, for a time $t < \tau$ the particle has not yet left the interval. Then we can write

$$G(x,t) = \text{Prob}(\tau \geq t) = \int_t^\infty p_{\text{exit}}(\tau)d\tau, \tag{4.3}$$

where $p_{\text{exit}}(\tau)$ is the probability density for the exit time τ, i.e., that the particle starting at the point x inside the interval $[a,b]$ at time $t = 0$ exits this interval at $t = \tau$.

Now, we will use the Kolmogorov backward equation (2.35) associated with the SDE (4.1),

$$\frac{\partial}{\partial t}p(x',t'|x,t) = -a(x)\frac{\partial}{\partial x}p(x',t'|x,t) - \frac{1}{2}b^2(x)\frac{\partial^2}{\partial x^2}p(x',t'|x,t). \tag{4.4}$$

Considering the system as stationary in the sense that it only depends on time intervals, we can shift the conditional probability by an arbitrary time difference $-t$. Therefore, $p(x',t|x,0) = p(x',0|x,-t)$. Substituting $p(x',t'|x,t)$ by $p(x',0|x,-t)$ in Eq. (4.4), we get

$$\frac{\partial}{\partial t}p(x',0|x,-t) = a(x)\frac{\partial}{\partial x}p(x',0|x,-t) + \frac{1}{2}b^2(x)\frac{\partial^2}{\partial x^2}p(x',0|x,-t). \tag{4.5}$$

Hence, $G(x,t)$ satisfies the following partial differential equation:

$$\frac{\partial}{\partial t}G(x,t) = a(x)\frac{\partial}{\partial x}G(x,t) + \frac{1}{2}b^2(x)\frac{\partial^2}{\partial x^2}G(x,t), \tag{4.6}$$

with boundary conditions

$$G(x,0) = \begin{cases} 1 & a \le x \le b, \\ 0 & x < a \text{ or } x > b. \end{cases} \tag{4.7}$$

Since $G(x,t)$ is the probability that $\tau \geq t$, we can conclude that $G(x,t)$ is the complement of the cumulative probability distribution of exit times. Therefore,

$$p_{\text{exit}}(t) = \frac{\partial}{\partial t}\Big(1 - G(x,t)\Big) = -\frac{\partial G(x,t)}{\partial t}, \tag{4.8}$$

and the *mean exit time* $\bar{\tau} \equiv \langle \tau \rangle$ can be calculated by

$$\bar{\tau} = -\int_0^\infty t\, \frac{\partial G(x,t)}{\partial t} dt = \int_0^\infty G(x,t) dt, \tag{4.9}$$

where we have applied integration by parts and made use of the condition

$$\lim_{t\to\infty}\; t\, G(x,t) = 0.$$

If we integrate Eq. (4.6) over t, from 0 to ∞, we get

$$\int_0^\infty dt \frac{\partial}{\partial t} G(x,t) = a(x)\frac{d}{dx}\bar{\tau}(x) + \frac{1}{2}b^2(x)\frac{d^2}{dx^2}\bar{\tau}(x). \tag{4.10}$$

We also have

$$\int_0^\infty dt \frac{\partial}{\partial t} G(x,t) = G(x,\infty) - G(x,0) = -1, \tag{4.11}$$

Since the particle will exit the region $[a,b]$ at some time, i.e., $G(0,\infty) = 0$ and $G(x,0) = 1$, which follows from the boundary conditions (4.7). Therefore, we obtain a second-order differential equation for the mean exit time $\bar{\tau}(x)$:

$$\frac{1}{2}b^2(x)\frac{d^2\bar{\tau}(x)}{dx^2} + a(x)\frac{d\tau(x)}{dx} = -1. \tag{4.12}$$

Equation (4.12) can be written as

$$\frac{du(x)}{dx} + p(x)u(x) = q(x), \tag{4.13}$$

where $u(x) = d\bar{\tau}(x)/dx$, $p(x) = 2a(x)/b^2(x)$, and $q(x) = -2/b^2(x)$. The homogeneous solution of Eq. (4.13) can be found by direct integration, and a particular solution can be found by the method of variation of the constants. Alternatively, we can apply the method of integrating factor. Thus, the general solution for Eq. (4.13) is

$$\bar{\tau}(x) = -\int_a^x \left(\frac{2}{\phi(x')}\int_a^{x'} \frac{\phi(x'')}{b^2(x'')}dx''\right)dx' + C_1\int_a^x \frac{dx'}{\phi(x')} + C_2, \tag{4.14}$$

where

$$\phi(x) = \exp\left(\int_a^x \frac{2a(x')}{b^2(x')}dx'\right), \tag{4.15}$$

with C_1 and C_2 being integration constants determined by the boundary conditions. The appropriate boundary conditions are determined according to the nature of the boundaries in a and b [45].

We are interested in the case where there are a reflecting boundary and an absorbing boundary. The reflecting boundary will be located at the left, in $x = a$, and the absorbing boundary will be located at the right, in $x = b$. This means that the particle can only exit the interval $[a, b]$ at $x = b$. The time when the particle exits the interval is called first passage time. The respective boundary conditions for this case are

$$\bar{\tau}(b) = 0 \quad \text{and} \quad \left.\frac{d\bar{\tau}(x)}{dx}\right|_{x=a} = 0. \tag{4.16}$$

Applying these boundary conditions in Eq. (4.14), we find

$$\begin{aligned} C_1 &= 0, \\ C_2 &= \int_a^b \left(\frac{2}{\phi(x)} \int_a^x \frac{\phi(x')}{b^2(x')} dx' \right) dx, \end{aligned} \tag{4.17}$$

and the complete solution is

$$\bar{\tau}(x) = 2 \int_x^b \frac{1}{\phi(x')} \left(\int_a^{x'} \frac{\phi(x'')}{b^2(x'')} dx'' \right) dx'. \tag{4.18}$$

The mean exit time in Eq. (4.18) is known as *mean first passage time* (MFPT) and determines the mean time for a particle, with trajectory described by the SDE (4.1), to pass through the boundary $x = b$ for the first time given that it started at a point $x \in [a, b]$ and is reflected at $x = a$.

4.1 APPLICATION TO NELSON'S FORMALISM

Now, let us apply Eq. (4.18) to the stochastic trajectory of a particle in Nelson's stochastic quantization, as defined in Eqs. (3.53). The resulting expression depends on whether the probability current density, given by $j(x) = \rho(x)v(x)$, vanishes or not. In what follows, we restrict our attention to stationary quantum states, for which the probability density $\rho(x)$ is time-independent. Consequently, both the osmotic velocity $u(x)$ and the current velocity $v(x)$ are also time-independent.

Within the framework of Nelson's stochastic quantization, every quantum particle is associated with a stochastic trajectory that represents its diffusive motion through space. Consider the one-dimensional forward stochastic trajectory described by

$$dx(t) = [v(x) + u(x)]dt + \sigma dW(t), \tag{4.19}$$

where $\sigma^2 = \hbar/m$ is the fluctuation coefficient associated with the stochastic dynamics. Recalling expression (4.18), the mean first passage time for a particle following the SDE

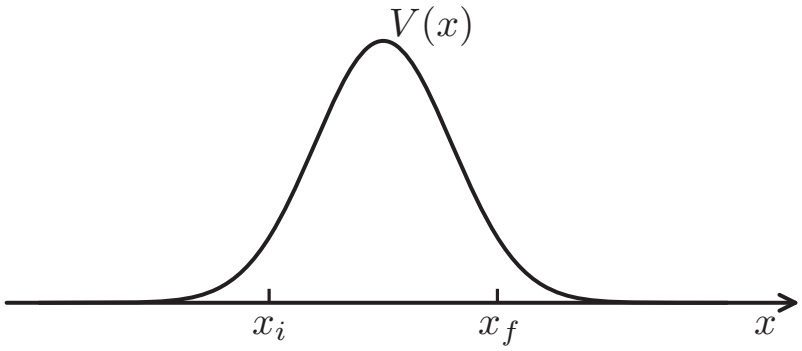


FIGURE 6 – Generic one-dimensional potential barrier $V(x)$ as a function of position. In the mean first passage time problem applying Nelson's formalism, the particle starts at position x_i at $t = 0$ and passes through x_f for the first time at $t = \tau$. The mean value $\bar{\tau}$ is calculated within the theory of stochastic processes.

(4.19) initially in the position $x \in [a, b]$ to exit through the boundary at $x = b$ is given by

$$\bar{\tau}(x) = \frac{2m}{\hbar} \int_x^b \frac{1}{\phi(y)} \left(\int_a^y \phi(z)\, dz \right) dy, \tag{4.20}$$

where

$$\phi(x) = \exp\left[\frac{2m}{\hbar} \int_a^x \Big(v(y) + u(y) \Big)\, dy \right]. \tag{4.21}$$

Under these conditions, two distinct situations arise. For *scattering states*, the presence of a net flux implies a non-vanishing $j(x)$. In contrast, for *bound states* the probability distribution is localized in such a way that the net current vanishes, yielding $j(x) = 0$. These two cases require separate treatments in the application of the mean first passage time formalism.

4.1.1 Scattering States

Consider a generic potential barrier as the one represented in Fig. 6. Initially, the particle is assumed to be within the region $[-\infty, x_f]$. The mean time required for the particle to pass through the potential barrier and reach the point x_f can then be evaluated using the MFPT expression given in Eq. (4.20), with the boundary values $a = -\infty$ and $b = x_f$. We consider that the particle starts on the left-hand side of the barrier, at an initial position $x_i \in [-\infty, x_f]$.

The stationary wave function can be expressed in polar form using the expression $\psi(x) = \sqrt{\rho(x)} \exp(iS(x)/\hbar)$, where $\rho(x) = |\psi(x)|^2$ denotes the probability density and $S(x)$ is the real phase function. Within Nelson's stochastic quantization framework, the associated current and osmotic velocities are respectively given by

$$v(x) = \frac{S'(x)}{m}, \qquad u(x) = \frac{\hbar}{2m} \frac{\rho'(x)}{\rho(x)}, \tag{4.22}$$

where primes denote derivatives with respect to the spatial coordinate. Consequently, the auxiliary function $\phi(x)$, see Eq. (4.21), introduced in the MFPT formula takes the form

$$\phi(x) = \exp\left[\frac{2m}{\hbar}\int_{-\infty}^{x}\left(\frac{S'(y)}{m} + \frac{\hbar}{2m}\frac{\rho'(y)}{\rho(y)}\right)dy\right], \tag{4.23}$$

Carrying out the integration of $\rho'(y)/\rho(y)$, we obtain

$$\phi(x) = C_0\,\rho(x)\exp\Big(\frac{2}{\hbar}\int_{-\infty}^{x} S'(y)\,dy\Big), \tag{4.24}$$

where C_0 is an integration constant. Next, carrying out the integration of $S'(y)$ yields

$$\begin{aligned}\phi(x) &= C_0\,\rho(x)\exp\Big[\frac{2}{\hbar}\big(S(x) - S(-\infty)\big)\Big] \\ &= C_0\,\rho(x)\exp\left(\frac{2}{\hbar}S(x)\right)\exp\left(-\frac{2}{\hbar}S(-\infty)\right),\end{aligned} \tag{4.25}$$

where $\exp\left(-\frac{2}{\hbar}S(-\infty)\right)$ is also constant. Consequently, defining $C = C_0\exp\left(-\frac{2}{\hbar}S(-\infty)\right)$, we get

$$\phi(x) = C\,\rho(x)\exp\left(\frac{2}{\hbar}S(x)\right), \tag{4.26}$$

Now, substituting Eq. (4.26) into expression (4.20) for $\bar{\tau}$, yields

$$\begin{aligned}\bar{\tau}(x_i, x_f) &= \frac{2m}{\hbar}\int_{x_i}^{x_f}\frac{1}{\rho(x)\exp\left(\frac{2}{\hbar}S(x)\right)}\left[\int_{-\infty}^{x}\rho(y)\exp\left(\frac{2}{\hbar}S(y)\right)dy\right]dx \\ &= \frac{2m}{\hbar}\int_{x_i}^{x_f}\frac{F(x)}{\rho(x)}\exp\left(-\frac{2}{\hbar}S(x)\right)dx,\end{aligned} \tag{4.27}$$

where we made the substitution

$$F(x) = \int_{-\infty}^{x}\rho(y)\exp\left(\frac{2}{\hbar}S(y)\right)dy. \tag{4.28}$$

Differentiating the exponential function yields

$$\begin{aligned}\frac{d}{dx}\exp\left(-\frac{2}{\hbar}S(x)\right) &= -\frac{2}{\hbar}S'(x)\exp\left(-\frac{2}{\hbar}S(x)\right) \\ &= -\frac{2m}{\hbar}v(x)\exp\left(-\frac{2}{\hbar}S(x)\right).\end{aligned} \tag{4.29}$$

Therefore,

$$\exp\left(-\frac{2}{\hbar}S(x)\right) = -\frac{\hbar}{2m}\frac{1}{v(x)}\frac{d}{dx}\exp\left(-\frac{2}{\hbar}S(x)\right). \tag{4.30}$$

Substituting this expression into Eq. (4.27) for $\bar{\tau}(x_i, x_f)$ and recalling that $j(x) = \rho(x)v(x)$, we obtain

$$\bar{\tau}(x_i, x_f) = -\int_{x_i}^{x_f}\frac{F(x)}{j(x)}\frac{d}{dx}\exp\left(-\frac{2}{\hbar}S(x)\right)dx. \tag{4.31}$$

Now we can perform an integration by parts, leading to

$$\bar{\tau}(x_i, x_f) = -\left[\frac{F(x)}{j(x)}\exp\left(-\frac{2}{\hbar}S(x)\right)\right]_{x_i}^{x_f} + \int_{x_i}^{x_f}\exp\left(-\frac{2}{\hbar}S(x)\right)\frac{d}{dx}\left(\frac{F(x)}{j(x)}\right)dx. \tag{4.32}$$

But the state $\psi(x)$ is stationary, i.e., it doesn't depend on time, then from the continuity equation, $j(x)$ must be a constant: $j(x) = j$. Additionally,

$$\frac{d}{dx}F(x) = \rho(x)\exp\left(\frac{2}{\hbar}S(x)\right). \tag{4.33}$$

Finally, we find

$$\begin{aligned}\bar{\tau}(x_i, x_f) = \int_{x_i}^{x_f}\frac{dx}{v(x)} + \frac{\exp\left(-\frac{2}{\hbar}S(x_i)\right)}{j}\int_{-\infty}^{x_i}\rho(x)\exp\left(\frac{2}{\hbar}S(x)\right)dx \\ - \frac{\exp\left(-\frac{2}{\hbar}S(x_f)\right)}{j}\int_{-\infty}^{x_f}\rho(x)\exp\left(\frac{2}{\hbar}S(x)\right)dx,\end{aligned} \tag{4.34}$$

for the mean passage time of a particle described by a scattering state in the stochastic quantization framework. When the particle energy lies below the barrier height, the quantity $\bar{\tau}$ corresponds to a tunneling time. This expression appears in Ref. [13], where the authors analyze the problem of the tunneling time through a square potential barrier.

4.1.2 Bound States

For bound states, arising from a confining potential such as the one illustrated in Fig. 7, the stationary wavefunction can always be chosen to be real implying that the complex phase $S(x)$ in the polar form of the wavefunction, $\psi(x) = \sqrt{\rho(x)}\exp(iS(x)/\hbar)$, vanishes. As discussed in the previous chapter, a vanishing phase leads to a null current velocity, $v(x) = \nabla S(x)/m = 0$, and consequently to zero probability current density $j = 0$. In this situation, the particle dynamics in Nelson's stochastic framework is governed solely by the osmotic velocity, and the associated forward SDE is

$$dx(t) = u(x)dt + \sqrt{\frac{\hbar}{m}}dW(t) \tag{4.35}$$

where, as before, $u(x) = (\hbar/m)\nabla\ln\psi(x)$ denotes the osmotic velocity.

Recalling the general expression for the MFPT in Nelson's formalism,

$$\bar{\tau}(x) = \frac{2m}{\hbar}\int_x^b \frac{1}{\phi(y)}\left(\int_a^y \phi(z)\,dz\right)dy, \tag{4.36}$$

where x is the initial position of the particle initially within the interval $[a, b]$, and we find that for $v(x) = 0$, the auxiliary function $\phi(x)$ in Eq. (4.21) simplifies to

$$\phi(x) = \exp\left[\frac{2m}{\hbar}\int_a^x u(y)\,dy\right]. \tag{4.37}$$

Substituting the expression for $u(x)$ into the expression above yields

$$\phi(x) = \exp\left[2\int_a^x \frac{d}{dy}\ln\psi(y)\,dy\right] = \frac{|\psi(x)|^2}{|\psi(a)|^2} = Cp(x), \tag{4.38}$$

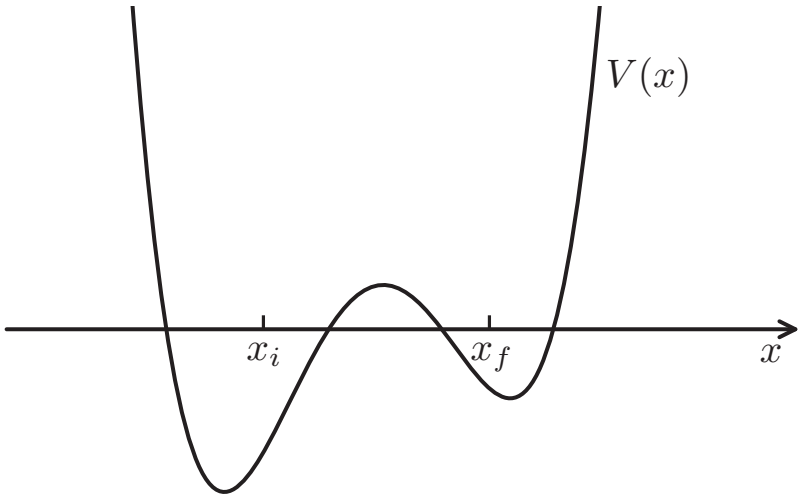


FIGURE 7 – Generic one-dimensional confining potential $V(x)$ as a function of position. In the mean first passage time problem applying Nelson's formalism,the particle starts at position x_i at $t = 0$ and passes through x_f for the first time at $t = \tau$. The mean value $\bar{\tau}$ is calculated within the theory of stochastic processes.

with $p(x) = |\psi(x)|^2$ being the probability density, and $C = 1/|\psi(a)|^2$ is a constant. Hence, for bound systems with $j = v = 0$, the mean passage time for a particle initially located at $x_i \in [-\infty, x_f]$ can be written as

$$\bar{\tau}(x_i, x_f) = \frac{2m}{\hbar} \int_{x_i}^{x_f} \frac{1}{p(x)} \left(\int_{-\infty}^{x} p(y)\, dy \right) dx. \tag{4.39}$$

Expression (4.39) represents the mean time a particle, initially at $x_i \in [-\infty, x_f]$, remains in the region $[-\infty, x_f]$ before escaping through the point x_f.

Note that in the classical limit, $\hbar/m \to 0$, Eq. (4.39) implies that $\bar{\tau} \to \infty$. This behavior is consistent with the fact that the osmotic velocity $u(x)$ vanishes in this limit. Consequently, since both the osmotic and current velocities go to zero, the particle remains at rest at the equilibrium position, and the tunneling time diverges.

4.2 EXPONENTIAL DECAY FOR FIRST PASSAGE TIME PROBABILITY

Previously, we have shown that the mean first passage time can be expressed as

$$\bar{\tau} = \int_0^{\infty} G(x, t) dt, \tag{4.40}$$

where the function $G(x, t)$ represents the probability that the particle has not yet exited the domain by time t. Hence, $G(x, t)$ is referred to as the *survival probability*. The function $G(x, t)$ satisfies the backward Fokker–Planck equation, see Eq. (4.6):

$$\frac{\partial G(x, t)}{\partial t} = \mathcal{L}_x G(x, t), \tag{4.41}$$

where the backward operator $\mathcal{L}_x$ is defined as

$$\mathcal{L}_x = a(x) \frac{\partial}{\partial x} + \frac{1}{2} b^2(x) \frac{\partial^2}{\partial x^2}. \tag{4.42}$$

Let us now assume a separable solution of the form $G(x,t) = \phi(x)T(t)$. Substituting this into the equation above yields

$$\frac{T'(t)}{T(t)} = \frac{\mathcal{L}_x\phi(x)}{\phi(x)} = -\lambda \tag{4.43}$$

where λ is a separation constant. The temporal part then satisfies the first-order differential equation $T'(t) = -\lambda T(t)$ whose general solution is

$$T(t) = T(0)e^{-\lambda t}. \tag{4.44}$$

The spatial component, in turn, satisfies $\mathcal{L}_x\phi(x) = -\lambda\phi(x)$ subjected to the boundary conditions $\phi'(a) = \phi(b) = 0$, see Eq. (4.16). This constitutes a Sturn-Liouville problem with eigenvalues $\lambda_1 < \lambda_2 < \ldots < \lambda_n < \ldots$ and corresponding eigenfunctions $\phi_1(x), \phi_2(x), \ldots, \phi_n(y), \ldots$.

Therefore, the general solution for the survival probability is given by the spectral expansion

$$G(x,t) = \sum_{i=1}^{\infty} c_i\phi_i(x)e^{-\lambda_i t}, \tag{4.45}$$

where the coefficients c_i are determined by the initial conditions. For long times, the term with the smallest eigenvalue λ_1 dominates, leading to

$$G(x,t) \approx c_1\phi_1(x)e^{-\lambda_1 t} = C(x)e^{-\lambda_1 t} \quad \text{as} \quad t \to \infty, \tag{4.46}$$

where $C(x) = c_1\phi_1(x)$. Note that λ_1 is the principal eigenvalue (the smallest in magnitude) of the operator $-\mathcal{L}_x$, which defines the characteristic timescale for the escape process, while the prefactor $C(x)$ encodes its spatial dependence. Thus, the survival probability exhibits exponential decay at large times, a hallmark of escape dynamics in bounded domains, with decay rate determined by the principal eigenvalue of the backward operator [102, 103].

Consequently, using Eq. (4.8), we can conclude that the first passage time density, or the probability density for the exit time τ, also exhibits an exponential tail for large τ:

$$p_{\text{exit}}(x,\tau) \approx \lambda_1 C(x)e^{-\lambda_1\tau}. \tag{4.47}$$

From a physical standpoint, the principal eigenvalue λ_1 represents the inverse of the characteristic lifetime of the particle within the confining region. In other words, $1/\lambda_1$ provides an approximation of the average time the particle remains confined before escaping, known as the mean first passage time.

5 TUNNELING TIMES I: SCATTERING STATES

The problem of defining and calculating passage time in quantum mechanics remains a longstanding and fundamental open question, primarily due to the absence of a self-adjoint time operator. This issue becomes particularly significant in the context of quantum tunneling, where one seeks to determine the time a particle spends traversing a potential barrier. Over the past decades, numerous theoretical approaches have been proposed to address this question [12, 104, 105, 106].

Among the most notable are the Büttiker-Landauer time, which estimates the traversal time from the response of a slowly modulated potential barrier [107], and the Larmor clock, which infers the tunneling duration from the precession of a particle's spin in a weak magnetic field applied within the barrier region [108]. Another widely discussed quantity is the phase delay time, derived from the stationary phase approximation, which measures the temporal shift of the transmitted wave packet peak relative to free propagation [109]. The dwell time, on the other hand, provides an average measure of the time a particle spends within a spatial region, independent of whether it is ultimately reflected or transmitted [110].

More recent developments have sought to construct a time-symmetric formulation of quantum mechanics, in which time is promoted to the status of an operator within an extended Hilbert space, akin to other canonical observables [106, 111, 112, 113]. Despite these efforts, the physical interpretation and consistency of such time definitions remain under discussion. In particular, issues related to causality, superluminal transmission, and the non-uniqueness of time observables continue to challenge the establishment of a universally accepted notion of tunneling time [114, 115, 116].

In this thesis, the tunneling time problem will be analyzed in the framework of Nelson's stochastic quantization, both in the present and in the following chapter. The discussion in this chapter is devoted to scattering (or unbound) states, specifically the case of a single potential barrier or well, where the particle dynamics are described by plane waves and localized wave packets. In contrast, the next chapter will focus on bound states, addressing the tunneling dynamics and corresponding tunneling times in double-well potentials.

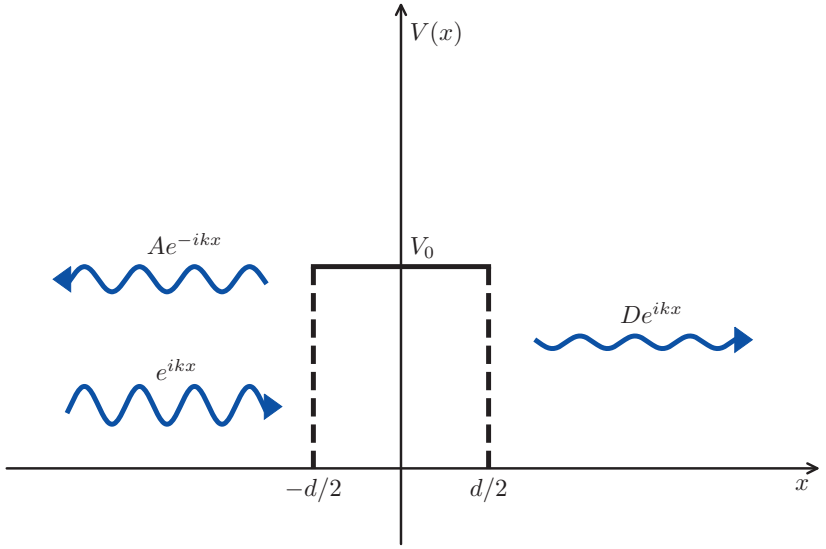


FIGURE 8 – Square barrier potential of height V_0 and width d. A particle with energy $E = \hbar^2 k^2/2m$ is incident from the left, represented by the wave e^{ikx}. The reflected and transmitted components are given by Ae^{-ikx} and De^{ikx}, respectively. The potential is defined as $V(x) = V_0$ for $-d/2 \leq x \leq d/2$ and $V(x) = 0$ otherwise.

5.1 PLANE WAVE AND SINGLE BARRIER/WELL

The system under consideration in this chapter consists of a quantum particle interacting with a single square potential barrier, defined as

$$V(x) = \begin{cases} 0, & |x| \geq d/2, \\ V_0, & -d/2 < x < d/2, \end{cases} \tag{5.1}$$

where $V_0 > 0$ and d denote, respectively, the height and width of the barrier. This potential is illustrated in Fig. 8. Quantum tunneling occurs when the particle has an energy $E < V_0$.

The time-independent Schrödinger equation can then be solved in the three spatial regions defined by the potential:

- **Region I:** $x < -d/2$;
- **Region II:** $-d/2 < x < d/2$;
- **Region III:** $x > d/2$.

Accordingly, for the case $E < V_0$, the stationary wave function takes the form

$$\psi(x) = \begin{cases} e^{ikx} + Ae^{-ikx}, & x < -d/2, \\ Be^{\kappa x} + Ce^{-\kappa x}, & -d/2 \leq x \leq d/2, \\ De^{ikx}, & x > d/2, \end{cases} \tag{5.2}$$

where the coefficients A, B, C, and D correspond, respectively, to the amplitudes of the reflected, decaying, growing, and transmitted components. The wave numbers are defined by

$$k = \frac{\sqrt{2mE}}{\hbar}, \qquad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}, \tag{5.3}$$

and by introducing

$$k_0 = \frac{\sqrt{2mV_0}}{\hbar}, \tag{5.4}$$

one finds the relation

$$\kappa^2 = k_0^2 - k^2. \tag{5.5}$$

Imposing the continuity of both the wave function and its first spatial derivative at the boundaries $x = \pm d/2$, the coefficients are obtained as follows:

$$A = -i\frac{1}{2F}\left(\frac{\kappa}{k} + \frac{k}{\kappa}\right)\sinh(\kappa d), \tag{5.6}$$

$$B = \frac{1}{2F}\left(1 + i\frac{k}{\kappa}\right)e^{-\kappa d/2 + ikd/2}, \tag{5.7}$$

$$C = \frac{1}{2F}\left(1 - i\frac{k}{\kappa}\right)e^{\kappa d/2 + ikd/2}, \tag{5.8}$$

$$D = \frac{1}{F}, \tag{5.9}$$

where

$$F = e^{ikd}\left(\cosh(\kappa d) + i\frac{1}{2}\left(\frac{\kappa}{k} - \frac{k}{\kappa}\right)\sinh(\kappa d)\right). \tag{5.10}$$

The transmission coefficient is $T = |D|^2$ and the reflection coefficient is $R = |A|^2$. An easy calculation shows that $R + T = 1$.

For the case $E > V_0$, the expressions obtained for the wave function remain valid under the substitution $\kappa \to ik_1$, where

$$k_1 = \frac{\sqrt{2m(E - V_0)}}{\hbar}. \tag{5.11}$$

The tunneling time problem can be naturally formulated as a mean first passage time (MFPT) problem, see Chapter 4, since it concerns the average time required for a particle to exit a specified spatial region. Recalling Eq. (4.34) for the MFPT of a particle in a scattering stationary state $\psi(x) = \sqrt{\rho(x)}\exp(iS(x)/\hbar)$, we obtain the following expression for the mean time $\bar{\tau}$ required for a particle initially located at $x_i \in [-\infty, x_f]$, to cross the point x_f:

$$\begin{aligned}\bar{\tau}(x_i, x_f) = \int_{x_i}^{x_f} \frac{dx}{v(x)} + \frac{\exp\left(-\frac{2}{\hbar}S(x_i)\right)}{j}\int_{-\infty}^{x_i}\rho(x)\exp\left(\frac{2}{\hbar}S(x)\right)dx \\ - \frac{\exp\left(-\frac{2}{\hbar}S(x_f)\right)}{j}\int_{-\infty}^{x_f}\rho(x)\exp\left(\frac{2}{\hbar}S(x)\right)dx,\end{aligned} \tag{5.12}$$

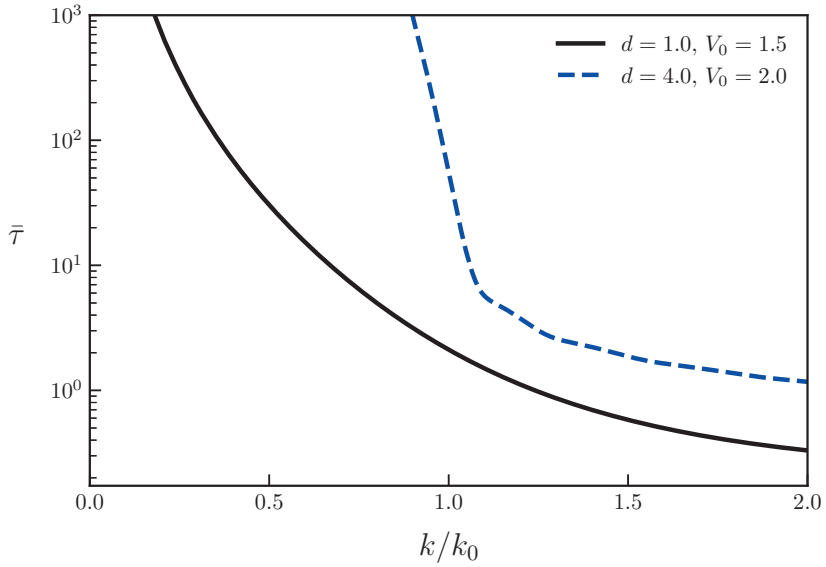


FIGURE 9 – Dimensionless mean passage time $\bar{\tau}$ from $x_i = -d/2$ to $x_f = d/2$ as a function of the normalized wave number k/k_0 for two square barrier configurations: $d = 1.0$, $V_0 = 1.5$ (solid line) and $d = 4.0$, $V_0 = 2.0$ (dashed line). As the particle energy increases (k/k_0 increases), the mean passage time decreases rapidly. The plots exhibit a pronounced growth in the opaque regime ($k/k_0 < 1$). Larger and higher barriers lead to exponentially longer mean passage times, consistent with the tunneling suppression in thicker or higher barriers.

where $v = \nabla S/m$ and $j = \rho(x)v(x)$.

In Eq. (5.12), it can be observed that the first term is analogous to the classical traversal time between the points x_i and x_f, a quantity that is often adopted as the definition of traversal time within the framework of Bohmian mechanics (pilot-wave theory) making the substitution of $v(x)$ for the proper Bohmian velocity [117, 118]. However, within the stochastic quantization approach, the definition of traversal time for scattering states naturally includes additional contributions. Specifically, two extra terms emerge that depend strongly on the phase of the wave function, reflecting the inherently quantum nature of the process.

Figure 9 presents the results obtained from the numerical integration of Eq. (5.12), considering $x_i = -d/2$ (the entrance of the barrier) and $x_f = d/2$ (the exit of the barrier), for two different potential configurations. For simplicity, all quantities are expressed in dimensionless units, setting $\hbar = m = 1$ and fixing d [1]. The computed mean traversal times show excellent agreement with the results previously reported in Ref. [13].

Let us denote, from now on, the mean first passage time across the barrier as $\bar{\tau} \equiv \bar{\tau}\left(x_i = -\frac{d}{2},\ x_f = \frac{d}{2}\right)$. Additionally, Eq. (4.34) can be conveniently rewritten in the

[1] The dimensionless units are defined as follows: $x = \tilde{x}/l$ (position), $E = \tilde{E}/g$ (energy) and $t = \tilde{t}/s$ (time), where $\tilde{x}$, $\tilde{E}$, and $\tilde{t}$ denote the dimensional quantities for position, energy and time, respectively. The characteristic scales are given by $g = \hbar^2/ml^2$ and $s = ml^2/\hbar$, while l is a characteristic length of the system such that the barrier width satisfies $d = \tilde{d}/l$.

form

$$\bar{\tau} = \tau_v + \tau_\rho, \tag{5.13}$$

where the first contribution represents the traversal time depending on $v(x)$,

$$\tau_v = \int_{-d/2}^{d/2} \frac{dx}{v(x)}, \tag{5.14}$$

and the second term,

$$\tau_\rho = \frac{e^{-\frac{2}{\hbar}S\left(-\frac{d}{2}\right)}}{j} \int_{-\infty}^{-d/2} \rho(x) e^{\frac{2}{\hbar}S(x)} dx - \frac{e^{-\frac{2}{\hbar}S\left(\frac{d}{2}\right)}}{j} \int_{-\infty}^{d/2} \rho(x) e^{\frac{2}{\hbar}S(x)} dx, \tag{5.15}$$

corresponds to the extra term arising from Nelson's formulation together with τ_v.

The first term, τ_v, can be evaluated analytically. The current velocity in region II (inside the barrier) is obtained from the wave function given by Eqs. (5.2)–(5.10), resulting in

$$v_{II}(x) = \frac{2k\hbar}{m} \left[\left(1 + \frac{k^2}{\kappa^2}\right) \cosh(\kappa d - 2\kappa x) + \left(1 - \frac{k^2}{\kappa^2}\right) \right]^{-1}. \tag{5.16}$$

Hence,

$$\begin{aligned} \tau_v &= \int_{-d/2}^{d/2} \frac{dx}{v(x)} = \int_{-d/2}^{d/2} \frac{dx}{v_{II}(x)} = \frac{m}{2k\hbar} \left[\left(1 + \frac{k^2}{\kappa^2}\right) \int_{-d/2}^{d/2} \cosh(\kappa d - 2\kappa x) dx + \left(1 - \frac{k^2}{\kappa^2}\right) d \right] \\ &= \frac{m}{2k\hbar} \left[\left(1 + \frac{k^2}{\kappa^2}\right) \frac{1}{2\kappa} \sinh(2\kappa d) + \left(1 - \frac{k^2}{\kappa^2}\right) d \right]. \end{aligned} \tag{5.17}$$

This expression can be further simplified to

$$\tau_v = \frac{mk}{\hbar\kappa} \frac{k_0^2 \sinh(2\kappa d) + 2\kappa d(\kappa^2 - k^2)}{4k^2\kappa^2}, \quad E < V_0. \tag{5.18}$$

In the regime $E > V_0$ the expression above remains valid with the substitution $\kappa \to ik_1$, then one obtains

$$\tau_v = \frac{mk}{\hbar k_1} \frac{2k_1 d(k_1^2 + k^2) - k_0^2 \sin(2k_1 d)}{4k^2 k_1^2}, \quad E > V_0. \tag{5.19}$$

Note that the expressions for $E > V_0$ correspond to a *passage time* of the particle with energy larger than the barrier potential. Otherwise, the expressions for $E < V_0$ correspond to a *tunneling time* of the particle with energy lower than the barrier potential.

The expression for τ_ρ involves a more intricate dependence on the spatial coordinate through both the probability density $\rho(x)$ and the phase function $S(x)$. This complexity prevents an analytical evaluation, and therefore τ_ρ must be computed numerically. Physically, this term encapsulates the corrections introduced by the stochastic dynamics and accounts for the phase interference on the traversal process.

A careful inspection of the definition of τ_v reveals a similarity with the definition of *dwell time*. The dwell time was introduced by Smith in 1960 [110] as a measure of time spent by the particle inside a region of space averaged over all scattering channels. For the one-dimensional case, the dwell time represents the mean time a particle spends strictly inside the barrier region, regardless of whether it is eventually reflected or transmitted, and it is defined as [12, 108]

$$\tau_{\mathrm{d}} = \frac{1}{j_{\mathrm{in}}} \int_{-d/2}^{d/2} |\psi(x)|^2 \, dx, \tag{5.20}$$

where j_{in} denotes the incident flux of particles. If the particles are incident as a plane wave, i.e., an incident wave function of the form e^{ikx}, see Eq. (5.2), then the incident flux is simply $j_{\mathrm{in}} = \hbar k/m$. Alternatively, the quantity τ_v can be expressed as

$$\tau_v = \frac{1}{j_{\mathrm{tr}}} \int_{-d/2}^{d/2} |\psi(x)|^2 \, dx, \tag{5.21}$$

where j_{tr} is the net flux of transmitted particles. Note that j_{tr} equals the difference between the incident and reflected fluxes in region I. Therefore, τ_v can be regarded as a kind of "transmission dwell time" directly related to the (total) dwell time τ_{d}.

The standard dwell time can be evaluated analytically, yielding

$$\tau_{\mathrm{d}} = \begin{cases} \dfrac{mk}{\hbar\kappa} \dfrac{k_0^2 \sinh(2\kappa d) + 2\kappa d(\kappa^2 - k^2)}{4k^2\kappa^2 + k_0^4 \sinh^2(\kappa d)}, & E < V_0, \\ \\ \dfrac{mk}{\hbar k_1} \dfrac{2k_1 d(k_1^2 + k^2) - k_0^2 \sin(2k_1 d)}{4k^2 k_1^2 + k_0^4 \sin^2(k_1 d)}, & E > V_0, \end{cases} \tag{5.22}$$

as reported in [108], where a detailed discussion on the relation between dwell time and other traversal time definitions for the single square barrier is provided. Moreover, the relation between τ_v and τ_{d} can be written as

$$\tau_v = \begin{cases} \tau_{\mathrm{d}} \left[1 + \dfrac{k_0^4}{4\kappa^2 k^2} \sinh^2(\kappa d) \right], & E < V_0, \\ \\ \tau_{\mathrm{d}} \left[1 + \dfrac{k_0^4}{4k_1^2 k^2} \sin^2(k_1 d) \right], & E > V_0, \end{cases} \tag{5.23}$$

which explicitly shows that τ_v is larger than τ_{d}. In Fig. 10, it is possible to see a comparison between $\bar{\tau}$, τ_v and τ_{d} for two different barrier configurations.

The definition of $\bar{\tau}$ obtained from stochastic quantization is clearly different from the dwell time. The time $\bar{\tau}$ represents a *tunneling* or *passage time*, corresponding to the mean time a particle spends diffusing through regions I and II before reaching region III. In contrast, the dwell time τ_{d} measures the average time the particle remains within the barrier region (region II), irrespective of whether it is ultimately transmitted or reflected.

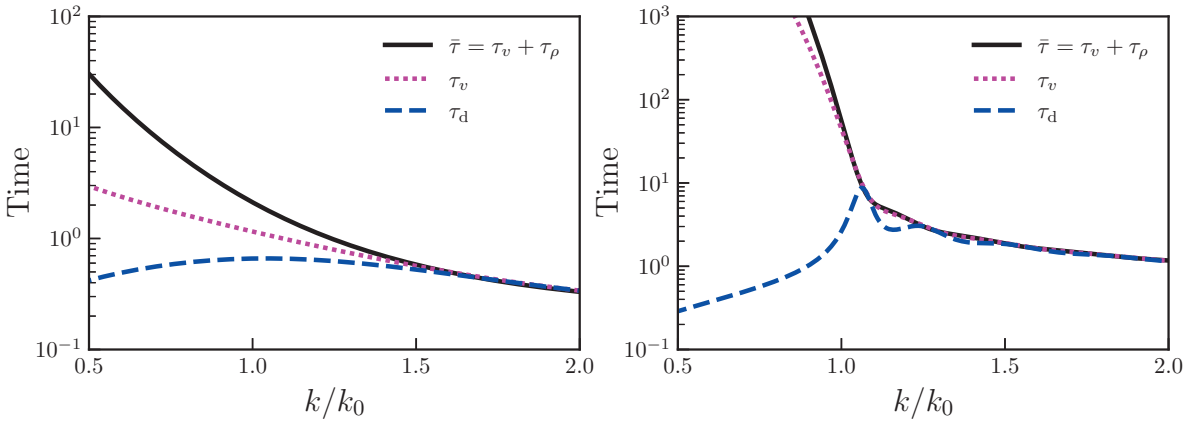


FIGURE 10 – Mean tunneling (passage) time $\bar{\tau}$, its component τ_v, and the dwell time τ_d for two different barrier configurations in dimensionless units. In the left panel, the barrier parameters are $d = 1.0$ and $V_0 = 1.5$, whereas in the right panel they are $d = 4.0$ and $V_0 = 2.0$ (setting $\hbar = m = 1$). Both plots use a semi-logarithmic scale. Note the exponential growth of τ_v in the region $k/k_0 < 1$ and the convergence between the three values in the region $k/k_0 > 1$.

The distinction between these two times becomes particularly clear in the limit of an *opaque barrier* ($V_0 \gg E$). In this regime, the probability density inside the barrier decays exponentially, implying that the particle scarcely penetrates the potential region. Consequently, the dwell time approaches zero, $\tau_\mathrm{d} \to 0$. Conversely, the probability of transmission through the barrier tends to vanish, leading to an infinite tunneling time, $\bar{\tau} \to \infty$. Thus, in the limit $V_0 \to \infty$, we obtain the physically consistent asymptotic behavior $\tau_\mathrm{d} \to 0$ and $\bar{\tau} \to \infty$.

This trend can be verified analytically from the asymptotic behavior of Eq. (5.18) in the limit $V_0 \gg E$. Since $\sinh(2\kappa d)$ grows exponentially with κd, we have

$$\tau_v \approx \frac{mk_0^2}{8\hbar k\kappa^3} e^{2\kappa d} \approx \frac{m}{8\hbar k k_0} e^{2k_0 d}, \quad V_0 \gg E. \tag{5.24}$$

This result is equal to one found in the literature [119] and equivalently presented in [120]. Similarly, the asymptotic limit of the dwell time obtained from Eq. (5.22) yields

$$\tau_\mathrm{d} \approx \frac{2mk}{\hbar\kappa k_0^2} \approx \frac{2mk}{\hbar k_0^3}, \quad V_0 \gg E. \tag{5.25}$$

Equations (5.24) and (5.25) confirm the physical interpretation: as the barrier becomes increasingly opaque, the dwell time rapidly vanishes while the tunneling time diverges exponentially. This asymptotic behavior is consistent with the intuitive picture of quantum tunneling and provides a clear validation of the stochastic quantization framework for describing tunneling time.

Another important limiting case to consider is that of a vanishing potential barrier, $V_0 \to 0$. In this limit, the system reduces to a free particle moving across a region of length

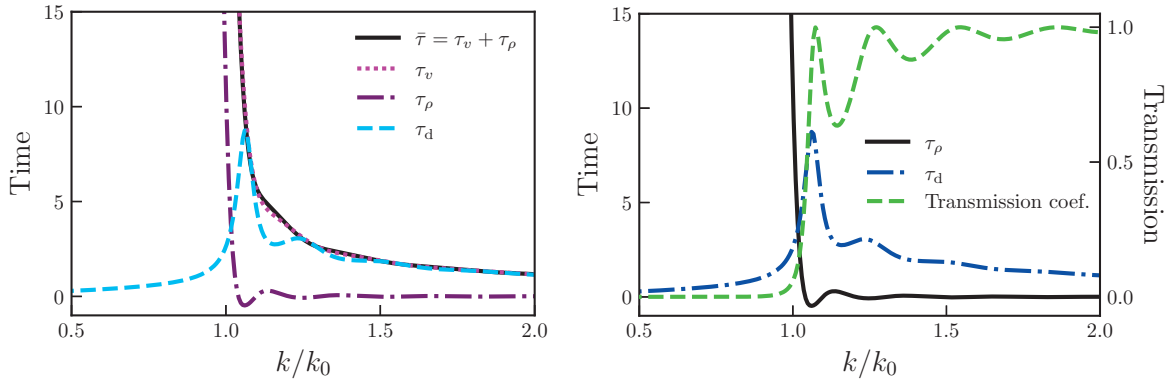


FIGURE 11 – Decomposition of the mean tunneling (passage) time into its components and its comparison with the dwell time and the transmission coefficient in dimensionless units. In the left panel, the mean time $\bar{\tau} = \tau_v + \tau_\rho$ is separated into the components τ_v and τ_ρ in comparison with the dwell time $\tau_{\rm d}$. In the right panel, the time τ_ρ and the dwell time $\tau_{\rm d}$ are shown together with the transmission coefficient, illustrating the correlation between resonant peaks in transmission and the times in question, in the scattering case. Both plots correspond to the same barrier configuration: $d = 4$, $V_0 = 2.0$, and setting $\hbar = m = 1$.

d. Substituting $V_0 = 0$ into expressions (5.19) and (5.22) for $E > V_0$, we find

$$\tau_v \approx \tau_{\rm d} \approx \frac{md}{\hbar k}, \tag{5.26}$$

which corresponds exactly to the classical expression for the traversal time of a free particle with momentum $p = \hbar k$ moving with constant velocity $v = \hbar k/m$.

In Fig. 11(a), a comparison between the mean passage (tunneling) time $\bar{\tau}$ and the dwell time $\tau_{\rm d}$ is presented, together with a comparison between the two contributions of $\bar{\tau}$, namely, the traversal time τ_v and the probability-dependent component τ_ρ. A comparison of the dwell $\tau_{\rm d}$ time and the probability-dependent component τ_ρ with the transmission coefficient is also shown in Fig. 11(b). It can be observed that the mean traversal time $\bar{\tau}$ as obtained within the framework of stochastic mechanics, exhibits a sharp decrease, with increasing wave number k, near the resonance condition $k \approx k_0$, where the transmission probability reaches its maximum. The component τ_ρ assumes small or even negative values for $k > k_0$, a behavior that originates from interference and phase effects within the barrier region. This term represents the fluctuating part of the total mean time, and its oscillatory structure close to $k/k_0 \approx 1$ reflects resonant contributions and constructive–destructive interference patterns inside the potential barrier. Note that the minimum points in τ_ρ coincide with the maximum values in the dwell time and in the transmission coefficient, indicating the resonant energies of the system. Beyond the resonance region, $\bar{\tau}$ decreases smoothly with increasing particle energy, remains strictly positive, and approaches the dwell time $\tau_{\rm d}$ for high energies.

The intrinsic difference in the physical interpretation of $\bar{\tau}$ and $\tau_{\rm d}$ for tunneling

states ($k/k_0 < 1$), as discussed above, is clearly illustrated in Figs. 10 and 11(a): while $\tau_{\rm d}$ goes to zero with decreasing k/k_0, $\bar{\tau}$ grows exponentially. In the high-energy limit, $k \gg k_0$, the contribution of the probability-dependent term τ_ρ vanishes, $\tau_\rho \to 0$ (quantum interference effects become negligible). Consequently, both the mean traversal time $\bar{\tau}$ (together with the dwell time $\tau_{\rm d}$) converge to the classical limit $md/\hbar k$ for a free particle crossing a region of width d. This asymptotic behavior reflects the recovery of classical dynamics from the stochastic quantum description: at sufficiently high energies (barrier-free limit), the particle effectively overcomes the barrier without significant reflection, and its motion can be described as nearly ballistic.

5.1.1 Hartman Effect

It is worth emphasizing that the traversal time $\bar{\tau}$ derived from stochastic quantization does not exhibit the so-called *Hartman effect* (after Thomas Hartman) [105, 109]. The Hartman effect is characterized by the independence of the tunneling time with respect to the barrier width, which leads to the unphysical implication of superluminal propagation for sufficiently thick barriers.

This counterintuitive behavior can be exemplified by the *phase delay time*, also known as Wigner delay time [12, 121]. This time can be defined in terms of the temporal delay in the phase of the wave function. It is calculated as the energy derivative of the phase of the transmission amplitude, summed with the traversal time of a free reference particle with the same incoming velocity and traveling between points x_1 and x_2 [122]. Mathematically:

$$\tau_\phi(E) = \hbar \frac{d\phi_T}{dE} + \frac{x_2 - x_1}{v(E)}, \tag{5.27}$$

where $\phi_T(E)$ is the phase of the complex transmission component $D(E) = |D(E)|e^{i\phi_T(E)}$ in the wave function in Eq. (5.2), and $E = \hbar^2 k^2/2m$ is the energy of the incident particle. The phase delay time has the following expression in the limit of an opaque barrier ($k_0 d \gg 1$) [12]:

$$\tau_\phi \approx \frac{2m}{\hbar k \kappa}. \tag{5.28}$$

Therefore, independent of the barrier width d.

For a long time, the phase delay time was thought of as a measure of traversal time. However, in Ref. [123], the author demonstrates that the phase time does not represent a genuine traversal time, but rather quantifies the lifetime of the energy (or probability density) temporarily stored within the barrier and subsequently released through both ends. This interpretation provides a consistent physical picture that resolves the apparent paradox associated with the Hartmann effect for the phase delay time.

Within the stochastic framework the traversal time $\bar{\tau}$ retains its dependence on the barrier width d, even in the limit of $k_0 d \gg 1$, see Eq. (5.24), ensuring consistency with

causality and relativistic constraints. This feature reinforces the physical interpretability of $\bar{\tau}$, free from paradoxical superluminal effects.

5.1.2 Numerical Simulations

The trajectories of particles undergoing tunneling through the potential barrier can be simulated numerically, enabling one to obtain the distribution of their passage times. These simulations are performed using the *Euler–Maruyama scheme*, which provides a numerical approximation to the solution of stochastic differential equations (SDEs). This method is the stochastic analogue of the classical Euler method for ordinary differential equations and is widely used due to its simplicity and stability for sufficiently small time steps [124].

Let X_t be a stochastic process governed by the SDE

$$\begin{aligned} dX(t) &= a(X(t),t)\,dt + b(X(t),t)\,dW(t), \quad t \in [0,T], \\ X(0) &= x_0 \in \mathbb{R}, \end{aligned} \tag{5.29}$$

where $W(t)$ denotes a Wiener process. As we have seen in Sec. 2.2.4, this equation can be expressed in integral form as

$$X(t) = X(0) + \int_0^t a(X(s),s)\,ds + \int_0^t b(X(s),s)\,dW(s), \tag{5.30}$$

where the last integral is understood in the Itô sense. To construct a discrete-time approximation, consider a uniform partition of the time interval $[0,T]$:

$$0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T, \tag{5.31}$$

with constant time step $\Delta t = t_{i+1} - t_i = T/n$. The Euler–Maruyama approximation of the process (5.30) is then given by

$$\begin{aligned} X_{i+1} &= X_i + a(X_i,t_i)\,\Delta t + b(X_i,t_i)\,\Delta W_i, \\ X_0 &= x_0, \quad 0 \le i \le n-1, \end{aligned} \tag{5.32}$$

where $X_i \equiv X(t_i)$ and $\Delta W_i = W(t_{i+1}) - W(t_i)$ is an independent Gaussian random variable with zero mean and variance Δt, i.e., ΔW_i has a distribution $\mathcal{N}(0,\Delta t)$. By iteratively applying Eq. (5.32) for a sufficiently large number of time steps (so that $\Delta t \ll 1$), one obtains a discrete approximation to the continuous stochastic trajectory $X(t)$, from which statistical quantities such as mean passage times can be computed.

In the case of a particle represented by a plane wave tunneling through a one-dimensional square potential barrier, the stochastic dynamics can be described by the SDE

$$dx(t) = v_+(x)dt + \sqrt{\frac{\hbar}{m}}\,dW(t). \tag{5.33}$$

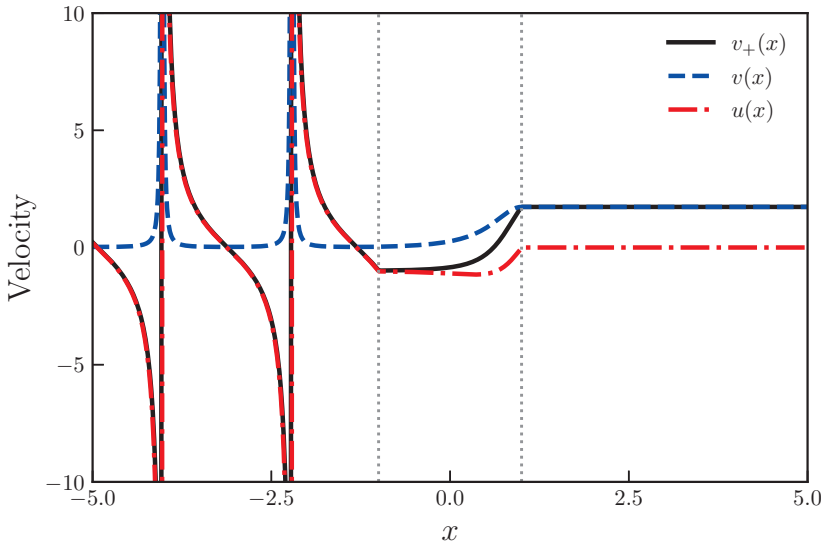


FIGURE 12 – Current, osmotic, and forward velocities for a particle interacting with a square barrier. The solid black line represents the forward velocity $v_+(x)$, the dashed blue line shows the current velocity $v(x)$, and the dash-dotted red line corresponds to the osmotic velocity $u(x)$. The vertical dotted lines indicate the spatial limits of the barrier region. The asymptotes on the left side of the barrier indicate the points where the wave function vanishes. The barrier parameters are: $d = 2.0$, $V_0 = 2.0$. Values in dimensionless units.

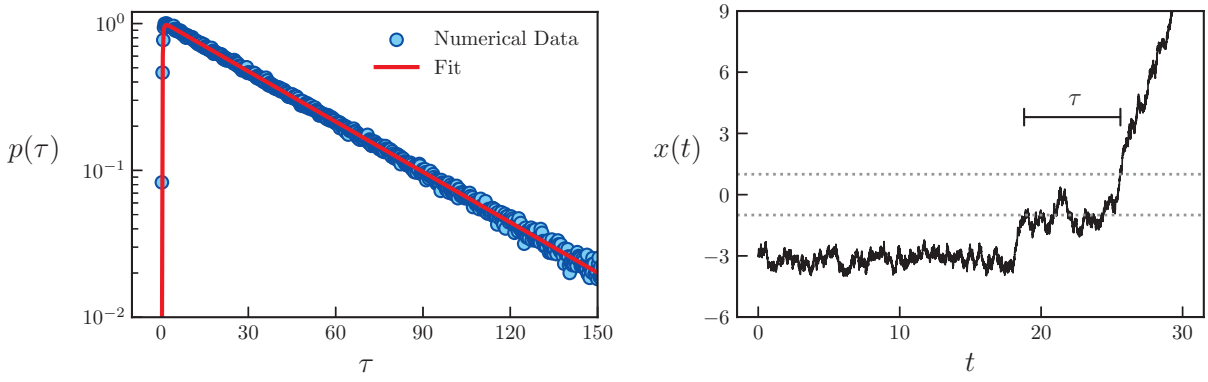
The corresponding forward drift, defined as $v_+(x) = u(x) + v(x)$, is obtained directly from the stationary wave function of the system, given in Eq. (5.2). Writing the wave function in polar form as $\psi(x) = \sqrt{\rho(x)}\exp(iS(x)/\hbar)$, the osmotic and current velocities in Nelson's stochastic mechanics can be respectively expressed as

$$u(x) = \frac{\hbar}{m}\,\mathrm{Re}\left(\frac{\psi'(x)}{\psi(x)}\right), \qquad v(x) = \frac{\hbar}{m}\,\mathrm{Im}\left(\frac{\psi'(x)}{\psi(x)}\right), \tag{5.34}$$

where primes denote spatial derivatives. This results in the following expression for $v_+(x) = u(x) + v(x)$ in terms of the constant complex coefficients in Eqs. (5.6)–(5.9) for $E < V_0$:

$$v_+(x) = \begin{cases} \dfrac{\hbar k}{m}\left[-\mathrm{Im}\left(\dfrac{1 - Ae^{-2ikx}}{1 + Ae^{-2ikx}}\right) + \mathrm{Re}\left(\dfrac{1 - Ae^{-2ikx}}{1 + Ae^{-2ikx}}\right)\right], & x < -d/2, \\ \dfrac{\hbar\kappa}{m}\left[\mathrm{Re}\left(\dfrac{Be^{\kappa x} - Ce^{-\kappa x}}{Be^{\kappa x} + Ce^{-\kappa x}}\right) + \mathrm{Im}\left(\dfrac{Be^{\kappa x} - Ce^{-\kappa x}}{Be^{\kappa x} + Ce^{-\kappa x}}\right)\right], & -d/2 \le x \le d/2, \\ \dfrac{\hbar k}{m}, & x > d/2. \end{cases} \tag{5.35}$$

Figure 12 shows the behaviors of the forward drift velocity $v_+(x)$, the current velocity $v(x)$, and the osmotic velocity $u(x)$. As we can see, the velocities develop asymptotes on the left side of the barrier at the points where the probability density vanishes, while on the right



(a) (b)

FIGURE 13 – Left: Probability distribution of the barrier passage times $p(\tau)$, normalized to have a unit value at its maximum, obtained from numerical simulations (blue circles) and compared with a fit (red line) given by Eq. (5.36) with parameters $\tau_\alpha = 0.493$, $\tau_\beta = 38.0$ and $\gamma = 3.27$. Right: Example of a single stochastic trajectory illustrating the definition of the passage time τ, measured as the interval between the first entrance and the exit of the particle from the barrier region (dotted lines). Values in dimensionless units.

side, the osmotic velocity vanishes and $v_+(x) = v(x)$ has a constant value corresponding to the particle's velocity after tunneling through the barrier.

Using the expression (5.35) for $v_+(x)$, we simulated the stochastic trajectories, according to Eq. (5.33), employing the Euler–Maruyama method described in Eq. (5.32), in order to obtain the tunneling time distribution. The particle begins its diffusive motion at $x = -d/2$ and time $t = 0$, and the tunneling time τ is defined as the time at which the particle first reaches $x = d/2$. The simulations were performed with the potential barrier characterized by the parameters $d = 2$ and $V_0 = 2$, the particle energy is $E = 1.5$. A total of 10^6 trajectories were simulated with a time step of $\Delta t = 10^{-4}$. Figure 13(a) shows the resulting tunneling time distribution, while Fig. 13(b) shows a representative example of an individual simulated trajectory. Note that the tunneling time τ obtained from stochastic quantization, simulating the trajectories, takes into account the "hesitation" of the particle around the barrier entrance before effectively tunnel through it as a consequence of the stochasticity of the trajectory. This effect is verified in [125] for a wave packet and is also clearly observed in the sample trajectory in Fig. 13 for the plane wave case considered here.

The mean value of the tunneling times τ can be calculated from the ensemble of simulated trajectories and with the expression (4.34). The mean tunneling time obtained from the simulations was $\bar{\tau}_{\text{num}} = 38.67$, in excellent agreement with the theoretical value of $\bar{\tau} = 38.55$ calculated from Eq. (5.13). The difference is due to finite statistics. This result validates the accordance between the theoretical and simulated results. From the numerical simulations, it was also verified that the standard deviation of the tunneling

time is approximately equal to its mean value, that is, $\Delta\tau \approx \bar{\tau}$. This result indicates that the tunneling time distribution is broad and exhibits significant fluctuations around the mean.

The obtained distribution exhibits a pronounced exponential tail at large times, in agreement with the theoretical prediction for the mean first-passage time in Sec. 4.2. This behavior reflects the presence of rare, long-lived trajectories that spend a significant time diffusing near or within the barrier region before successfully crossing it. The tunneling time distribution obtained from the simulated trajectories can be fitted by the function proposed in [83], given by

$$p(\tau) = C \exp\left[-\left(\frac{\tau_\alpha}{\tau}\right)^\gamma + \frac{\tau}{\tau_\beta}\right], \tag{5.36}$$

where τ_α, τ_β, and γ are fitting parameters. The normalization constant C is chosen such that the distribution attains a unit value at its maximum, i.e., the most probable tunneling time is normalized to one.

At short times, the distribution displays a significantly low probability density. Physically, this corresponds to the fact that, for a particle to traverse the barrier in a very short time, it would require a highly improbable sequence of fluctuations leading to an almost ballistic motion through the potential region. Since the trajectories are influenced by the diffusive term and the drift $v_+(x)$, the probability of observing such "fast-tunneling" events is exponentially suppressed. Therefore, the combined structure of the distribution, with a sharp rise followed by an exponential tail, characterizes the quantum tunneling, as described within Nelson's framework.

5.1.3 Simple Square Well

From the same analytical solution obtained previously for the square barrier, we can directly derive the corresponding expressions for the mean passage time of a particle through a square well by considering $V_0 < 0$. In this case, the particle energy always satisfies $E > V_0$, and the stationary solution of the Schrödinger equation for a well of width d and depth $-V_0$, considering $V_0 > 0$, see Fig. 14, is written as

$$\psi(x) = \begin{cases} e^{ikx} + Ae^{-ikx}, & x < -d/2, \\ Be^{ik_1 x} + Ce^{-ik_1 x}, & -d/2 \le x \le d/2, \\ De^{ikx}, & x > d/2, \end{cases} \tag{5.37}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}, \quad k_0 = \frac{\sqrt{2mV_0}}{\hbar}, \quad k_1 = \frac{\sqrt{2m(E+V_0)}}{\hbar}. \tag{5.38}$$

The coefficients A, B, C and D are given by the same expressions as in Eqs. (5.6)–(5.9), but with the substitution $\kappa \to ik_1$. The transmission coefficient is again given by $T = |D|^2$.

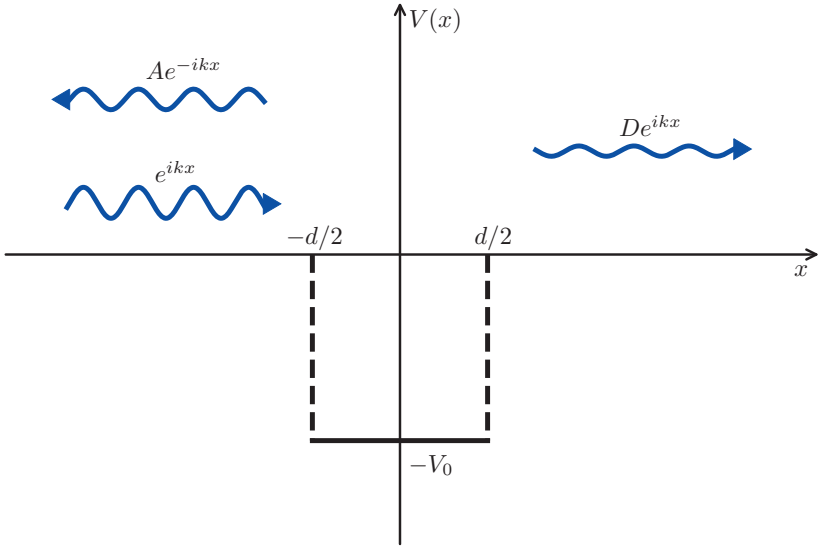


FIGURE 14 – Square well potential of depth V_0 and width d. A particle with energy $E = \hbar^2k^2/2m$ is incident from the left, represented by the wave e^{ikx}. The reflected and transmitted components are given by Ae^{-ikx} and De^{ikx}, respectively. The potential is defined as $V(x) = -V_0$ for $-d/2 \leq x \leq d/2$ ans $V(x) = 0$ otherwise.

The component dependent on $v(x)$ of the mean passage time τ_v, see Eq. (5.14), for a square well takes the form

$$\tau_v = \frac{mk}{\hbar k_1}\left[\frac{2k_1 d(k_1^2 + k^2) + k_0^2 \sin(2k_1 d)}{4k^2 k_1^2}\right], \tag{5.39}$$

and the total mean passage time for the square well is expressed (as for the barrier) as the sum

$$\bar{\tau} = \tau_v + \tau_\rho, \tag{5.40}$$

where the term τ_ρ has the same structure as in Eq. (5.15). The dwell time in the region of the well ($-d/2 \leq x \leq d/2$) has the expression

$$\tau_{\mathrm{d}} = \frac{mk}{\hbar k_1}\frac{2k_1 d(k_1^2 + k^2) + k_0^2 \sin(2k_1 d)}{4k^2 k_1^2 + k_0^4 \sin^2(k_1 d)}. \tag{5.41}$$

Figure 15 presents the mean passage time $\bar{\tau}$ for a square well of width $d = 4$ for several values of the potential depth V_0 (in adimensional units: $\hbar = m = 1$ and fixing d). The results show that $\bar{\tau}$ decreases with increasing wave number k, but exhibits a pronounced peak followed by small oscillations. As illustrated in Fig. 16 (for $V_0 = 20$), this peak is in some way related to the resonance observed in the transmission coefficient T, and both have their origin in interference between the forward and backward traveling waves confined within the well.

At very low energies, the particle is predominantly reflected by the potential, and consequently, the mean passage time is large. In this regime, only a small fraction of trajectories contribute to transmission, and those that succeed in crossing the well tend

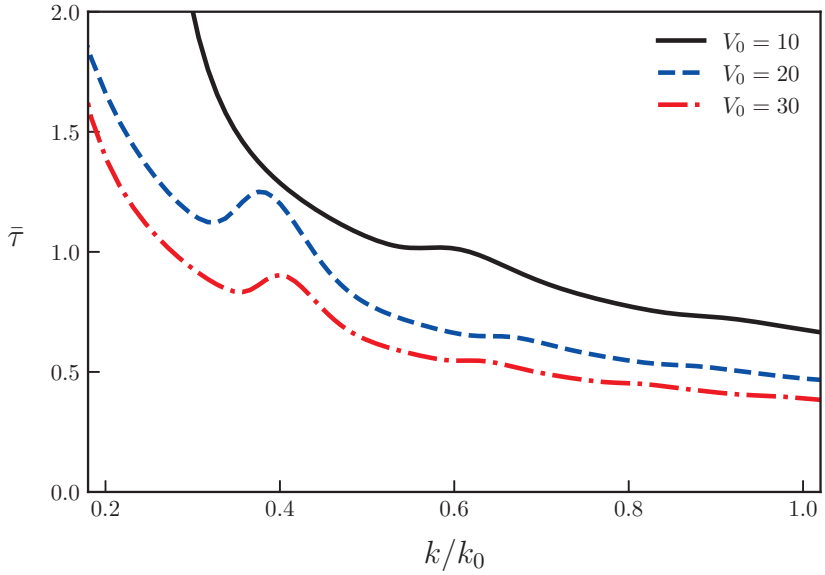


FIGURE 15 – Mean passage time $\bar{\tau}$ as a function of the normalized wave number k/k_0 for a square well potential of fixed width $d = 4$ and different fixed depths V_0. The decrease in $\bar{\tau}$ with increasing V_0 reflects the enhancement of the transmission probability due to the stronger confinement, while the local oscillations are related to resonant conditions within the well. Values in dimensionless units.

to take longer on average. As the energy increases, the particle penetrates more easily through the potential region, and the mean passage time decreases overall.

In the high-energy limit, $k/k_0 \gg 1$, the system approaches the classical regime, and the traversal time converges to the classical value $md/\hbar k$ corresponding to a free particle moving across the distance d. However, before reaching this asymptotic behavior, the mean passage time $\bar{\tau}$ exhibits a pronounced maximum before the first resonance in the transmission coefficient T, and after that, other tiny, almost imperceptible, peaks can be noted, see Fig. 16. This pre-resonant maximum arises from *non-resonant interference* effects inside the well, which increase the probability density within the potential region and lead to a temporary trapping of the particle in quasi-stationary (metastable) states [126]. In other words, as the energy approaches a resonant value, the internal interference pattern becomes almost constructive, enhancing the particle's dwell time in the well. Once the resonance condition is exactly satisfied, constructive interference becomes complete, a quasi-bound state is formed, and the transmission probability reaches its maximum. In this state, the particle passes through the well more efficiently, and consequently, the mean passage time decreases.

This interplay between interference-induced delay and resonant transmission is a signature of quasi-bound states in one-dimensional scattering. It provides a clear physical picture: before resonance, the particle spends more time within the potential due to partial constructive interference; at resonance, the transmission becomes optimal and the residence time inside the well is minimized.

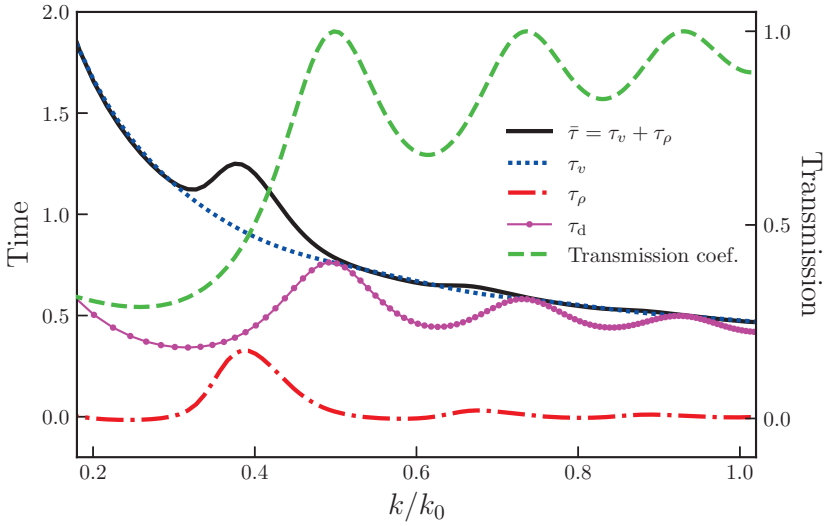


FIGURE 16 – Comparison of the mean passage time $\bar{\tau} = \tau_v + \tau_\rho$ and its components, τ_v and τ_ρ, with the dwell time τ_d and the transmission coefficient as a function of the ratio k/k_0. The potential well has width $d = 4$ and depth $V_0 = 20$. Values in dimensionless units.

In Fig. 16 it is possible to note that, as observed in the barrier case (see Fig. 11), when the transmission reaches its maximum value, the dwell time τ_d tends to coincide with the mean passage time $\bar{\tau}$. This agreement occurs because the dwell time intrinsically accounts for the total probability density accumulated within the potential region, including both transmitted and reflected components. At resonance, where reflection is minimal and transmission dominates, the average duration that the particle spends inside the well is determined almost entirely by the transmitted trajectories, which concerns the mean passage time.

5.2 WAVE PACKET AND SINGLE BARRIER

Let us now discuss the problem of the tunneling time of a quantum particle described by a wave packet, as it interacts with a square potential barrier, such as the one defined in Eq. (5.1). The time evolution of the wave packet is governed by the time-dependent Schrödinger equation, whose formal solution can be written as

$$\Psi(x,t) = \int_{-\infty}^{\infty} \mathcal{A}(k)\psi(x,k)e^{-iE(k)t/\hbar}\,dk, \tag{5.42}$$

where

$$E(k) = \frac{\hbar^2 k^2}{2m} \tag{5.43}$$

and $\psi(x,k)$ denotes the stationary solution of the time-independent Schrödinger equation, given by Eqs. (5.2)–(5.10). The spectral amplitude $\mathcal{A}(k)$ defines the momentum-space structure of the wave packet and is expressed by

$$\mathcal{A}(k) = \left(\frac{1}{2\pi(\Delta k)^2}\right)^{1/4} \exp\left[-\frac{(k-\langle k\rangle)^2}{4(\Delta k)^2} - ik\langle x_0\rangle\right], \tag{5.44}$$

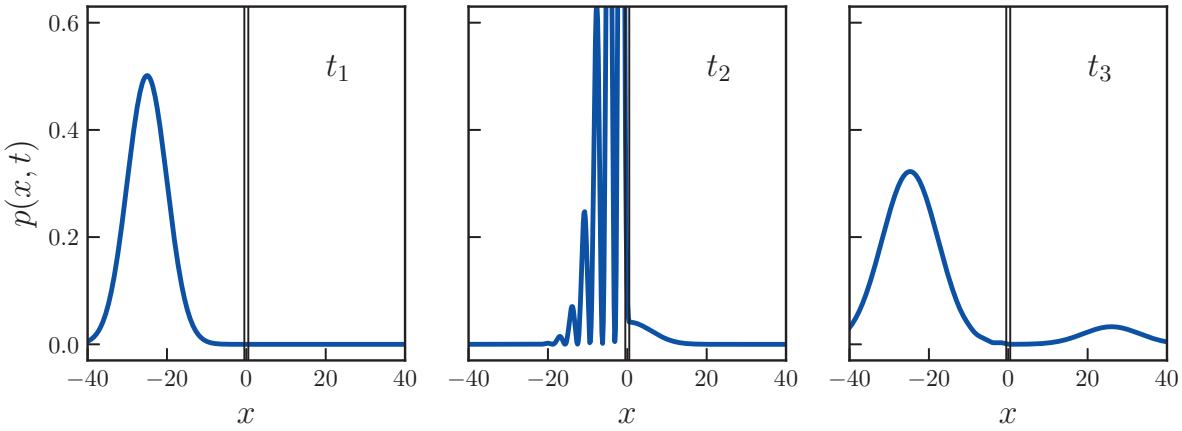


FIGURE 17 – Time evolution of the probability density $p(x,t) = |\Psi(x,t)|^2$ for a wave packet incident on a square barrier potential. At t_1, the packet is localized on the left, approaching the barrier. At t_2, the packet interacts with the barrier, giving rise to strong interference patterns inside and close to the potential region. At t_3, the transmitted and reflected components are clearly separated. The vertical line indicates the position of the potential barrier.

which ensures that the initial distribution of the particle momentum k is Gaussian with mean $\langle k\rangle$ and standard deviation Δk. The quantity $\langle x_0\rangle$ in Eq. (5.44) represents the mean initial position (the center of the wave packet), at time $t = 0$. The value of $\langle x_0\rangle$ is chosen so that at the initial instant $t = 0$ the wave packet $\Psi(x,t)$ is far away from the barrier and reproduces the spatial profile of a freely propagating Gaussian wave packet, which can be written as

$$\Psi(x,0) = \left(\frac{1}{2\pi(\Delta x)^2}\right)^{1/4} \exp\left[-\frac{(x-\langle x_0\rangle)^2}{4(\Delta x)^2} + i\langle k\rangle(x-\langle x_0\rangle)\right], \tag{5.45}$$

where the position and momentum standard deviations are related by the minimum uncertainty relation $\Delta x = \hbar/(2\Delta k)$. Equation (5.42) was evaluated numerically to obtain the complete time evolution of the wave packet as it interacts with the barrier. Figure 17 illustrates the resulting probability density $p(x,t) = |\Psi(x,t)|^2$ at three distinct time instants, showing the incident, reflected, and transmitted components of the packet.

In this dynamical setting, the probability density $p(x,t) = |\Psi(x,t)|^2$ depends on time; therefore, the expression for the mean first-passage time, Eq. (4.20), is not directly applicable. Nevertheless, the tunneling times can be analyzed numerically by simulating the stochastic trajectories associated with the particle's motion, as discussed in Sec. 5.1.2.

Analogously to the stationary case of plane waves, one can define the osmotic and current velocities in the framework of Nelson's stochastic mechanics by

$$u(x,t) = \frac{\hbar}{m}\,\mathrm{Re}\left(\frac{\Psi'(x,t)}{\Psi(x,t)}\right), \quad v(x,t) = \frac{\hbar}{m}\,\mathrm{Im}\left(\frac{\Psi'(x,t)}{\Psi(x,t)}\right), \tag{5.46}$$

where primes denote spatial derivatives. In Fig. 18 it is possible to see the behavior of the drift $v_+(x,t) = v(x,t) + u(x,t)$ for three different values of time. These two quantities were

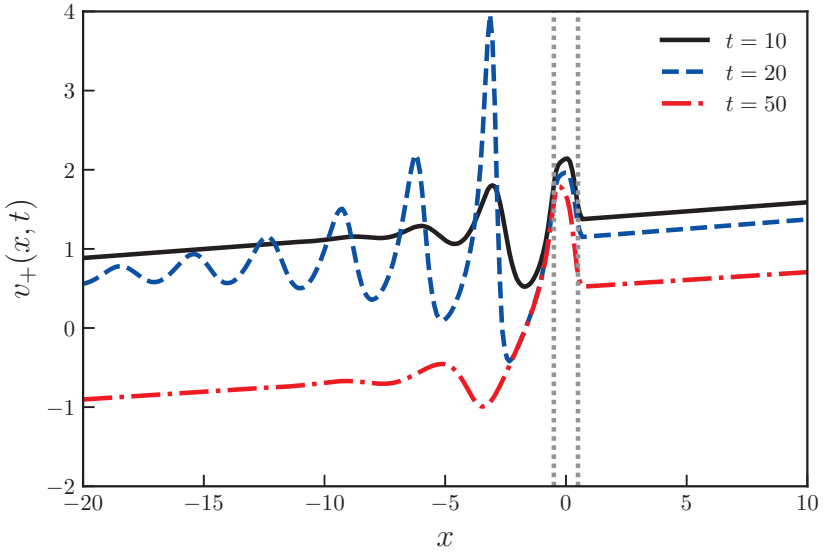


FIGURE 18 – Forward drift velocity $v_+(x,t) = v(x,t) + u(x,t)$ as a function of position x at different times. The curves correspond to $t = 10$ (black solid line), $t = 20$ (blue dashed line), and $t = 50$ (red dash-dotted line). The vertical dotted lines indicate the position of the potential barrier. The average momentum is $\langle k \rangle = 1.0$ and its standard deviation is $\Delta k = 0.1$, the barrier height is $V_0 = 2.0$ and the barrier width is $d = 1.0$ in dimensionless units. Oscillations near the barrier at intermediate times reflect interference between incident and reflected components of the wave packet.

used to compute the tunneling times by numerical simulations of the particle trajectory described by the SDE

$$dx(t) = [v(x,t) + u(x,t)]dt + \sqrt{\frac{\hbar}{m}}dW(t). \tag{5.47}$$

In order to analyze the stochastic properties of the tunneling process for a particle represented by a wave packet, an ensemble of trajectories is generated. The initial position of each particle is chosen randomly with probability density

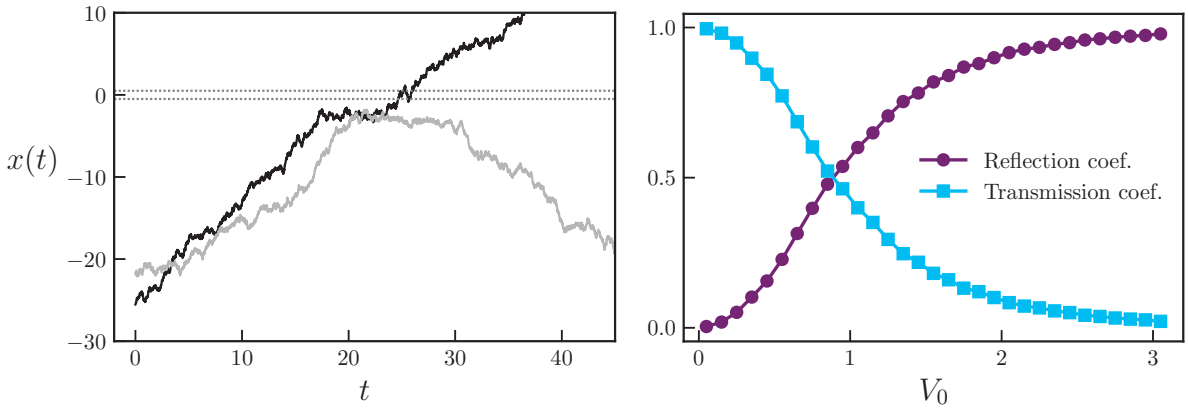
$$p(x,0) = |\Psi(x,0)|^2 = \frac{1}{\sqrt{2\pi(\Delta x)^2}} \exp\left[-\frac{(x - \langle x_0 \rangle)^2}{2(\Delta x)^2}\right], \tag{5.48}$$

which represents the Gaussian wave packet at $t = 0$ centered at $\langle x_0 \rangle$ and characterized by spatial width Δx. Each stochastic trajectory $x_i(t)$ evolves in time according to the Nelson equation (5.47) and is computed using the Euler-Maruyama scheme described in Sec. 5.1.2.

For each transmitted particle, the time spent inside the potential barrier defines an individual time computed as in [127], i.e.,

$$\tau_i = \int_0^{t_f} \Theta(x_i(t))\, dt, \quad i = 1, 2, \ldots, N, \tag{5.49}$$

where $x_i(t)$ denotes the i-th sample path corresponding to a transmitted trajectory, t_f is the final simulation time, and $\Theta(x)$ is a rectangular window function that takes the



(a) (b)

FIGURE 19 – Left: Sample trajectories of particles evolving according to Nelson's stochastic dynamics for the mean energy of the incoming wave packet $\langle E \rangle$ below the potential height V_0. The dashed lines indicate the boundaries of the potential barrier region. Some trajectories are reflected while others are transmitted. Right: Reflection and transmission coefficients, obtained from numerical simulations, as functions of the barrier height V_0. As V_0 increases, the reflection probability approaches unity, while the transmission coefficient decreases accordingly.

value unity when the particle is located inside the barrier region ($-d/2 \leq x \leq d/2$) and zero otherwise. This time does not have the same interpretation as the MFPT used in the previous section. The quantity τ_i in Eq. (5.49) may be regarded as a partial dwell time associated exclusively with the transmitted fraction of the ensemble, thus quantifying the residence time of particles that successfully cross the barrier. In Ref. [127], the time defined in Eq. (5.49) is treated as a measure of the tunneling time.

The ensemble average of the individual times τ_i defines the mean partial dwell time, denoted by $\bar{\tau}$. Depending on the mean energy of the incoming wave packet, this quantity acquires distinct physical interpretations. For $\langle E \rangle > V_0$, the mean particle's energy exceeds the barrier height, and $\bar{\tau}$ represents a *mean traversal (dwell) time*—the average duration spent above the barrier by the transmitted particles. Conversely, when $\langle E \rangle < V_0$, the process involves quantum tunneling, and the mean time $\bar{\tau}$ corresponds to a type of *mean tunneling (dwell) time*.

The total simulation time t_f must be sufficiently large to ensure that all trajectories have reached their asymptotic state—either transmitted or reflected. Figure 19(a) illustrates typical examples of reflected and transmitted stochastic trajectories obtained from the numerical simulations, while Fig. 19(b) presents the corresponding transmission and reflection coefficients. These coefficients were determined statistically as the fraction of trajectories that successfully crossed the barrier or were reflected back. It is worth noting that these coefficients display the expected behavior, with reflection increasing and transmission decreasing as the barrier height grows. All the simulations were performed using a momentum average of $\langle k \rangle = 1.0$, corresponding to a mean particle energy of

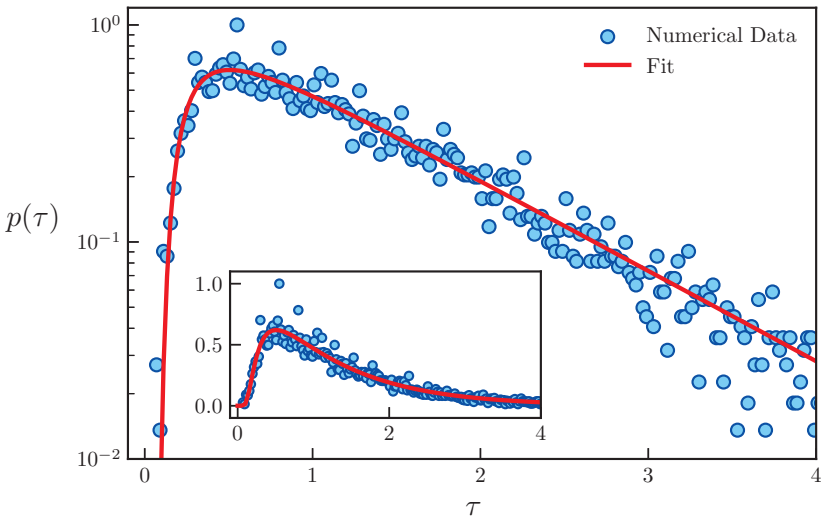


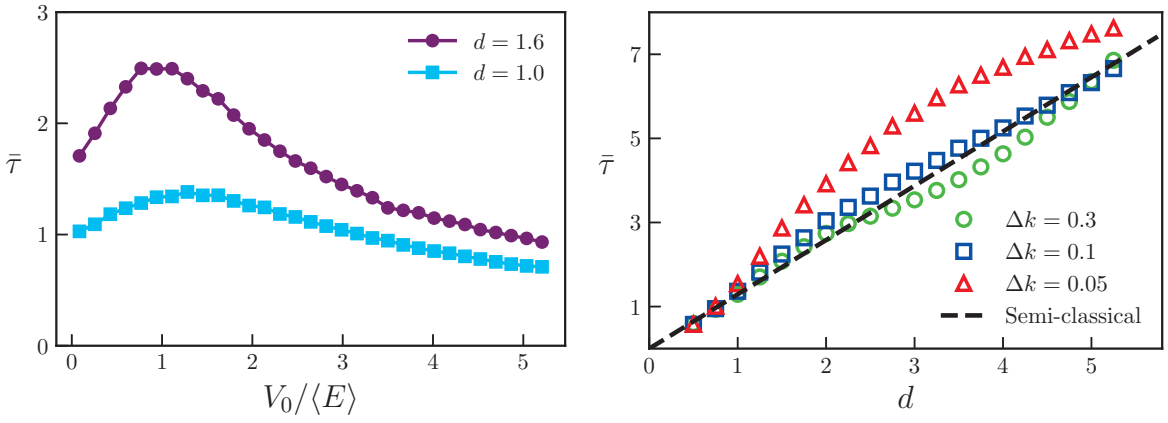
FIGURE 20 – Probability density function $p(\tau)$ of the tunneling times obtained from stochastic simulations (blue circles) and its analytical fit (red solid line). A total of 10^4 transmitted trajectories were simulated with a time-step of 0.01 and $V_0 = 1.05$, $\langle k \rangle = 1.0$, $\Delta k = 0.1$, $\langle E \rangle = 0.505$. The distribution exhibits a sharp rise at short times followed by a long exponential tail, indicating the presence of rare long-duration tunneling events. The inset shows the same data in linear scale for clarity. The fit is given by Eq. (5.36) with parameters $\tau_\alpha = 0.244$, $\tau_\beta = 1.04$ and $\gamma = 1.72$. The mean tunneling time is $\bar{\tau} = 1.30$. Values in dimensionless units.

$\langle E \rangle = 0.505$ approximately, and a momentum standard deviation of $\Delta k = 0.1$.

The probability distribution of the tunneling time obtained from the numerical ensemble is shown in Fig. 20. A total of 10^4 transmitted trajectories were obtained with a time-step of 0.01 and barrier height of $V_0 = 1.05$. The distribution exhibits an exponential tail and the entire distributions can be fitted by the exponential function defined in Eq. (5.36), as shown in Fig. 20. In Ref. [127], the authors proposed a fit using a gamma distribution for the tunneling-time statistics; however, in the present study, the exponential form (5.36) was found to provide a better agreement with the numerical data.

Figure 21(a) presents the dependence of the mean traversal (tunneling) time $\bar{\tau}$ on the barrier height, for two different barrier widths d. Note that for the barrier height smaller than the mean particle energy, the mean traversal time $\bar{\tau}$ increases with increasing V_0. Otherwise, for tunneling states, when the barrier height is larger than the mean particle energy, the tunneling time $\bar{\tau}$ decreases with increasing V_0. In general, $\bar{\tau}$ has a peak when $V_0 \approx \langle E \rangle$, as is possible to see in the figure.

This result reveals a counterintuitive feature of the tunneling regime. For wave packets whose mean energy $\langle E \rangle$ lies below the barrier height V_0, the mean tunneling time $\bar{\tau}$ decreases as the barrier height increases. In other words, the higher the barrier—and consequently the lower the transmission probability—the shorter the average traversal time, as defined by Eq. (5.49), spent by those particles that successfully tunnel through it.



(a) (b)

FIGURE 21 – Dependence of the mean tunneling (passage) time $\bar{\tau}$ on the system parameters. In both plots the wave packet has parameter $\langle k\rangle = 1.0$. Left: Variation of $\bar{\tau}$ with the ratio $k_0/\langle k\rangle$ for two barrier widths, $d = 1.0$ and $d = 1.6$. The parameters are $\Delta k = 0.1$, $\langle E\rangle = 0.505$. The time increases with $V_0 < \langle E\rangle$ and decreases with $V_0 > \langle E\rangle$. Right: Mean tunneling time as a function of barrier width d for three different values of the momentum standard deviation Δk: 0.3, 0.1, and 0.05. The barrier height is $V_0 = 0.8$. The dashed line represents the classical-like estimate $\bar{\tau} = d/\sqrt{2(V_0 - E_0)}$ where $E_0 = \langle k\rangle^2/2$ (setting dimensionless units: $\hbar = m = 1$).

This behavior implies that when the tunneling process becomes less probable, the rare transmission events that occur tend to happen more rapidly. Moreover, this behavior is in agreement with the notion of a dwell time, since the mean tunneling time $\bar{\tau}$ obtained here can be interpreted as a transmission dwell time—that is, the mean residence time of the transmitted fraction of the ensemble inside the barrier region.

Figure 21(b) also shows the mean tunneling time $\bar{\tau}$ of the Gaussian wave packet as a function of the barrier width d for different momentum spreads Δk and barrier height $V_0 = 0.8$. In all cases, $\bar{\tau}$ increases with d, as expected from the longer traversal distance inside the classically forbidden region. The results asymptotically approach the semiclassical estimate $md/\hbar\kappa$, where the decay constant inside the barrier is given by $\kappa = \sqrt{2m(V_0 - E_0)}/\hbar$ with $E_0 = \hbar^2\langle k\rangle^2/2m$. Note that $\langle k^2\rangle \approx \langle k\rangle^2$ if the momentum distribution is narrow enough, then $E_0 \approx \langle E\rangle$, which is valid for the cases considered here. Superimposed on this general trend, variations emerge, particularly for narrower spectral widths, revealing the formation of quasi-bound states within the barrier. These resonances correspond to conditions of constructive interference and are more evident for spectrally narrow wave packets, emphasizing the role of coherence in the tunneling dynamics. Broader wave packets (Δk large) average over energy components, thereby smoothing out such resonant features. The semiclassical prediction reproduces only the monotonic component of the behavior, failing to capture the interference-induced variations.

The overall dependence of $\bar{\tau}$ on d is consistent with the results reported by Hara and Ohba [127], who investigated the same quantity within Nelson's stochastic quantization

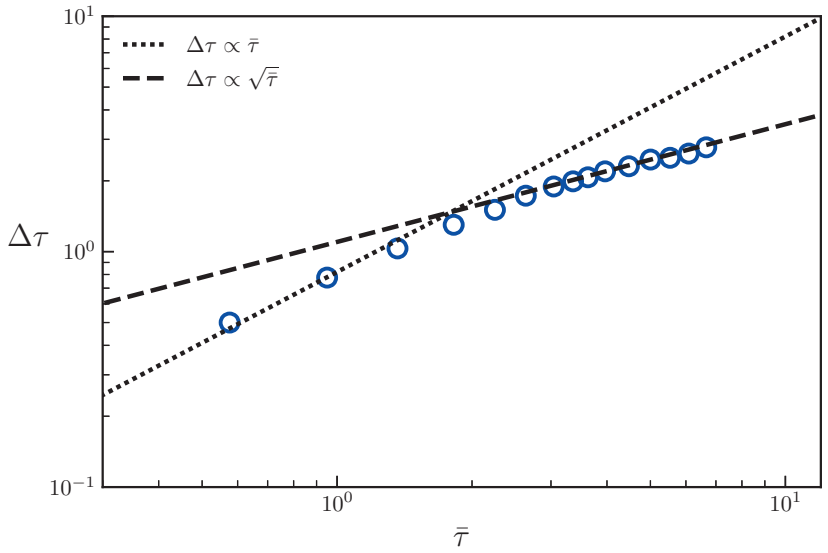


FIGURE 22 – Standard deviation of the tunneling time $\Delta\tau$ as a function of the mean tunneling time $\bar{\tau}$, in dimensionless units, obtained by varying the barrier width d. The wave packet parameters are $\langle k\rangle = 1.0$ and $\Delta k = 0.1$ ($\langle E\rangle = 0.505$), with barrier height $V_0 = 0.8$. The numerical results (blue circles) exhibit a crossover between two regimes: for short times, $\Delta\tau \propto \bar{\tau}$ (dotted line), characteristic of coherent wave packet propagation, while for longer times, the scaling approaches $\Delta\tau \propto \sqrt{\bar{\tau}}$ (dashed line), indicative of diffusive stochastic behavior.

framework. As they have shown, the mean tunneling time grows with d and approaches the semi-classical limit in the opaque regime ($\kappa d \gtrsim 2$), while deviations appear for thinner barriers, where the semi-classical approximation breaks down. Their results indicate that the mean tunneling time encodes a transition from a coherent, interference-dominated regime to an incoherent, quasiclassical one, illustrating the wave–particle duality inherent in the tunneling process.

Finally, Fig. 22 shows the dependence of the standard deviation of the tunneling time, $\Delta\tau$, on its mean value $\bar{\tau}$ as the barrier width is varied. A transition is observed between two distinct regimes: for thin barriers, $\Delta\tau$ scales linearly with $\bar{\tau}$, i.e., $\Delta\tau \propto \bar{\tau}$, whereas for thick barriers, the scaling follows $\Delta\tau \propto \sqrt{\bar{\tau}}$ (similar to the Brownian motion). The transition between these two regimes happens at $\kappa d \approx 2$. This crossover behavior was also reported by Hara and Ohba in Ref. [127] and can be interpreted as a transition from a ballistic regime—where the wave packet crosses the barrier coherently—to a diffusive regime, characterized by multiple internal reflections and interference processes within the barrier. In contrast, for the case of a particle described by a stationary plane wave, the proportionality $\Delta\tau \propto \bar{\tau}$ persists across all barrier widths, since the process is fully coherent.

This analysis of the tunneling behavior of wave packets within the framework of Nelson's stochastic mechanics still requires further investigation, particularly through refined numerical methods and the exploration of a broader range of parameter regimes.

It would also be valuable to compare the results obtained here—using the time defined in Eq. (5.49)—with MFPT estimates extracted directly from trajectory simulations. Moreover, we may compare these results with alternative formulations of tunneling time, such as Larmor precession times [128].

6 TUNNELING TIMES II: BOUND STATES

This chapter is devoted to the analysis of tunneling times for bound states in double-well potentials. We begin by examining the case of the double square well, which admits an analytical treatment and thus serves as a useful reference model. The results for the tunneling time in this system are then compared with those obtained from the two-state approximate approach from quantum mechanics based on the half-period of oscillation of non-stationary states. This comparison reveals an intriguing relationship between the two characteristic times.

Subsequently, the analysis is extended to other classes of double-well potentials, allowing us to identify common dynamical features and the influence of potential shape on the tunneling process. In the opaque-barrier limit, the results are further generalized to arbitrary double-well configurations using the WKB approximation.

The tunneling dynamics in quartic double wells have been previously investigated in Refs. [14, 83], where some results qualitatively resemble those obtained in this work. Our approach, however, aims to provide a more general and systematic treatment, extending the discussion to a broader class of potential profiles.

Finally, the formalism for tunneling time developed within Nelson's stochastic quantization framework is applied to a concrete physical system: the inversion dynamics of the ammonia molecule, modeled as a double-well potential. The inversion frequency of ammonia obtained through the stochastic quantization approach exhibits excellent agreement with experimental measurements.

6.1 DOUBLE SQUARE WELL

We consider an infinite double square well potential defined as

$$V(x) = \begin{cases} \infty, & |x| \geq b/2, \\ V_0, & -d/2 < x < d/2, \\ 0, & \text{otherwise.} \end{cases} \tag{6.1}$$

and illustrated schematically in Fig. 23. The potential consists of two identical wells of width $L = (b-d)/2$ separated by a central barrier of width d and height V_0. Accordingly, we call this potential a double square well (DSW). For bound states satisfying $E < V_0$, the time-independent Schrödinger equation can be solved analytically. The even (symmetric)

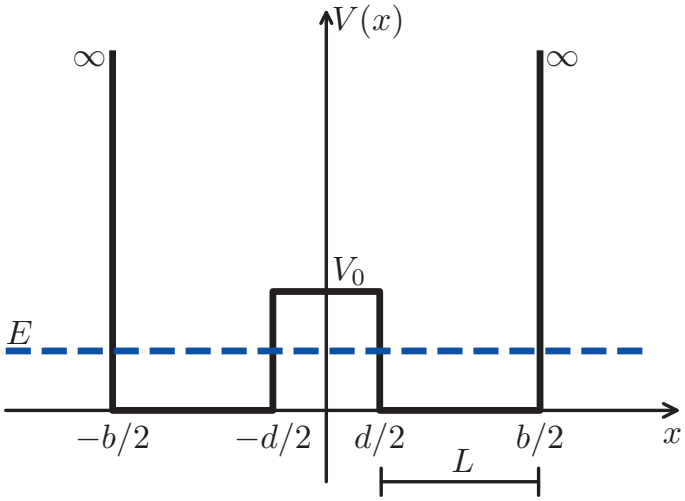


FIGURE 23 – Double square well potential with arbitrary parameters. This potential can be built with two infinity walls at the positions $\{-\frac{b}{2}, \frac{b}{2}\}$ and with a barrier of thickness d and height V_0 centered on the origin. The dashed line indicates the particle's energy E.

solutions take the form

$$\psi(x) = \begin{cases} A\sin[k(x+b/2)], & -b/2 \le x \le -d/2, \\ C\cosh(\kappa x), & -d/2 < x < d/2, \\ -A\sin[k(x-b/2)] & d/2 \le x \le b/2, \end{cases} \tag{6.2}$$

where the parameters are defined as $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}/\hbar$, or equivalently $\kappa^2 = k_0^2 - k^2$ with $k_0 = \sqrt{2mV_0}/\hbar$. Applying the continuity conditions of the wavefunction and its derivative at $x = \pm d/2$ yields the following relation:

$$\frac{C}{A} = \frac{\sin(kL)}{\cosh(\kappa d/2)}, \tag{6.3}$$

and the transcendental equation

$$k\cot(kL) + \kappa\tanh(\kappa d/2) = 0, \tag{6.4}$$

which determines the allowed energy eigenvalues, or equivalently the quantized wave numbers k, for the symmetric states.

Similarly, the antisymmetric (odd) stationary solutions of the time-independent Schrödinger equation can be written as

$$\psi(x) = \begin{cases} A'\sin[k(x+b/2)], & -b/2 \le x \le -d/2, \\ C'\sinh(\kappa x), & -d/2 < x < d/2, \\ A'\sin[k(x-b/2)], & d/2 \le x \le b/2, \end{cases} \tag{6.5}$$

where the continuity conditions yield the relation

$$\frac{C'}{A'} = \frac{\sin(kL)}{\sinh(\kappa d/2)}, \tag{6.6}$$

and the quantization condition

$$\kappa \tan(kL) + k \tanh(\kappa d/2) = 0, \tag{6.7}$$

which determines the allowed energy eigenvalues for the antisymmetric states. The two transcendental equations, (6.4) and (6.7), governing the symmetric and antisymmetric eigenstates, respectively, can be combined into the unified form

$$\frac{k^2}{\kappa^2} \cot(kL) + \tan(kL) = -2\frac{k}{\kappa} \coth(\kappa d), \tag{6.8}$$

which can be used to obtain the entire energy spectrum of the double square well potential.

It is worth noting that for $E > V_0$, the solutions can be straightforwardly extended by substituting $\kappa \to ik_1$, where $k_1 = \sqrt{2m(E - V_0)}/\hbar$. In this case, the exponential behavior of the wavefunction inside the barrier region ($-d/2 < x < d/2$) becomes oscillatory. Nevertheless, in the present work we shall not pursue this regime further, as our main interest lies in the tunneling case $E < V_0$, where the particle effectively "tunnels" through the barrier and transits between the two wells.

Equation (6.8) can be conveniently rewritten in dimensionless form as

$$f(\epsilon) \equiv \frac{\epsilon}{1-\epsilon} \cot(k_0 L\sqrt{\epsilon}) + \tan(k_0 L\sqrt{\epsilon}) + 2\sqrt{\frac{\epsilon}{1-\epsilon}} \coth(k_0 d\sqrt{1-\epsilon}) = 0, \tag{6.9}$$

where $\epsilon = E/V_0$ and $\epsilon \in (0, 1)$. Thus, finding the quantized energy levels of the system reduces to determining the roots of the function $f(\epsilon)$ within the domain $(0, 1)$. Since Eq. (6.9) cannot be solved analytically, the roots are obtained numerically for given potential parameters V_0, L, and d.

Recall Eq. (4.39) for the mean first passage time in bound states. In the case of the double-square well discussed here, this equation can be written as

$$\bar{\tau} = \frac{2m}{\hbar} \int_{-d/2}^{d/2} \frac{1}{p(x)} \left(\int_{-b/2}^{x} p(y)\, dy \right) dx \tag{6.10}$$

for a particle initially localized at $x = -d/2$ and undergoing a diffusive motion within the region $[-b/2, d/2]$ until it crosses the point $x = d/2$ (see Fig. 23). Equation (6.10) for the double-square well potential can be evaluated analytically. This makes it an excellent model for investigating the relationship between the mean first passage time and the structure of the stationary quantum states in a double-well configuration.

For a particle in the ground state, the wave function is even, as given by Eq. (6.2). Accordingly, the stationary probability density $p(x) = |\psi(x)|^2$ takes the form

$$p(x) = \begin{cases} A^2 \sin^2(k(x + b/2)), & -b/2 \le x \le -d/2, \\ C^2 \cosh^2(\kappa x), & -d/2 < x < d/2, \\ A^2 \sin^2(k(x - b/2)), & d/2 \le x \le b/2. \end{cases} \tag{6.11}$$

Substituting this probability density into Eq. (6.10), the inner integral can be separated into two contributions, corresponding to the well region on the left and the barrier region in the center:

$$\int_{-b/2}^{x} p(y)\, dy = \int_{-b/2}^{-d/2} p(y)\, dy + \int_{-d/2}^{x} p(y)\, dy. \tag{6.12}$$

Let us consider the first integral in Eq. (6.12). Using the identity $\sin^2(\theta) = \frac{1}{2}\Big[1 - \cos(2\theta)\Big]$, we obtain

$$\begin{aligned} \int_{-b/2}^{d/2} p(y)\, dy &= A^2 \int_{-b/2}^{-d/2} \sin^2\Big(k(y + b/2)\Big) dy \\ &= A^2 \int_{-b/2}^{-d/2} \frac{1 - \cos\Big(2k(y + b/2)\Big)}{2}\, dy \\ &= A^2 \left(\frac{L}{2} + \frac{\sin\Big(2k(d/2 - b/2)\Big)}{4k} \right) \\ &= A^2 \left(\frac{L}{2} - \frac{\sin(2kL)}{4k} \right). \end{aligned} \tag{6.13}$$

Next, for the second integral in Eq. (6.12), we use the identity $\cosh^2(\theta) = \frac{1}{2}[1 + \cosh(2\theta)]$, obtaining

$$\begin{aligned} \int_{-d/2}^{x} p(y)\, dy &= C^2 \int_{-d/2}^{x} \cosh^2(\kappa y)\, dy \\ &= C^2 \int_{-d/2}^{x} \frac{1 + \cosh(2\kappa y)}{2}\, dy \\ &= C^2 \left(\frac{x + d/2}{2} + \frac{\sinh(2\kappa x) - \sinh(-\kappa d)}{4\kappa} \right). \end{aligned} \tag{6.14}$$

Combining the two results, the full expression for the integral in Eq. (6.12) becomes

$$\begin{aligned} \int_{-b/2}^{x} p(y)\, dy =& A^2 \left(\frac{L}{2} - \frac{\sin(2kL)}{4k} \right) + C^2 \left(\frac{d}{4} + \frac{\sinh(\kappa d)}{4\kappa} \right) \\ &+ C^2 \left(\frac{x}{2} + \frac{\sinh(2\kappa x)}{4\kappa} \right). \end{aligned} \tag{6.15}$$

Substituting this result into Eq. (6.10), the mean tunneling time can be expressed as

$$\begin{aligned} \bar{\tau} =& \frac{2m}{\hbar} \int_{-d/2}^{d/2} \frac{1}{C^2 \cosh^2(\kappa x)} \left[A^2 \left(\frac{L}{2} - \frac{\sin(2kL)}{4k} \right) \right. \\ &\left. + C^2 \left(\frac{d}{4} + \frac{\sinh(\kappa d)}{4\kappa} \right) + C^2 \left(\frac{x}{2} + \frac{\sinh(2\kappa x)}{4\kappa} \right) \right] dx. \end{aligned} \tag{6.16}$$

The integrand in Eq. (6.16) can be separated into even and odd parts with respect to x. Since $\cosh^2(\kappa x)$ is an even function, the third term inside the square brackets, which is odd in x, vanishes under integration over the symmetric interval $[-d/2,\, d/2]$. The result is therefore

$$\bar{\tau} = \frac{2m}{\hbar}\left[\frac{A^2}{C^2}\left(\frac{L}{2} - \frac{\sin(2kL)}{4k}\right) + \frac{d}{4} + \frac{\sinh(\kappa d)}{4\kappa}\right]\int_{-d/2}^{d/2}\frac{dx}{\cosh^2(\kappa x)}. \tag{6.17}$$

The remaining integral is straightforward and yields

$$\int_{-d/2}^{d/2}\frac{dx}{\cosh^2(\kappa x)} = \frac{2}{\kappa}\tanh\left(\frac{\kappa d}{2}\right). \tag{6.18}$$

Thus, the mean tunneling time becomes

$$\bar{\tau} = \frac{2m}{\hbar}\left[\frac{A^2}{C^2}\left(\frac{L}{2} - \frac{\sin(2kL)}{4k}\right) + \frac{d}{4} + \frac{\sinh(\kappa d)}{4\kappa}\right]\frac{2}{\kappa}\tanh\left(\frac{\kappa d}{2}\right). \tag{6.19}$$

Using the relation between the coefficients A and C from Eq. (6.3), we obtain

$$\bar{\tau} = \frac{m}{\hbar\kappa}\tanh\left(\frac{\kappa d}{2}\right)\left[\left(\frac{\cosh(\kappa d/2)}{\sin(kL)}\right)^2\left(2L - \frac{\sin(2kL)}{k}\right) + \frac{\sinh(\kappa d)}{\kappa} + d\right]. \tag{6.20}$$

Now, Eq. (6.20) can be further simplified to eliminate the trigonometric functions. Considering the transcendental equation for the even states in (6.4), one can derive the relations

$$\frac{1}{\sin^2(kL)} = 1 + \frac{\kappa^2}{k^2}\tanh^2\left(\frac{\kappa d}{2}\right), \tag{6.21}$$

and

$$\sin(2kL) = 2\sin(kL)\cos(kL) = -\frac{2\kappa\tanh(\frac{\kappa d}{2})}{k\left(1 + \frac{\kappa^2}{k^2}\tanh\left(\frac{\kappa d}{2}\right)\right)}, \tag{6.22}$$

where it should be noted that, from Eq. (6.4), $\tan(kL) > 0$ must be valid.

Substituting Eqs. (6.21) and (6.22) into Eq. (6.20), and using the identity $\kappa^2 = k_0^2 - k^2$, results in

$$\bar{\tau} = \frac{m}{\hbar\kappa}\tanh\left(\frac{\kappa d}{2}\right)\left[2L\left(1 + \frac{k_0^2}{k^2}\sinh^2\left(\frac{\kappa d}{2}\right)\right) + \frac{k_0^2}{k^2\kappa}\sinh(\kappa d) + d\right]. \tag{6.23}$$

Finally, making use of the identity $2\sinh^2(x) = \cosh(2x) - 1$, the result can be written in the form

$$\bar{\tau} = \frac{m}{\hbar\kappa}\tanh\left(\frac{\kappa d}{2}\right)\left[L\left(2 - \frac{k_0^2}{k^2} + \frac{k_0^2}{k^2}\cosh(\kappa d)\right) + \frac{k_0^2}{k^2\kappa}\sinh(\kappa d) + d\right]. \tag{6.24}$$

Equation (6.24) provides an exact analytical expression for the mean tunneling time of a particle in the symmetric ground state of a double-square well potential.

6.1.1 High Barrier Limit

Let us now analyze the behavior of the mean tunneling time for the double-square well potential given by Eq. (6.24) in the limit of an opaque barrier, that is, when $V_0 \gg E$ or $\kappa d \gg 1$. In this regime, the hyperbolic functions can be approximated by their asymptotic forms

$$\tanh\left(\frac{\kappa d}{2}\right) \approx 1, \quad \cosh(\kappa d) \approx \frac{e^{\kappa d}}{2}, \quad \sinh(\kappa d) \approx \frac{e^{\kappa d}}{2}. \tag{6.25}$$

Substituting these approximations into Eq. (6.24) yields

$$\bar{\tau} \overset{\kappa d \gg 1}{\approx} \frac{m}{\hbar\kappa}\left[\frac{Lk_0^2}{k^2}\left(\frac{e^{\kappa d}}{2} - 1\right) + \frac{k_0^2}{2k^2\kappa}e^{\kappa d} + 2L + d\right]. \tag{6.26}$$

In this limit, the exponential terms dominate the expression, allowing us to neglect all non-exponential contributions. This leads to the simplified form

$$\bar{\tau} \approx \frac{mk_0^2}{2\hbar k^2\kappa^2}e^{\kappa d}\left(L\kappa + 1\right). \tag{6.27}$$

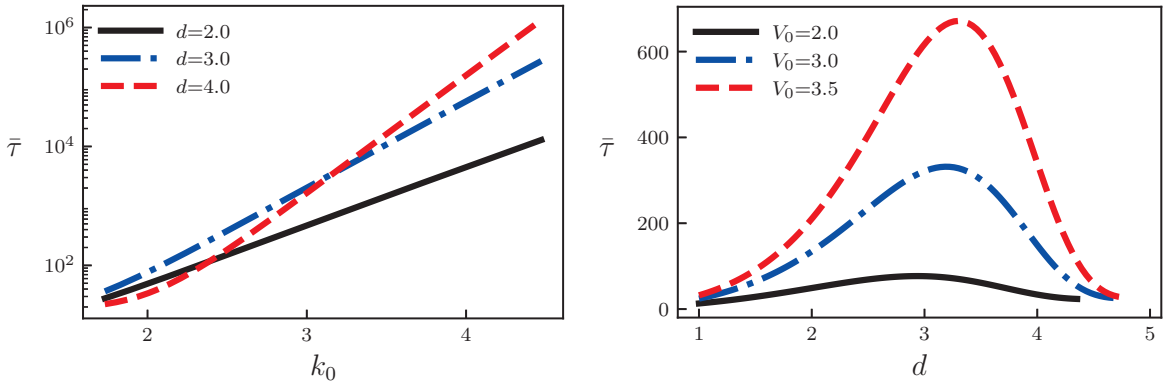
If we further assume that $L\kappa \gg 1$, which is consistent with the high barrier condition $V_0 \gg E$, the expression reduces to

$$\bar{\tau} \approx \frac{mLk_0^2}{2\hbar k^2\kappa}e^{\kappa d} \approx \frac{mLk_0}{2\hbar k^2}e^{k_0 d}, \tag{6.28}$$

where in the last step we used the approximation $\kappa \approx k_0$. The exponential factor in Eq. (6.28) shows the characteristic suppression of tunneling probability, and hence the increase in tunneling time, with the barrier width d and with the square root of the potential in $k_0 = \sqrt{2mV_0}/\hbar$. This result is consistent with the intuitive expectation that the mean time required for a particle to tunnel through a barrier increases rapidly as the barrier becomes higher or wider.

In Fig. 24(a), we present, in a semi-logarithmic plot, the behavior of $\bar{\tau}$ given by Eq. (6.24) as a function of k_0 (recall that $k_0 = \sqrt{2mV_0}/\hbar$) for three values of d, namely $d = 2.0$, 3.0, and 4.0, with fixed $b = 6$ in dimensionless units: setting $\hbar = m = 1$ and fixing b. We see from this figure that $\bar{\tau}$ increases monotonically with k_0, as expected, and exhibits an exponential growth at large k_0, in agreement with Eq. (6.28)—a behavior clearly reflected by the linear asymptotic trend in the semi-logarithmic plot.

Figure 24(b) shows $\bar{\tau}$ as a function of d, for three different values of V_0. One sees from this figure that, starting from a small value of d, the mean tunneling time first increases with the barrier width, as expected, then reaches a maximum value, and decreases after that. This behavior is explained by the fact that increasing d, for fixed b, leads to a reduction in the distance, L, between the impenetrable walls and the barrier, see Fig. 23, so that for sufficiently small L the particle becomes "compressed" in a narrow



(a) (b)

FIGURE 24 – Left: mean tunneling time as a function of k_0 for three values of the barrier thickness $d = \{2.0, 3.0, 4.0\}$ with fixed $b = 6.0$. Note the exponential growth with increasing k_0. Right: mean tunneling time as a function of d for three values of the barrier height $V_0 = \{2.0, 3.0, 3.5\}$ with $b = 6.0$ fixed. Note that the mean tunneling time has a maximum. Values in dimensionless units.

region between the infinite wall and the barrier wall. In such a situation, reducing the classically allowed region (i.e., decreasing L) increases the kinetic energy—the ground state energy eigenvalue increases as the L decreases—causing the particle to traverse the allowed region more rapidly and encounter the barrier more frequently. In other words, the particle "ricochets" ever so more rapidly between these two vertical walls, which leads to an increase in the tunneling probability and a decrease in the tunneling time.

6.1.2 Numerical Simulations

For the double-square well potential, the forward drift velocity is composed solely of the osmotic component, which takes the form

$$u(x) = \begin{cases} \dfrac{\hbar k}{m}\cot[k(x+b/2)], & -b/2 \le x \le -d/2, \\ \dfrac{\hbar \kappa}{m}\tanh(\kappa x), & -d/2 < x < d/2, \\ \dfrac{\hbar k}{m}\cot[k(x-b/2)], & d/2 \le x \le b/2. \end{cases} \tag{6.29}$$

calculated from the stationary symmetric wave function given by Eq. (6.2). Using the forward SDE in (4.35), together with the expression above for $u(x)$, one can simulate the stochastic trajectories of a particle in the ground state as it tunnels between the two wells using the Euler-Maruyama method, as described in Sec. 5.1.2. Examples of such simulated trajectories are displayed in Fig. 25, illustrating the stochastic oscillations of the particle between the two wells separated by the central barrier.

The total instantaneous energy of the system, in this case, can be written as

$$E(x) = \frac{1}{2}mu^2(x) + V(x), \tag{6.30}$$

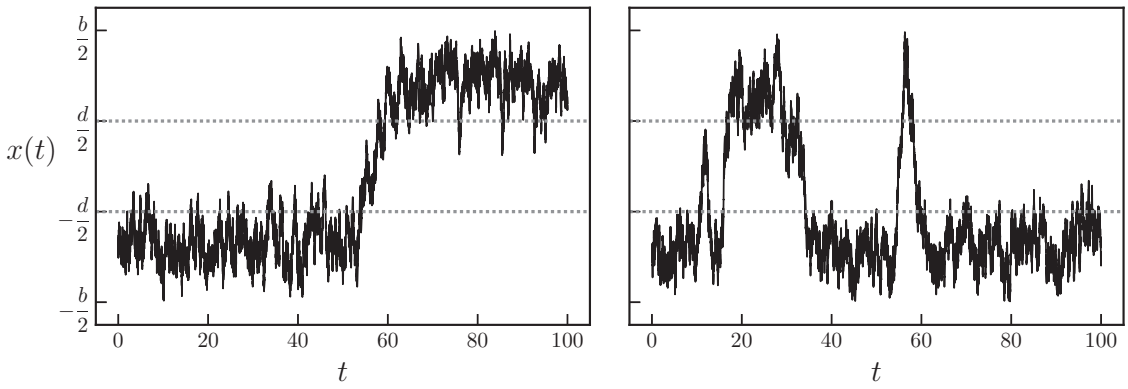


FIGURE 25 – Sample stochastic trajectories for a particle evolving in a double square well potential obtained via Nelson's stochastic quantization. The dotted lines indicate the barrier edges.

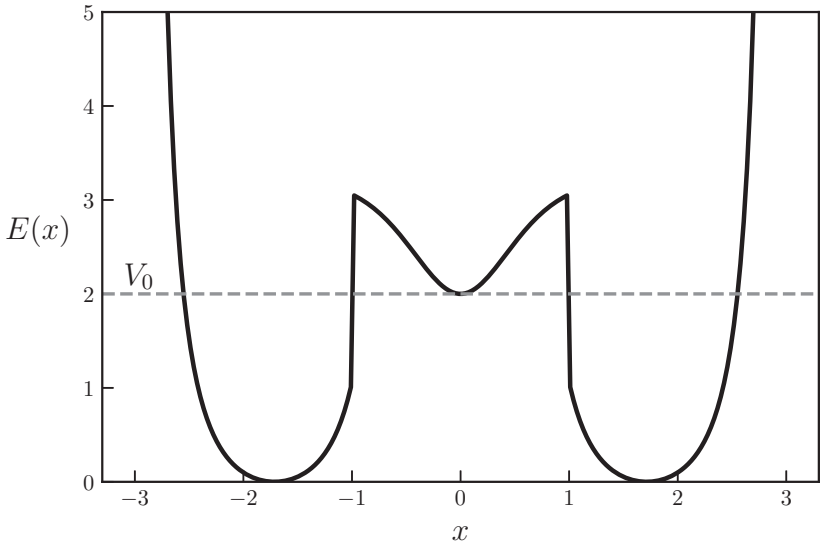


FIGURE 26 – Instantaneous energy $E(x)$ of the system as a function of position in the double square well potential. The parameters of the double square well are $d = 2.0$, $b = 6.0$, and $V_0 = 2.0$ in dimensionless units ($\hbar = m = 1$). The quantized energy of the particle in the ground state of this system is $E_0 \approx 0.7462$. The horizontal dashed line indicates the barrier height V_0.

which, upon substituting the explicit forms of $u(x)$ and $V(x)$, yields

$$E(x) = \begin{cases} \dfrac{\hbar^2 k^2}{2m} \cot^2[k(x + b/2)], & -b/2 < x \leq -d/2, \\ \dfrac{\hbar^2 \kappa^2}{2m} \tanh^2(\kappa x) + V_0, & -d/2 < x < d/2, \\ \dfrac{\hbar^2 k^2}{2m} \cot^2[k(x - b/2)], & d/2 \leq x < b/2. \end{cases} \tag{6.31}$$

The energy $E(x)$ in Eq. (6.31) as a function of the position is shown in Fig. 26. Due to the behavior of the cotangent function, $\cot(x) \to \infty$ as $x \to 0$, the kinetic energy diverges near the infinite potential walls at both boundaries of the well. Consequently, the particle is dynamically repelled from these regions, rarely approaching the walls. Moreover, since

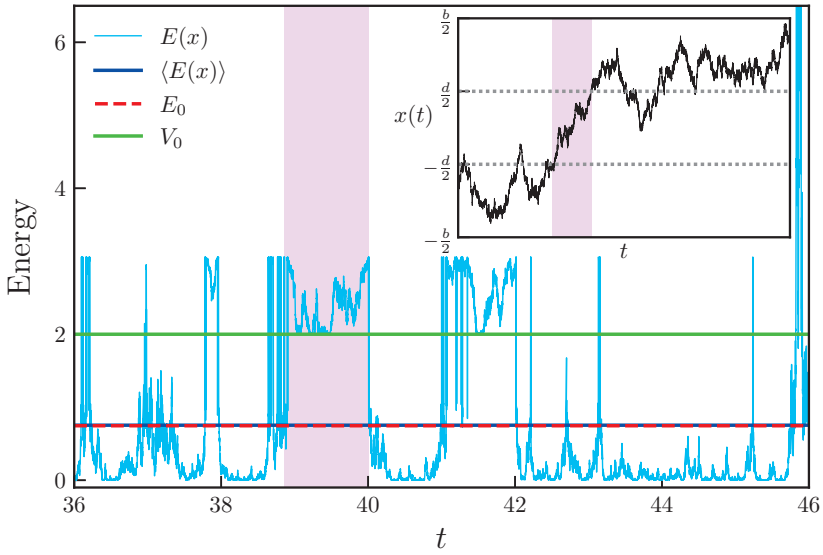


FIGURE 27 – Sample time series of the particle's instantaneous energy $E(x)$ in the double square well potential obtained via stochastic quantization. The mean energy $\langle E(x)\rangle$ coincides with the ground-state eigenenergy E_0 of the system. The inset displays the corresponding stochastic trajectory over the same time interval as the main plot, with the barrier edges indicated by the dotted lines. The highlighted region illustrates that the instantaneous energy exceeds the barrier height V_0 whenever the particle enters the barrier region. The instantaneous energy also exhibits a sharp rise whenever the particle tries to approach the infinite walls of the potential.

$\cot(\pm\pi/2) = 0$, the energy vanishes at the points

$$x_\pm = \pm\frac{\pi}{2k} \mp \frac{b}{2},$$

i.e., at a distance of $\pi/(2k)$ from the infinite walls. At these positions, both the energy and the osmotic velocity vanish, leaving the motion governed solely by the stochastic (diffusive) component of the dynamics. Note that the points $x_\pm$ are exactly the points where the probability distribution, given by Eq. (6.11), is maximum. A similar situation occurs at the midpoint of the barrier, $x = 0$, where the energy equals the barrier height, $E(x = 0) = V_0$. At this point, both the kinetic energy and osmotic velocity are zero, and the motion results purely from the Wiener process fluctuations. This does not violate the uncertainty principle, since the position remains indeterminate due to the inherent stochasticity of the dynamics. As discussed in Chapter 3, the uncertainty relations emerge naturally within the framework of stochastic quantization.

It is also worth emphasizing that, in the stochastic description, when the particle is within the barrier region, its instantaneous energy satisfies $E(x) \geq V_0$ at all times. Thus, strictly speaking, the conventional notion of quantum tunneling does not apply here: the particle does not traverse a classically forbidden region with insufficient energy. Instead, the stochastic dynamics continuously exchange energy with the background noise, allowing the particle to transiently acquire enough energy to cross the barrier. Figure 27 shows

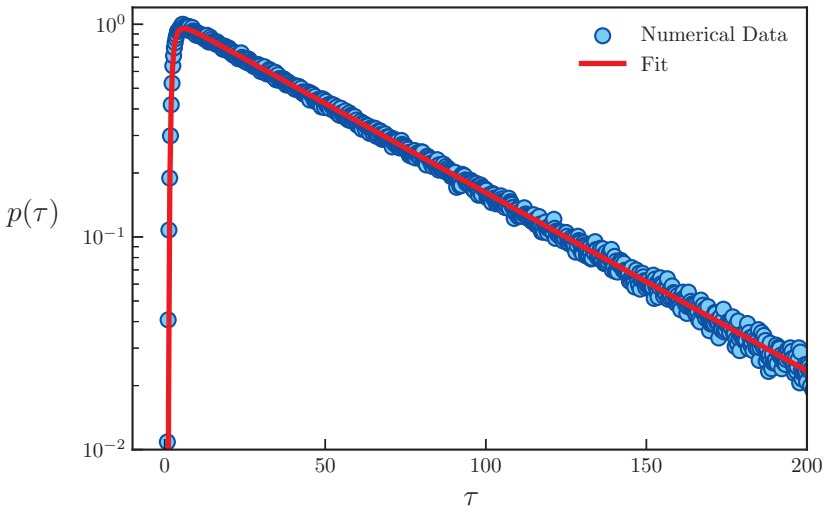


FIGURE 28 – Tunneling time distribution (blue circles) for the double square well potential with dimensionless parameters $d = 2.0$, $b = 6.0$, and $V_0 = 2.0$, obtained from 10^6 simulated trajectories using a time step of 10^{-4}. The red line represents the fit given by Eq. (5.36), with fitting parameters $\tau_\alpha = 1.97$, $\tau_\beta = 51.80$ and $\gamma = 2.92$.

the variation of the particle's total energy for an interval of a representative trajectory, along with the averaged energy along the trajectory. The mean value closely matches the ground-state eigenenergy, $E_0 = \hbar^2 k_0^2/2m$, confirming the consistency between the stochastic simulations and the quantum solution.

From the ensemble of simulated trajectories, we can also obtain the tunneling time distribution, which is shown in Fig. 28. In the simulations, a total of 10^6 trajectories were generated with a time step $\Delta t = 10^{-4}$. The initial position of each particle was set at $x = -(b+d)/4$, corresponding to the center of the left well, and the dynamics was followed until the particle reached $x = (b+d)/4$, the center of the right well. As it can be observed in Fig. 28, the distribution exhibits the characteristic exponential tail. The numerical data were fitted using the expression given in Eq. (5.36), showing an excellent agreement. The mean tunneling time extracted from the numerical simulations of $\bar{\tau}_{\text{num}} = 54.45$ is in very good agreement with the theoretical value of $\bar{\tau} = 55.90$ obtained from Eq. (6.24), thus validating the analytical treatment of the problem within the stochastic quantization framework.

6.1.3 Quantum Mechanics Prediction

In the standard formalism of quantum mechanics, the tunneling process in a symmetric double-well potential can be interpreted as the temporal evolution of a quantum superposition between two stationary states of opposite parity. In particular, the ground state (even parity) and the first excited state (odd parity), given respectively by Eqs. (6.2) and (6.5), constitute a pair of quasi-degenerate states that define the fundamental tunneling dynamics of the system [129]; see Fig. 29.

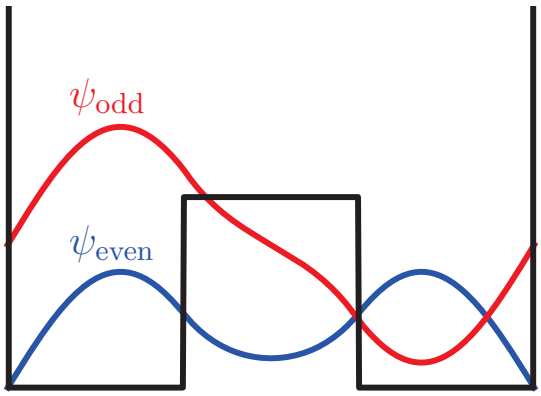


FIGURE 29 – Even (ψ_{even}) and odd (ψ_{odd}) stationary states of the symmetric double square well potential (usually the ground and first excited states). The even state is symmetric with respect to the center of the well, while the odd state displays a single node at the midpoint. For clarity, the odd state has been vertically shifted to improve visualization. These two eigenstates form the basis for tunneling dynamics and determine the energy splitting ΔE responsible for coherent oscillations between the wells.

From these two stationary states, one can construct localized states predominantly confined in the left or right wells of the potential. These localized wave functions are defined as

$$\begin{aligned} \psi_{\text{left}}(x) &= \frac{1}{\sqrt{2}}\Big[\psi_{\text{even}}(x) + \psi_{\text{odd}}(x)\Big], \\ \psi_{\text{right}}(x) &= \frac{1}{\sqrt{2}}\Big[\psi_{\text{even}}(x) - \psi_{\text{odd}}(x)\Big]. \end{aligned} \tag{6.32}$$

The states $\psi_{\text{left}}(x)$ and $\psi_{\text{right}}(x)$ are not eigenstates of the Hamiltonian; instead, they represent localized combinations that approximate the physical situation of a particle initially confined in one of the wells. At $t = 0$, let the particle be in the left-localized state $\psi_{\text{left}}(x)$. The time evolution of this state is governed by the action of the time evolution operator in the odd and even states, leading to

$$\begin{aligned} \psi(x,t) &= \frac{1}{\sqrt{2}}\Big[e^{-iE_0 t/\hbar}\psi_{\text{even}}(x) + e^{-iE_1 t/\hbar}\psi_{\text{odd}}(x)\Big] \\ &= \frac{1}{\sqrt{2}}e^{-iE_0 t/\hbar}\Big[\psi_{\text{even}}(x) + e^{-i(E_1-E_0)t/\hbar}\psi_{\text{odd}}(x)\Big], \end{aligned} \tag{6.33}$$

where E_0 and E_1 are the energy eigenvalues associated with the ground (even) and first excited (odd) states, respectively. The evolution in Eq. (6.33) describes an oscillatory transfer of probability amplitude between the two wells. To see this explicitly, let us compute the probability that the particle, evolving according to the state in Eq. (6.33), is found in one of the two localized states, say $\psi_{\text{left}}(x)$. Using the orthonormality of the even

and odd eigenstates, ψ_{even} and ψ_{odd}, we obtain

$$\begin{aligned} |\langle\psi_{\text{left}}|\psi\rangle|^2 &= \left|\frac{1}{2}e^{-iE_0t/\hbar}\left[\langle\psi_{\text{even}}|\psi_{\text{even}}\rangle + e^{-i(E_1-E_0)t/\hbar}\,\langle\psi_{\text{odd}}|\psi_{\text{odd}}\rangle\right]\right|^2 \\ &= \frac{1}{4}(1+e^{-i\Delta Et/\hbar})(1+e^{i\Delta Et/\hbar}) \\ &= \frac{1+\cos\left(\frac{\Delta E}{\hbar}t\right)}{2} = \cos^2\left(\frac{\Delta E}{2\hbar}t\right), \end{aligned} \tag{6.34}$$

where $\Delta E = E_1 - E_0$. This result shows that the probability of finding the particle in the left well arises from the coherent interference between the even and odd components of the wavefunction, leading to an oscillatory population transfer between the two wells. The oscillation frequency is determined by the energy splitting ΔE, and the corresponding period of oscillation is

$$T = \frac{2\pi\hbar}{\Delta E}. \tag{6.35}$$

From Eq. (6.33), we also observe that if the system is initially prepared in the localized state $\psi_{\text{left}}(x)$, it evolves coherently into the opposite localized state $\psi_{\text{right}}(x)$ after a time interval $\Delta t = T/2 = \pi\hbar/\Delta E$ since the factor $e^{-iE_0t/\hbar}$ is an irrelevant global phase. This result establishes that the tunneling period is directly related to the energy splitting between the symmetric and antisymmetric eigenstates. A larger barrier height V_0 increases the separation between the two wells, thereby reducing the overlap between $\psi_{\text{even}}(x)$ and $\psi_{\text{odd}}(x)$ inside the barrier and exponentially suppressing the energy difference ΔE. Consequently, the tunneling period T grows rapidly as the barrier becomes more opaque.

In the limiting case where $V_0 \to \infty$, the two wells become completely isolated, effectively forming two independent infinite square wells. In this limit, $\Delta E \to 0$, the states $\psi_{\text{left}}(x)$ and $\psi_{\text{right}}(x)$ become exact eigenstates of the Hamiltonian with identical eigenvalues (degeneracy). The tunneling dynamics ceases, and the particle remains indefinitely localized in its initial well.

Figure 30 schematically illustrates this coherent oscillation process between the two wells, showing the evolution of the probability density from the left to the right well as a function of time. This simple two-state picture captures the essence of tunneling in double-well systems in quantum mechanics.

6.1.4 Comparison between Quantum and Stochastic Tunneling Times

We now proceed to estimate the energy splitting between the ground (symmetric) and the first excited (antisymmetric) states of a particle confined in a one-dimensional double square well potential, under the assumption of a high and wide central barrier. Specifically, we consider the limit in which the barrier height is much greater than the energies of the two lowest bound states, $V_0 \gg E_1$, ensuring that tunneling between the wells is weak and that the two lowest levels are nearly degenerate.

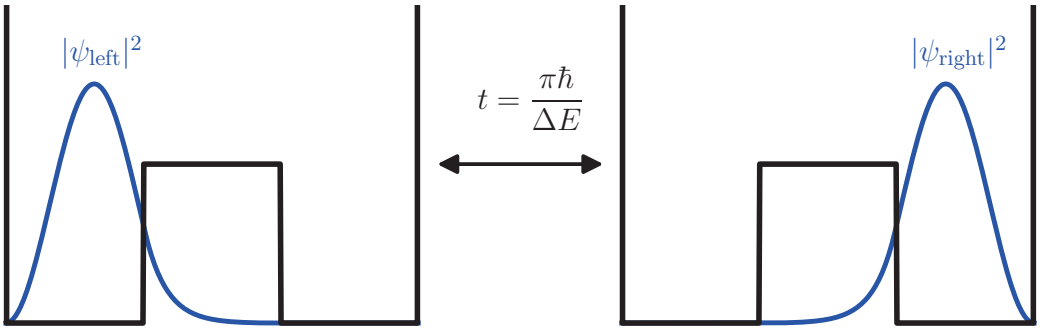


FIGURE 30 – Quantum oscillation between the left and right wells of a symmetric double square well potential. The probabilities $|\psi_{\text{left}}|^2$ and $|\psi_{\text{right}}|^2$ oscillate coherently with period $T = 2\pi\hbar/\Delta E$, where ΔE is the energy splitting between the two lowest eigenstates. This illustrates the tunneling-induced population transfer characteristic of a two-level system.

The quantization conditions for the allowed wave numbers k of even and odd states are given by the transcendental Eqs. (6.4) and (6.7). Introducing the dimensionless quantities $z_0 = k_0 L$ and $z_1 = k_1 L$ for the ground and first excited states, respectively, with $E_0 = \hbar^2 k_0^2/2m$ and $E_1 = \hbar^2 k_1^2/2m$, these equations can be rewritten as

$$\begin{aligned} \tan(z_0) + \frac{k_0}{\kappa_0}\coth(\kappa_0 d/2) = 0, \\ \tan(z_1) + \frac{k_1}{\kappa_1}\tanh(\kappa_1 d/2) = 0, \end{aligned} \tag{6.36}$$

where $\kappa_i = \sqrt{2m(V_0 - E_i)}/\hbar$ for $i = 0, 1$.

In the limit $V_0 \to \infty$, both energy levels E_0 and E_1 approach the lowest energy level of a single infinite potential well, $E_\infty = \hbar^2\pi^2/(2mL^2)$, corresponding to $k = \pi/L$. Thus, both z_0 and z_1 tend to π, allowing us to perform a first-order Taylor expansion of $\tan(z)$ around $z = \pi$. Moreover, for $\kappa d \gg 1$, we can approximate the hyperbolic functions as

$$\tanh(\kappa d/2) \approx 1 - 2e^{-\kappa d}, \quad \coth(\kappa d/2) \approx 1 + 2e^{-\kappa d}. \tag{6.37}$$

Substituting these approximations into Eqs. (6.36), we obtain, in the limit of an opaque barrier,

$$\begin{aligned} z_0 - \pi = -\frac{k}{\kappa}(1 + 2e^{-\kappa d}), \\ z_1 - \pi = -\frac{k}{\kappa}(1 - 2e^{-\kappa d}), \end{aligned} \tag{6.38}$$

where we have used $k_1 \approx k_0 = k$ and $\kappa_1 \approx \kappa_0 = \kappa$. The difference between the wave numbers of the first excited and ground states can then be expressed as

$$\Delta k = k_1 - k_0 = \frac{z_1 - z_0}{L} = \frac{4k}{L\kappa}e^{-\kappa d}. \tag{6.39}$$

Consequently, the energy difference between the two lowest states is given by

$$\Delta E = \frac{\hbar^2}{2m}(k_1^2 - k_0^2) = \frac{\hbar^2}{2m}(k_1 + k_0)(k_1 - k_0) \approx \frac{\hbar^2 k}{m}\Delta k, \tag{6.40}$$

Substituting the expression for Δk, we finally obtain

$$\Delta E \approx \frac{4\hbar^2 k^2}{mL\kappa}e^{-\kappa d} \approx \frac{4\hbar^2 k^2}{mLk_0}e^{-k_0 d}, \tag{6.41}$$

where, in the last step, we made the approximation $\kappa \approx k_0$. Equation (6.41) shows the expected exponential suppression of the energy splitting with the barrier width and height, a hallmark of tunneling phenomena in double-well systems.

In the framework of standard quantum mechanics, the period of oscillation between the localized states $\psi_{\text{left}}(x)$ and $\psi_{\text{right}}(x)$ is given by Eq. (6.35), and the characteristic tunneling time can be identified as half this period,

$$\tau_{\text{QM}} \equiv \frac{T}{2} = \frac{\pi\hbar}{\Delta E} \approx \frac{m\pi Lk_0}{4k^2\hbar}e^{k_0 d}. \tag{6.42}$$

On the other hand, the mean tunneling time obtained from Nelson's stochastic quantization, in the high-barrier limit, is given by

$$\bar{\tau} \approx \frac{mLk_0}{2\hbar k^2}e^{k_0 d}. \tag{6.43}$$

Comparing the two expressions, we find a simple proportionality relation between the two characteristic times:

$$\frac{\tau_{\text{QM}}}{\bar{\tau}} \approx \frac{\pi}{2} \tag{6.44}$$

or equivalently, $T \approx \pi\bar{\tau}$.

This result establishes an intriguing quantitative connection between the tunneling time derived from standard quantum mechanics and the mean tunneling time obtained within Nelson's stochastic formulation. Figure 31 shows the convergence of the ratio $\tau_{\text{QM}}/\bar{\tau}$ to the constant value $\pi/2$ as the barrier height increases for three values of the parameter ratio b/d. Remarkably, this convergence is relatively rapid.

In the following section, we extend this analysis to other types of double-well potentials in order to test the robustness and universality of this correspondence.

6.2 FINITE DEPTH DOUBLE SQUARE WELL

For completeness, we now present the results concerning the tunneling time for the finite depth double square well potential (FD-DSW), defined as

$$V(x) = \begin{cases} 0, & d/2 \leq |x| \leq b/2, \\ V_0, & d/2 \geq |x|, \\ V_D, & b/2 \leq |x|, \end{cases} \tag{6.45}$$

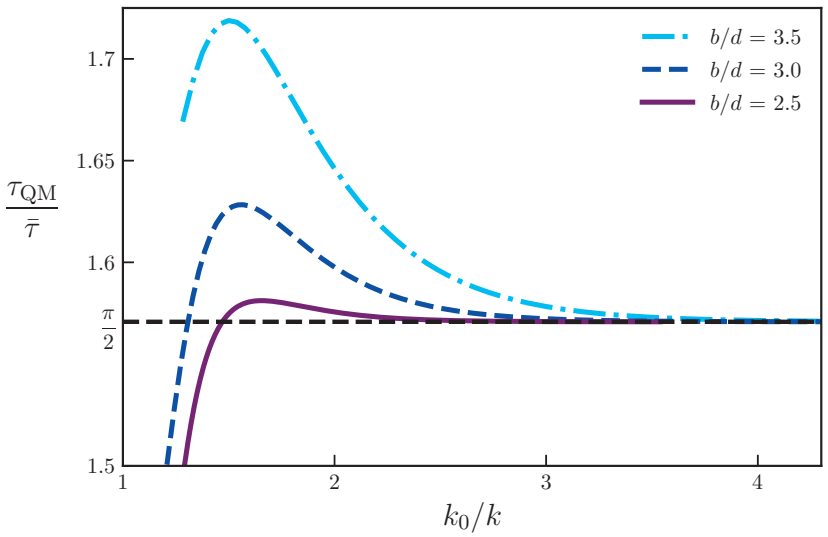


FIGURE 31 – Ratio between the quantum-mechanical half period of oscillation $T/2$ and the stochastic prediction for the tunneling time $\bar{\tau}$, as a function of the dimensionless wave number k_0/k for the double square well potential. Results are shown for three parameter ratios b/d: $\{3.5, 3.0, 2.5\}$.

and schematically represented in Fig. 32. Note that for $V_D \to \infty$, the infinite double square well potential is recovered. Solving the time-independent Schrödinger equation for this potential, and considering the case in which the particle energy is smaller than the barrier height, i.e., $E < V_0$, the symmetric (even) wave function can be written as

$$\psi(x) = \begin{cases} Ae^{\eta x}, & x < -b/2, \\ B\sin(kx) + C\cos(kx), & -b/2 < x < -d/2, \\ D\cosh(\kappa x), & -d/2 < x < d/2, \\ -B\sin(kx) + C\cos(kx), & d/2 < x < b/2, \\ Ae^{-\eta x}, & x > b/2, \end{cases} \tag{6.46}$$

where $\eta = \sqrt{2m(V_D - E)}/\hbar$, $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}\hbar$.

By imposing the continuity of the wave function and its first derivative at $x = \pm d/2$, we obtain the relations

$$\frac{C}{D} = \left[\cos(kd/2)\cosh(\kappa d/2) - \frac{\kappa}{k}\sin(kd/2)\sinh(\kappa d/2)\right], \tag{6.47}$$

and

$$\frac{B}{D} = -\left[\frac{\kappa}{k}\cos(kd/2)\sinh(\kappa d/2) + \sin(kd/2)\cosh(\kappa d/2)\right]. \tag{6.48}$$

Applying the same continuity conditions at $x = \pm b/2$ gives

$$\frac{A}{D} = \left[\frac{\kappa}{k}\sin(kL)\sinh(\kappa d/2) + \cos(kL)\cosh(\kappa d/2)\right] e^{\eta b/2}, \tag{6.49}$$

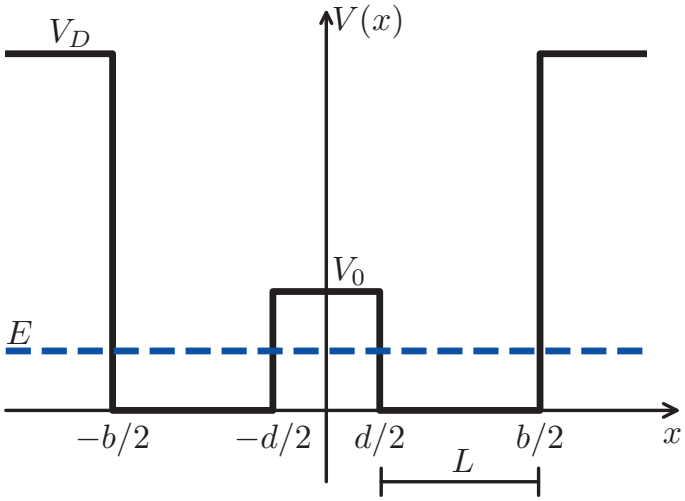


FIGURE 32 – Finite depth double square well potential characterized by the well width L, barrier width d, well depth V_D, and barrier height V_0. The dashed line indicates the particle's energy E.

where $L = (b-d)/2$ is the width of each well. The transcendental equation determining the quantized energy eigenvalues is

$$\frac{k - \kappa \cot(kL)\tanh(\kappa d/2)}{\eta} = \frac{\kappa}{k}\tanh(\kappa d/2) + \cot(kL). \tag{6.50}$$

In the limit $V_D \gg V_0 > E$, implying $\eta \gg k$ and $\eta \gg \kappa$, the left-hand side of Eq. (6.50) tends to zero, and we recover Eq. (6.4), corresponding to the energy quantization condition for the infinite double square well potential in the previous section.

From the wave function given in Eq. (6.46), we can now derive the expression for the mean tunneling time in the FD-DSW. Recalling Eq. (4.39), the mean tunneling time is now defined as

$$\bar{\tau} = \frac{2m}{\hbar}\int_{-d/2}^{d/2}\frac{1}{p(x)}\left(\int_{-\infty}^{x} p(y)\,dy\right)dx, \tag{6.51}$$

where $p(x) = |\psi(x)|^2$ represents the probability density. The inner integral in Eq. (6.51) can be decomposed into three parts as

$$\begin{aligned}\int_{-\infty}^{x} p(y)dy =& A^2\int_{-\infty}^{-b/2} e^{2\eta y}dy + \int_{-b/2}^{-d/2}\left|B\sin(ky) + C\cos(ky)\right|^2 dy \\ &+ D^2\int_{-d/2}^{x}\cosh^2(\kappa y)dy.\end{aligned} \tag{6.52}$$

All the integrals in Eq. (6.52) can be evaluated analytically, yielding

$$\int_{-\infty}^{x} p(y)dy = \mathcal{Z} + \frac{D^2}{2}x + \frac{D^2}{2}\frac{\sinh(2\kappa x)}{2\kappa}, \tag{6.53}$$

where $\mathcal{Z}$ is a constant with respect to x and is given by

$$\begin{aligned}\mathcal{Z} =&\frac{A^2}{2\eta}e^{-\eta b} + \frac{B^2}{2}\left[L + \frac{\sin(kd)}{2k} - \frac{\sin(kb)}{2k}\right] \\ &+ \frac{C^2}{2}\left[L - \frac{\sin(kd)}{2k} + \frac{\sin(kb)}{2k}\right] + \frac{BC}{2k}\left[\cos(kb) - \cos(kd)\right] \\ &+ \frac{D^2}{2}\left[\frac{d}{2} + \frac{\sinh(\kappa d)}{2\kappa}\right].\end{aligned} \tag{6.54}$$

Since both x and $\sinh(2\kappa x)$ are odd functions and only the even part of the integrand in Eq. (6.51) contributes to the integral, we obtain

$$\begin{aligned}\bar{\tau} &= \frac{2m}{\hbar}\int_{-d/2}^{d/2}\frac{\mathcal{Z}}{p(x)}dx = \frac{2m}{\hbar}\frac{\mathcal{Z}}{D^2}\int_{-d/2}^{d/2}\frac{1}{\cosh^2(\kappa x)}dx \\ &= \frac{2m}{\hbar}\frac{\mathcal{Z}}{D^2}\frac{2}{\kappa}\tanh(\kappa d/2).\end{aligned} \tag{6.55}$$

By substituting Eq. (6.54) for $\mathcal{Z}$ and using the relations for A/D, B/D, and C/D from Eqs. (6.49), (6.48), and (6.47), respectively, we obtain, after some algebraic simplifications,

$$\begin{aligned}\bar{\tau} = \frac{2m}{\hbar\kappa}\tanh\left(\frac{\kappa d}{2}\right)\Bigg\{&\frac{1}{\eta}\left[\frac{\kappa}{k}\sin(kL)\sinh\left(\frac{\kappa d}{2}\right) + \cos(kL)\cosh\left(\frac{\kappa d}{2}\right)\right]^2 \\ &+ L\left[\frac{\kappa^2}{k^2}\sinh^2\left(\frac{\kappa d}{2}\right) + \cosh^2\left(\frac{\kappa d}{2}\right)\right] \\ &- \frac{1}{2k}\left[\frac{\kappa^2}{k^2}\sinh^2\left(\frac{\kappa d}{2}\right) - \cosh^2\left(\frac{\kappa d}{2}\right)\right]\sin(2kL) \\ &+ \frac{\kappa}{k^2}\sinh(\kappa d)\sin^2(kL) + \frac{d}{2} + \frac{\sinh(\kappa d)}{2\kappa}\Bigg\}.\end{aligned} \tag{6.56}$$

In the limit of an infinite confining potential, $\eta \to \infty$, the first term in Eq. (6.56) vanishes. Applying the corresponding transcendental equation (6.50) in this limit, we obtain

$$\bar{\tau} = \frac{2m}{\hbar\kappa}\tanh\left(\frac{\kappa d}{2}\right)\left\{\left[\frac{\cosh(\kappa d/2)}{\sin(kL)}\right]^2\left[L - \frac{\sin(2kL)}{2k}\right] + \frac{d}{2} + \frac{\sinh(\kappa d)}{2\kappa}\right\}, \tag{6.57}$$

which exactly coincides with Eq. (6.20), corresponding to the mean tunneling time for the infinite double square well potential.

Therefore, the tunneling time obtained for the finite depth double square well smoothly converges to the infinite well result when $V_D \to \infty$, confirming the consistency of the formalism. Consequently, the same limiting relations discussed in the previous section apply here as well—in particular, the proportionality between the mean tunneling time from Nelson's framework and the oscillation period from standard quantum mechanics, $\tau_{\mathrm{QM}}/\bar{\tau} = \pi/2$.

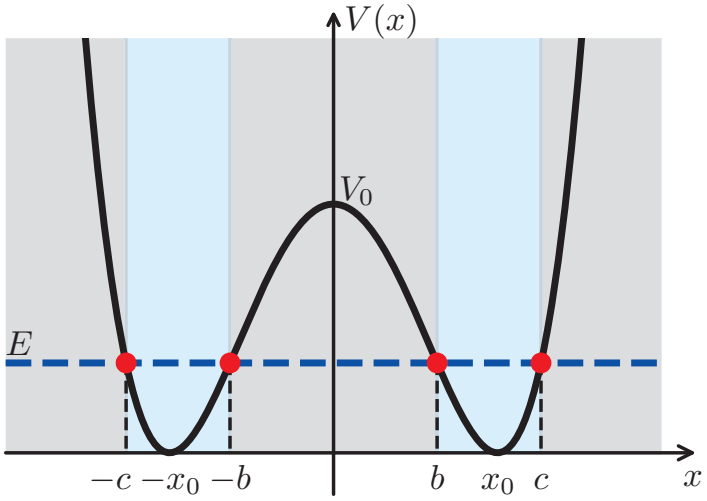


FIGURE 33 – Quartic double-well potential with barrier height V_0 and minimum point at $\pm x_0$. The dashed blue line represents the particle energy E. The red points located at $\pm c$ and $\pm b$ are the classical turning points. The blue areas correspond to the classically allowed regions, and the grey areas correspond to the classically forbidden regions. Classically, a particle with energy E will oscillate between b and c (or equivalently, between $-c$ and $-b$) and will never be found in the forbidden regions. In quantum mechanics, the particle can be in the interval $[-c, -b]$ as well as in the interval $[b, c]$ with equal probability and can travel from one interval to another through the forbidden region $[-b, b]$, this is the tunnel effect.

6.3 QUARTIC DOUBLE-WELL

Let us now analyze the case of the quartic double-well potential. Differently from the DSW and the FD-DSW discussed previously, this potential is continuous and smooth. It is defined by

$$V(x) = \frac{V_0}{x_0^4}(x^2 - x_0^2)^2 \tag{6.58}$$

and is illustrated in Fig. 33, where the classically allowed and forbidden regions are highlighted. This potential exhibits two symmetric minima located at $x = \pm x_0$ separated by a barrier of height V_0.

Unlike the double square wells, for which analytical solutions for the stationary states can be obtained, the quartic double-well does not admit closed-form expressions for its eigenfunctions or eigenenergies. Consequently, both the wave functions and the corresponding mean tunneling times must be determined numerically. In this work, the stationary wave functions were computed using the Numerov method [130, 131], which provides a highly accurate integration scheme for the one-dimensional time-independent Schrödinger equation.

The tunneling dynamics in the quartic double-well has also been analyzed within

Nelson's stochastic quantization framework in Refs. [14, 17]. The results presented there are in good agreement with those obtained in the present study. In particular, Köeppe [83] reported that the tunneling time distributions display the characteristic exponential tail typical of stochastic escape processes, and that the ratio $\tau_{\mathrm{QM}}/\bar{\tau}$ converges to a constant value close to $\pi/2$ in the limit of an opaque barrier. However, that study did not explore in detail the origin or universality of this limiting behavior, which we further investigate here.

An important question that arises when dealing with a continuous potential, such as the quartic double-well, concerns the definition of the starting point of the tunneling process or where the particle starts to interact with the barrier. Unlike the case of the double square well, where the barrier and wells are sharply defined, in a smooth potential the boundaries between classically allowed and forbidden regions are not sharply localized. Several reference points can be considered as the onset of the tunneling process: the classical turning point, the potential minimum, or the position of the maximum of the probability density, which in general is slightly displaced from the potential minimum. This displacement between the potential minimum and the probability maximum is a consequence of the continuous coupling between the wells and the barrier, which should therefore not be regarded as distinct subsystems.

A useful strategy to address this issue was proposed by Köppe in Ref. [14], where the mean tunneling time is averaged over all possible starting points $x \in (-\infty, -x_t]$ within the left well, with $x_t > 0$ being the classical turning point on the barrier. This point satisfies the condition $V(x_t) = E$, where E denotes the particle energy, as illustrated in Fig. 33 with $x_t = b$.

The averaged mean tunneling time over the starting positions can be expressed as [14]

$$\bar{\tau}_{\mathrm{avg}} = \frac{2m}{\hbar} \int_{-\infty}^{-x_f} \tilde{p}(x) \int_{x}^{x_f} \frac{1}{p(y)} \left(\int_{-\infty}^{y} p(z)\, dz \right) dy\, dx, \tag{6.59}$$

where $\tilde{p}(x)$ is the probability density renormalized within the interval $(-\infty, -x_f]$ and the upper limit x_f defines the region $[-x_f, x_f]$ where the particle is considered to be certainly in the tunneling regime. In Ref. [14] the value of this upper limit was fixed as $x_f = x_t$. This choice of fixing the upper integration limit to the classical turning point is physically well justified. Nevertheless, in order to investigate the sensitivity of the tunneling time to this choice, we generalize the analysis by allowing the upper limit to vary as $x_f \in [x_0, x_t]$ where x_0 denotes the position of the potential minimum.

In this way, we can explore how the mean tunneling time $\bar{\tau}$ changes as a function of the point x_f. This analysis helps to clarify as to what extent the tunneling process depends on the precise choice of the region that separates the wells from the barrier. It is worth noting that, in principle, one could also perform an averaging procedure over the final

TABLE 1 – Mean tunneling time $\bar{\tau}$, averaged tunneling time $\bar{\tau}_{\rm avg}$, and percentage deviation $\Delta\%$ of $\bar{\tau}_{\rm avg}$ with respect to $\bar{\tau}$ for increasing values of the barrier height V_0 with minimum point $x_0 = 1.2$. The values are dimensionless units.

V_0	$\bar{\tau}$	$\bar{\tau}_{\rm avg}$	$\Delta\%$
2.0	4.324	5.011	15.88
4.0	8.879	9.507	7.08
6.0	17.069	17.643	3.36
8.0	31.275	31.797	1.67
10.0	54.966	55.444	0.87

positions in the right well, in analogy with the averaging over the starting points. However, in the present analysis, we assume that the final position is well defined, corresponding to the presence of a detector placed at a fixed location x_f in the right well in order to simplify the treatment.

We have also investigated the influence of averaging the mean tunneling time over the initial positions of the particle. The mean tunneling times for the quartic double well were computed using both the averaged expression in Eq. (6.59) and the non-averaged expression in Eq. (4.39), that is,

$$\bar{\tau} = \frac{2m}{\hbar} \int_{-x_f}^{x_f} \frac{1}{p(x)} \left(\int_{-\infty}^{x} p(y)\, dy \right) dx, \tag{6.60}$$

A comparison between these two procedures is presented in Table 1, where we adopt $x_f = x_t$, fix the potential minimum at $x_0 = 1.2$, and vary the barrier height V_0. As the table shows, the inclusion of the averaging over initial positions produces noticeable changes in the mean tunneling time only for relatively small barriers. The differences between the averaged and non-averaged results become progressively smaller as the barrier height increases.

Figure 34 presents the results for the ratio $\tau_{\rm QM}/\bar{\tau}$, as discussed in Sec. 6.1.4, where the mean tunneling time $\bar{\tau}$ is calculated from Eqs. (6.59) and (6.60), corresponding respectively to the averaged and non-averaged formulations. The ratio is plotted as a function of the initial cutoff position $-x_f$, varying from the location of the minimum potential, $-x_0$, to the classical turning point, $-x_t$, for different barrier heights V_0 in the quartic double-well potential. As it can be observed, as the barrier height increases, the ratio approaches the constant value of $\pi/2$, becoming essentially independent of the specific choice of x_f. This result indicates that, in the opaque-barrier limit, the definition of the boundaries that delineate the tunneling region does not significantly affect the mean tunneling time. However, as shown in Fig. 34, when x_f is chosen to coincide with the classical turning point x_t, the convergence toward the asymptotic value $\pi/2$ occurs more rapidly. We also observe that the closer x_f is to the potential minimum x_0, the less relevant

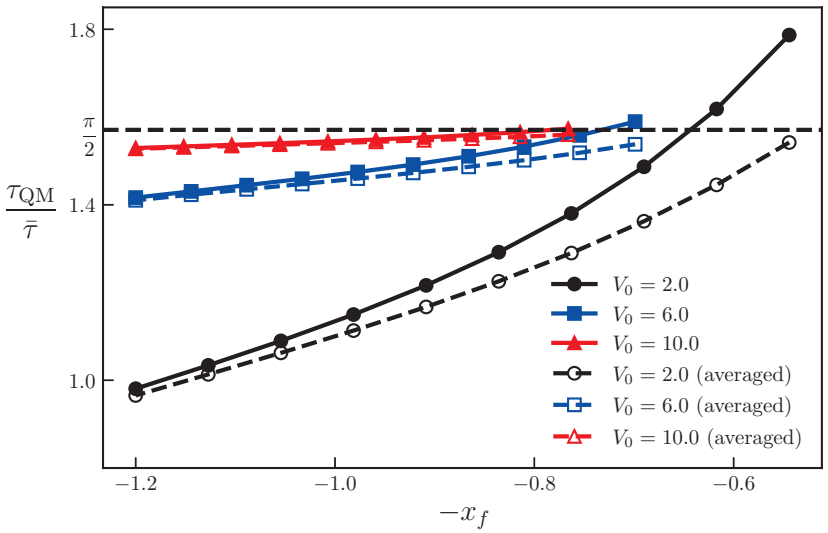


FIGURE 34 – Ratio $\tau_{QM}/\bar{\tau}$ as a function of the left barrier limit $-x_f$ varying from the minimum potential point to the classical turning point in the left well for a quartic double-well potential, Eq. (6.58), for different barrier heights $V_0 = \{2.0,\ 6.0,\ 10.0\}$ and $x_0 = 1.2$ fixed in dimensionless units. The curves are presented with and without the initial position average.

the averaging over initial positions becomes. In particular, when choosing $x_f = x_t$ and performing the averaging procedure, the ratio $\tau_{QM}/\bar{\tau}$ already approaches the value of $\pi/2$ even for relatively small barriers.

It is also important to note that the concept of tunneling becomes less meaningful for very small barrier heights. In such cases, it is difficult to ensure that the particle's energy eigenvalue remains below the barrier height in a realistic experimental setup. Consequently, the tunneling regime is physically relevant only for moderate to high barriers, where the potential effectively confines the particle within a well and separates the classically allowed regions. A similar reasoning applies to the barrier width: the notion of tunneling is only meaningful for sufficiently thick barriers, where quantum penetration through the classically forbidden region can be properly characterized.

We conclude this section by emphasizing that, in the high-barrier limit, averaging over the initial positions in the calculation of the mean tunneling time becomes essentially irrelevant. In this regime, the specific choice of the spatial limits that define the tunneling region also has a negligible influence on the results. Nevertheless, defining these limits by the classical turning points remains the most physically consistent and conceptually transparent approach, as it naturally separates the classically allowed and forbidden regions. Therefore, in the subsequent analyses involving continuous potentials, we adopt $x_f = x_t$ and Eq. (6.60) as a natural and physically consistent choice.

Additional tests performed with other double-well potentials, such as the Rosen-Morse potential [132] (to be discussed later), revealed a behavior qualitatively similar to that observed for the quartic double well. Having established these general features, we

now proceed to analyze the tunneling process in a more general framework by employing the WKB approximation, which allows us to obtain analytical insights into the behavior of the tunneling time for a generic double-well potential.

6.4 GENERIC DOUBLE-WELLS: WKB ANALYSIS

For simplicity (but without loss of generality), we consider a symmetric double-well potential, $V(x) = V(-x)$, with two minima at $x = \pm x_0$, i.e., $V'(\pm x_0) = V(\pm x_0) = 0$, and a local maximum (barrier) at the origin, i.e., $V'(0) = 0$ and $V(0) = V_0 > 0$. For a particle in a state of energy E, the classical turning points are denoted by $\pm c$ and $\pm b$, where $V(\pm c) = V(\pm b) = E$. The classically allowed regions are therefore the intervals $[-c, -b]$ and $[b, c]$ in the left and right wells of the potential, respectively, whereas the interval $[-b, b]$ corresponds to the classically forbidden region (inside the barrier); see Fig. 33. We assume furthermore that V_0 is sufficiently high, so that $E_0, E_1 < V_0$, where E_0 and E_1 denote the energies of the ground state and first excited state, respectively. We now investigate the tunneling time predicted by stochastic quantization for a particle in the ground state.

According to the discussion presented in the previous section, the tunneling time can be calculated using Eq. (4.39), which in our case is given simply by

$$\bar{\tau} = \frac{2m}{\hbar} \int_{-b}^{b} \frac{1}{p(x)} \left(\int_{-\infty}^{x} p(y)\, dy \right) dx, \tag{6.61}$$

where $p(x) = |\psi(x)|^2$ is the probability density of the ground (symmetric) state. We can effectively set to zero the probability of finding the particle in the classically forbidden region to the left of the potential well, which is a justified approximation in the high-barrier limit. Furthermore, in this limit, the probability of finding the particle inside the barrier is negligible, so we can further simplify Eq. (6.61):

$$\bar{\tau} = \frac{2m}{\hbar} \int_{-b}^{b} \frac{1}{p(x)} \left(\int_{-c}^{-b} p(y)\, dy \right) dx. \tag{6.62}$$

We thus see that in order to estimate $\bar{\tau}$ we only need to know the wavefunction in the classically allowed and forbidden regions, $-c < x < -b$ and $-b < x < b$, respectively, which can easily be accomplished within the Wentzel-Kramers-Brillouin (WKB) approximation (for standard expositions of the WKB method and the derivation of the connection formulas, see, e.g., Refs. [133, 134]).

We recall that the WKB approximation is valid when the potential changes very slowly compared to the particle wavelength, which implies the condition:

$$\frac{\hbar^2}{2m} \frac{|V'(x)|}{|E - V(x)|^{3/2}} \ll 1. \tag{6.63}$$

We shall suppose throughout this section that this condition is satisfied by our generic potential $V(x)$ in the regions of interest. Let us also introduce some required quantities:

$$k(x) = \frac{\sqrt{2m(E - V(x))}}{\hbar}, \qquad E > V(x), \tag{6.64}$$

$$\kappa(x) = \frac{\sqrt{2m(V(x) - E)}}{\hbar}, \qquad V(x) > E, \tag{6.65}$$

$$\Phi = \int_{-b}^{b} \kappa(x')\, dx'. \tag{6.66}$$

Using the standard connection formulas for the WKB wavefunctions [133, 134], we can write the symmetric wavefunction within the relevant regions as

$$\psi(x) \approx \begin{cases} \dfrac{A}{\sqrt{k(x)}} \cos\Big(\int_{-b}^{x} k(x')dx' + \frac{\pi}{4}\Big), & -c < x < -b, \\ \dfrac{B}{\sqrt{\kappa(x)}} \cosh(\int_{0}^{x} \kappa(x')dx'), & -b < x < b, \\ \dfrac{A}{\sqrt{k(x)}} \cos\Big(\int_{b}^{x} k(x')dx' - \frac{\pi}{4}\Big), & b < x < c. \end{cases} \tag{6.67}$$

where

$$A = B \exp\left(\frac{\Phi}{2}\right), \tag{6.68}$$

with Φ given in Eq. (6.66). The constant A can be fixed through the normalization $\int_{-c}^{c} p(x)dx \approx 1$. The antisymmetric (odd) wavefunction are given as above, with the only change that cosh is replaced with sinh.

Neglecting the probability of finding the particle inside the barrier and noting that the probability distributions in both wells are identical, we can write

$$\int_{-c}^{-b} p(x)dx = \int_{b}^{c} p(x)dx \approx 1/2. \tag{6.69}$$

We also have that, in the right well, the probability density in the WKB approximation is given by

$$\begin{aligned} \int_{b}^{c} p(x)dx &= \int_{b}^{c} \frac{A^2}{k(x)} \cos^2\left(\int_{b}^{x} k(x')dx' - \frac{\pi}{4}\right) dx \\ &\approx \frac{A^2}{2} \int_{b}^{c} \frac{dx}{k(x)}, \end{aligned} \tag{6.70}$$

where we have used the fact that the squared cosine term oscillates rapidly under the WKB condition, Eq. (6.63), and can therefore be replaced by its average value $\langle \cos^2 \rangle = 1/2$. Next, we define the classical oscillation period in the classically allowed regions as

$$T_{\mathrm{cl}} = 2 \int_{b}^{c} \frac{dx}{v(x)} = \frac{2m}{\hbar} \int_{b}^{c} \frac{dx}{k(x)}, \tag{6.71}$$

which allows us to express the integral of the probability density as

$$\int_b^c p(x)dx \approx \frac{A^2}{4m}\hbar T_{\rm cl}. \tag{6.72}$$

Combining this result with Eq. (6.69), we obtain

$$A^2 \approx \frac{2m}{\hbar T_{\rm cl}}, \tag{6.73}$$

and consequently, using the standard WKB matching condition through the barrier, Eq. (6.68),

$$B^2 \approx \frac{2m}{\hbar T_{\rm cl}} e^{-\Phi}. \tag{6.74}$$

Having obtained the WKB wavefunctions, we can now proceed to evaluate the mean tunneling time. Substituting Eqs. (6.67) and (6.69) into Eq. (6.62), we find

$$\bar{\tau} \approx \frac{m}{\hbar B^2}\int_{-b}^{b} \frac{\kappa(x)}{\cosh^2(\int_0^x \kappa(x')dx')}dx. \tag{6.75}$$

To make analytical progress, let us assume that $\kappa(x)$ varies slowly across the barrier region, which is in agreement with the WKB condition in Eq. (6.63), so that it can be approximated by its average value, $\kappa(x) \approx \kappa_0$. Under this approximation, we can write $\int_0^x \kappa(x')\,dx' \approx \kappa_0 x$. Inserting these approximations into the expression above yields

$$\bar{\tau} \approx \frac{m\kappa_0}{\hbar B^2}\int_{-b}^{b} \frac{dx}{\cosh^2(\kappa_0 x)}. \tag{6.76}$$

The integral can be evaluated exactly, giving

$$\int_{-b}^{b} \frac{dx}{\cosh^2(\kappa_0 x)} = \left[\frac{\tanh(\kappa_0 x)}{\kappa_0}\right]_{-b}^{b} = \frac{2}{\kappa_0}\tanh(\kappa_0 b). \tag{6.77}$$

Hence,

$$\bar{\tau} \approx \frac{2m}{\hbar B^2}\tanh(\kappa_0 b). \tag{6.78}$$

In the high-barrier limit, $\kappa_0 b \gg 1$, the hyperbolic tangent approaches unity, $\tanh(\kappa_0 b) \approx 1$, and the mean tunneling time simplifies to

$$\bar{\tau} \approx \frac{2m}{\hbar B^2}. \tag{6.79}$$

Using the expression for B^2 obtained previously in Eq. (6.74), we finally obtain the WKB estimate for the mean tunneling time:

$$\bar{\tau} \approx e^{\Phi} T_{\rm cl}, \tag{6.80}$$

This result shows that the mean tunneling time grows exponentially with the barrier integral, reflecting the exponential suppression of the transmission probability with increasing barrier width or height.

As mentioned in Sec. 6.1.3, in the quantum mechanics two-state approximation, the oscillation period T between localized states inside each of the two wells is determined by the energy splitting, $\Delta E = E_1 - E_0$, for the antisymmetric and symmetric states. It is well known [133, 135] that in WKB approximation the energy splitting for a symmetric double well in the high barrier limit ($\Phi \gg 1$) is given by

$$\Delta E \approx \frac{2\hbar}{T_{\rm cl}} e^{-\Phi}. \tag{6.81}$$

Inserting this into Eq. (6.35) for the oscillation period T, we get

$$T = \frac{2\pi\hbar}{\Delta E} \approx \pi e^{\Phi} T_{\rm cl}. \tag{6.82}$$

A we can see from Eqs. (6.61) and Eq. (6.82), in the high barrier limit, both $\bar{\tau}$ and T have the same dependences differing only by a multiplicative constant equal to π. Using the definition $\tau_{\rm QM} \equiv T/2$, we then recover the relation deduced in Sec. 6.1.4:

$$\frac{\tau_{\rm QM}}{\bar{\tau}} = \frac{\pi}{2}, \tag{6.83}$$

for the ratio (in the high-barrier limit) between the tunneling time, $\tau_{\rm QM}$, estimated from quantum mechanics and the mean tunneling time, $\bar{\tau}$, predicted by stochastic quantization. Note, however, that the WKB calculation presented above is valid regardless of the specific shape of the potential or energy level in the WKB limit.

6.5 APPLICATION TO AMMONIA

A well-known example of quantum tunneling is the inversion of the ammonia molecule (NH_3). In this process, the nitrogen atom can penetrate the potential barrier formed by the plane of the three hydrogen atoms, effectively oscillating between two equivalent configurations on either side of the plane. Within quantum mechanics, this inversion is understood as the time evolution of a localized state that arises from the coherent superposition of the system's symmetric (even) and antisymmetric (odd) energy eigenstates as discussed in Sec. 6.1.3.

The transition frequency—here denoted by $\nu_{\rm QM}$—for such localized states is related to the energy splitting ΔE, between the ground and first excited states of ammonia, or more exactly, from Eq. (6.35)

$$\nu_{\rm QM} = \frac{\Delta E}{2\pi\hbar}. \tag{6.84}$$

The experimental value for the ammonia inversion frequency is approximately 24 GHz [136].

Using the correspondence given in Eq. (6.83) between the mean tunneling time, $\bar{\tau}$, obtained from stochastic quantization and the quantum-mechanical tunneling time, $\tau_{\rm QM} = T/2$, defined as half the oscillation period of the probability of finding the particle

in either well, we can then write a stochastic-quantization prediction for the inversion frequency as follows:

$$\nu_{\mathrm{SQ}} \equiv \frac{1}{\pi\bar{\tau}}. \tag{6.85}$$

As argued above, ν_{SQ} should in general be relatively close to the inversion frequency, ν_{QM}, predicted by quantum mechanics.

Indeed, we will see below that the prediction for the inversion frequency defined in Eq. (6.85) agrees remarkably well with the quantum-mechanical value for the ammonia inversion frequency, thus validating the calculation of the mean tunneling time within the stochastic quantization formalism.

6.5.1 Rosen-Morse Potential

To investigate the tunneling dynamics of ammonia within the framework of stochastic quantization, we shall model the system as a particle of mass m—the reduced mass of the molecule—moving in a symmetric double-well potential. In what follows, we shall consider the double Rosen–Morse potential (RMP), which has been extensively used to model the ammonia molecule [132, 137].

The double Rosen-Morse potential was introduced by Rosen and Morse [132] to model the vibration of polyatomic molecules, with special attention to the ammonia inversion problem, which is the prototypical example of this kind of problem. The double Rosen-Morse potential has the following form:

$$V(x) = \begin{cases} A\tanh\left(\dfrac{x}{d}-k\right) - B\,\mathrm{sech}^2\left(\dfrac{x}{d}-k\right), & x \geq 0, \\ -A\tanh\left(\dfrac{x}{d}+k\right) - B\,\mathrm{sech}^2\left(\dfrac{x}{d}+k\right), & x \leq 0, \end{cases} \tag{6.86}$$

where A, B, d and k are adjustable parameters. This potential is illustrated in Fig. 35. The reduced mass of the nitrogen atom relative to the hydrogen atoms is

$$m = \frac{3m_H m_N}{3m_H + m_N} \tag{6.87}$$

where m_H and m_N are the masses of the hydrogen and nitrogen atoms, respectively. The values used for their respective masses were: $m_H = 1.66 \times 10^{-27}$ kg and $m_N = 2.33 \times 10^{-26}$ kg.

To choose the potential parameters one typically uses three experimental data [138], namely: the energy separation, $\Delta E^0 = W_1^+ - W_0^- = 950\ \mathrm{cm}^{-1}$, between the two lowest pair of levels, and the level separations within each such pair of levels, $\Delta E = \Delta W_0 = W_0^+ - W_0^- = 0.8\ \mathrm{cm}^{-1}$ and $\Delta W_1 = W_1^+ - W_1^- = 33\ \mathrm{cm}^{-1}$ (where $1\ \mathrm{cm}^{-1} = 1\,hc\ \mathrm{J} \approx 1.988 \times 10^{-23}$ J), see Fig. 35. Since there are four parameters and only three experimental data to fit, the best that can be done in this case is to determine a range of values for each

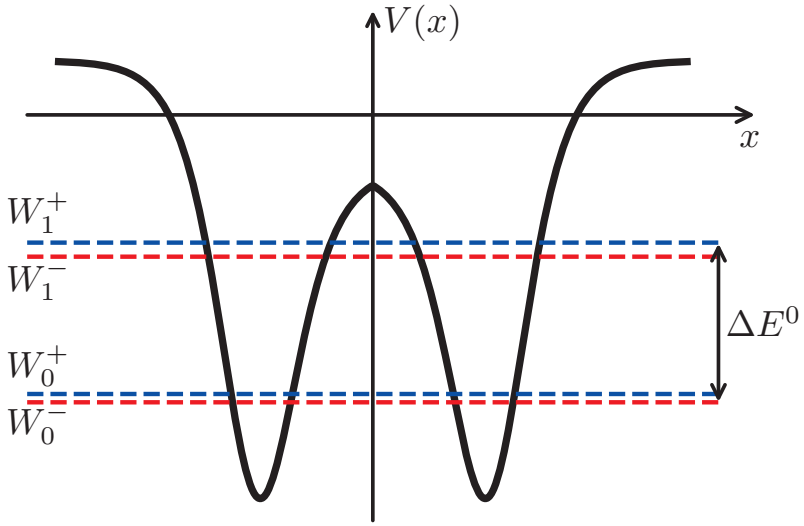


FIGURE 35 – Double Rosen-Morse potential defined by expression (6.86). The first two pairs of energy levels are shown. The red lines are the energies of pair states and the blue lines are the energies of odd states. The ΔE^0 represents the splitting between these two pairs.

parameter based on the reasonable shape of the potential, as described in [132]. These restrictions provide the following ranges of possible values for the RMP parameters:

$$0 < A < 1000 \text{ cm}^{-1},$$

$$2200 \text{ cm}^{-1} < B < 3000 \text{ cm}^{-1},$$

$$0.16 \text{ Å} < d < 0.185 \text{ Å},$$

$$2.20 < k < 2.24.$$

From Eq. (6.86) one finds that the two potential minima are located at $x = \pm x_0$, where [1]

$$x_0 = kd - \tanh^{-1}\left(\frac{A}{2B}\right) d, \tag{6.88}$$

with the condition $A/2B < 1$. Whereas the barrier height, $V_0 = V(0) - V(x_0)$, can be calculated to be

$$V_0 = \frac{A^2}{2B} - A\tanh k + B\tanh^2 k. \tag{6.89}$$

The dissociation energy (or well depth), V_D, corresponding to the difference between the potential asymptotic value, $V(x \to \infty) = A$, and its minimum, $V(x_0)$, is given by

$$V_D = A + B + \frac{A^2}{4B}. \tag{6.90}$$

Within the ranges of allowed parameters mentioned above, one can verify that the values of x_0 and V_0 differ at most by eight percent. So, any form of the potential (6.86) within

[1] In the paper by Rosen and Morse where this potential was introduced [132], the expression for the minimum point x_0 is missing the multiplication by d.

the acceptable range of parameters will have x_0 near 0.38 Å and V_0 near 2050 cm^{-1} or 0.25 eV [132].

With these considerations in mind, we choose the values of the parameters in order to get a value of ΔW_0 very close to the experimental value of 0.8 cm^{-1} for the ammonia molecule, since this is the energy splitting that determines the quantum-mechanical tunneling frequency. To do so, we compute numerically the energy eigenvalues of the RMP by the Numerov method [130] and apply a fit procedure to determine the optimal RMP parameters, where we fix $d = 0.17$ Å and $k = 2.22$, and vary A and B. The values obtained are as follows: $A = 398$ cm^{-1} and $B = 2810$ cm^{-1}, which of course are within the allowed ranges, as expected [2].

Having determined the relevant parameter values for the double Rosen-Morse potential, we can proceed to compute the mean tunneling time predicted by stochastic quantization for the ground state of the ammonia molecule. The classical turning points are $x = \pm b$ and $x = \pm c$, where $V(\pm c) = V(\pm b) = W_0^-$. The ground state wave function, $\psi_0(x)$, and its energy, W_0^-, were calculated numerically using the Numerov method. With these quantities, we then numerically performed the integrations in Eq. (6.61) to obtain the mean tunneling time, $\bar{\tau}$, for a particle with reduced mass m, given by Eq. (6.87), in the ground state of the RMP. We find $\bar{\tau} = 13.4578$ ps, which in view of Eq. (6.85) corresponds to a tunneling frequency $\nu_{\text{SQ}} = 23.7$ GHz, see Table 2, which is indeed very close to the experimental value of 23.8 GHz [136]. This agreement is quite remarkable, when considering that the "conversion formula" (6.83) between tunneling time and quantum oscillation period, which led to Eq. (6.85), was derived in the asymptotic limit $V_0 \gg E$. Our results thus suggest that this correspondence is expected to hold for any practical tunneling situation where the quantum mechanical two-state approximation is valid, as in the inversion dynamics of the ammonia molecule.

We also show in Fig. 36 the distribution of tunneling times for the ground state of the RMP with the parameters chosen above, obtained from simulating 10^6 trajectories of our Brownian particle moving under the appropriate stochastic quantization diffusion process. The simulations were carried out using the Euler–Maruyama method (see Sec. 5.1.2) with a time step of 10^{-3} in dimensionless units (or approximately 10^{-5} ps). For each trajectory, the particle was initialized at $t = 0$ at the right classical turning point of the left potential well, and the simulation was terminated when the particle reached the left classical turning point of the right well. The elapsed time between these two events defines the tunneling time for the trajectory.

One sees again from Fig. 36 the distinct exponential decay of the probability

[2] The calculations and simulations were performed in dimensionless units: $x = \tilde{x}/d$ (position), $E = \tilde{E}/g$ (energy) and $t = \tilde{t}/s$ (time), where $\tilde{x}$, $\tilde{E}$, and $\tilde{t}$ denote the dimensional quantities, $g = \hbar^2/md^2$, and $s = md^2/\hbar$.

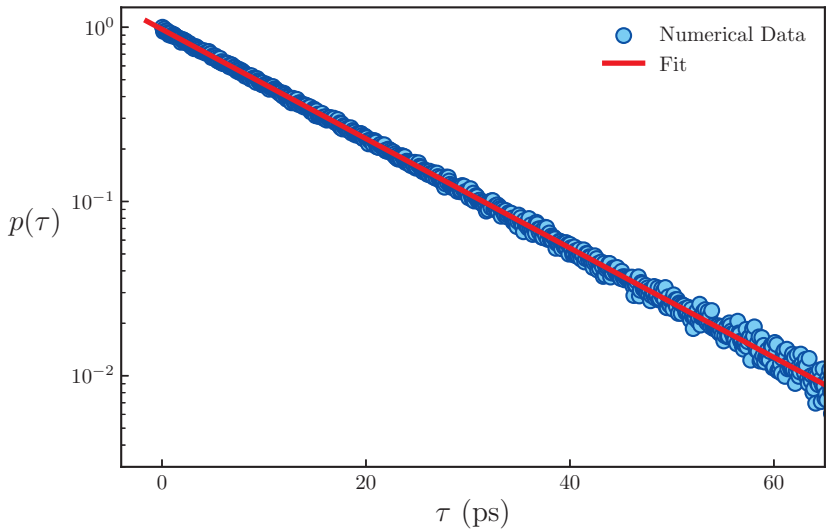


FIGURE 36 – Tunneling time distribution (blue circles) for the double Rosen-Morse potential with parameters $A = 398$ cm^{-1}, $B = 2810$ cm^{-1}, $k = 2.22$ and $d = 17$ pm, computed from 10^6 trajectories and time step of approximately 10^{-5} ps (10^{-3} in dimensionless units). An exponential fit (red line), $p(\tau) = C\exp[-(\tau/\tau_l)]$ with $\tau_l = 13.84$ ps, adjusts remarkably well the entire data.

distribution, as predicted theoretically in Sec. 4.2. This indicates that stochastic trajectories effectively sample barrier-crossing events as a Poisson-like process characterized by a single mean scale $\bar{\tau}$. This provides a concrete dynamical interpretation of tunneling as a rare-event diffusion process underlying the coherent oscillations described by quantum mechanics. Note, also, that in contrast with similar distribution for the double square well (see Fig. 28), for the RMP there is a much sharper rise from $p(0) = 0$ to the exponential curve for $\tau > 0$, with no event outside the exponential region detected within our run of 10^6 simulations, so much so that an exponential fit (red line) was capable to adjust remarkably well the entire data. Here the theoretical value for the mean tunneling time, computed from Eq. (6.61), is $\bar{\tau} = 13.46$ ps, again in very good agreement with the corresponding value, $\bar{\tau}_{\rm num} = 13.86$ ps, obtained from the simulations.

The proportionality $\tau_{\rm QM}/\bar{\tau} = \pi/2$, derived analytically for the square double-well and confirmed through a WKB analysis for arbitrary smooth potentials, establishes a precise correspondence between the stochastic and conventional quantum descriptions in the high-barrier limit. It should be noted, however, that in general the proportionality between $\bar{\tau}$ and $\tau_{\rm QM}$ may depend somewhat on the potential shape and on the specific stopping rule adopted to define the tunneling time. This dependence on the potential shape is illustrated in Fig. 37, which shows the ratio $\tau_{\rm QM}/\bar{\tau}$ as a function of the barrier height V_0 for the Rosen–Morse potential. Here, the parameters are fixed at $A = 398$ cm^{-1}, $k = 2.22$, and $d = 17$ pm, while B is varied in the range 680 cm$^{-1} < B < 2810$ cm^{-1}. Remarkably, the prefactor approaches the universal value $\pi/2$ already at moderate values of the barrier height, as shown in Fig. 37 (see, e.g., point B). Note that point C in this

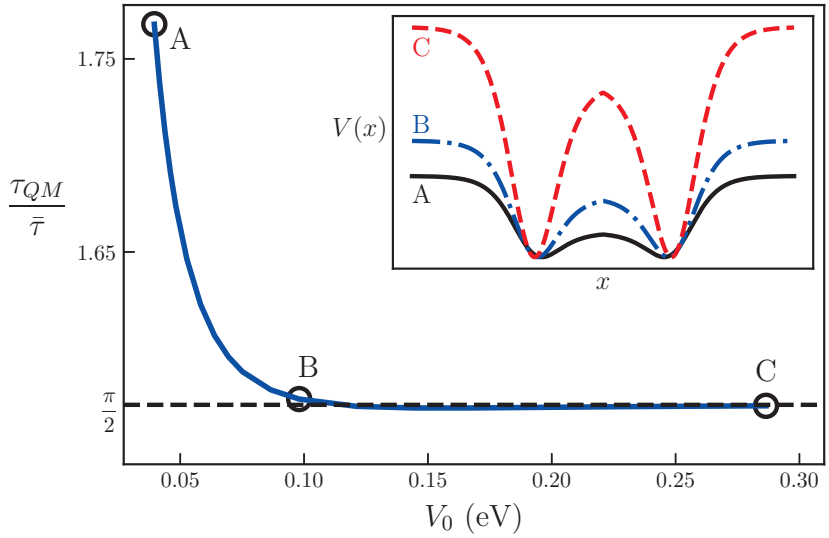


FIGURE 37 – Ratio $\tau_{\mathrm{QM}}/\bar{\tau}$ between the quantum-mechanical tunneling time and the mean stochastic tunneling time as a function of the barrier height V_0 for the double Rosen–Morse potential. The parameters are fixed at $A = 398$ cm^{-1}, $k = 2.22$, and $d = 17$ pm, while B is varied in the range 680 cm$^{-1} < B <$ 2810 cm^{-1}. The inset displays the potential profiles corresponding to points A, B, and C indicated on the main curve, where the barrier heights are 39.5 meV (A), 98.0 meV (B), and 286.5 meV (C), which correspond to 28.8%, 48.4%, and 71.6% of the well depth V_D, respectively.

figure refers to the optimal parameter values for the RMP mentioned above. For this point the barrier height, V_0, is approximately 72% of the well depth, V_D, which indeed corresponds to a relatively high barrier, as seen in the inset of Fig. 37.

Physically, the proportionality between τ_{QM} and $\bar{\tau}$ indicates that the diffusive motion intrinsic to stochastic quantization reproduces the same characteristic timescale that, in quantum mechanics, governs coherent oscillations between the two localized states of the double-well. The fact that τ_{QM} exceeds $\bar{\tau}$ may be understood as reflecting the distinction between two complementary descriptions of the tunneling process. In the stochastic picture, $\bar{\tau}$ represents the mean first passage time obtained as an average over an ensemble of stochastic trajectories crossing the barrier from one well to the other, whereas in quantum mechanics τ_{QM} relates to the collective oscillation period of the entire probability distribution. The latter entails a coherent redistribution of probability density between the wells—a process inherently slower than the stochastic transition of single trajectories. Within the high-barrier and two-level approximation, this interpretation provides a consistent physical link between single-trajectory diffusion dynamics and the collective evolution of quantum probability. However, whether a physical explanation exists for the emergence of $\pi/2$ as the universal ratio remains unclear at present.

In Fig. 38 we plot $\bar{\tau}(x_f)$, as defined in Eq. (6.60), as a function of the initial tunneling point, $-x_f$, for the RMP potential, using parameters corresponding to points A, B, and C in Fig. 37. For the three curves shown, $-x_f$ is varied from the minimum

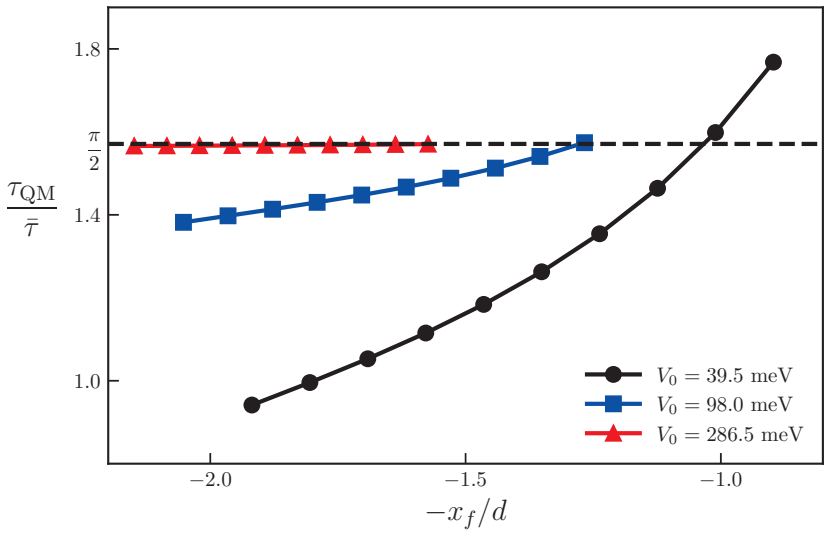


FIGURE 38 – Ratio $\tau_{QM}/\bar{\tau}$ as a function of x_f for the Rosen-Morse potential, Eq. (6.86), with $V_0 = \{39.5$ meV, 98.0 meV, 286.5 meV$\}$ corresponding to points A, B and C in Fig. 37. The x_f parameter, which delimits the tunneling region, varies from the classical turning point on the barrier (b) to the minimum potential point (x_0). If V_0 is high, then the ratio gets close to the value $\pi/2$ despite the choice of the parameter x_f.

point of the left well ($-x_0$) to the right classical turning point ($-b$). Since τ_{QM} is fixed for each curve, one sees from Fig. 38 that $\bar{\tau}$ decreases as x_f decreases, as expected, since the distance traveled within the tunneling region $(-x_f, x_f)$ becomes smaller. As expected, for a low barrier (black circles), the ratio $\tau_{QM}/\bar{\tau}$ changes more significantly with x_f. As the barrier height increases—see, for instance, the upper curve in Fig. 38—this ratio becomes insensitive to the precise definition of the tunneling stopping rule, thereby confirming the universal character of the factor $\pi/2$ in this limit. This result provides further evidence that the classical turning points on both sides of the barrier can be safely used as reference positions in defining the quantum tunneling process, as argued above.

The successful application of the stochastic quantization formalism to the inversion dynamics of the ammonia molecule further illustrates its predictive power. Using the double Rosen–Morse potential and the formula for the stochastic-mechanical tunneling frequency ν_{SQ} in terms of $\bar{\tau}$, see Eq. (6.85), we obtained an inversion frequency for ammonia of about 24 GHz, in remarkable agreement with the expected value. This quantitative concordance demonstrates that the stochastic quantization framework captures not only the qualitative behavior of tunneling but also its measurable spectroscopic signature. It also reinforces the view that the stochastic representation is not merely an interpretational alternative but a dynamically consistent formulation of quantum mechanics at the level of wavefunction evolution and associated single-time statistics, while offering practical computational advantages in certain contexts.

TABLE 2 – Comparison of key parameters for different model potentials describing the ammonia lowest energy splitting: the symmetric double square well (DSW), the finite-depth double square well (FD-DSW), the quartic double-well potential, and the Rosen-Morse potential. Listed quantities include the well depth V_D, barrier height V_0, minimum position x_0, well length L, ground-state splitting ΔW_0, distance from the ground state to the barrier height $V_0 - W_0$, and the corresponding tunneling frequencies obtained from quantum mechanical calculation ν_{QM} and from stochastic quantization ν_{SQ}.

	DSW	FD-DSW	Quartic	Rosen-Morse
V_0 [eV]	0.1905	0.1905	0.2399	0.2865
V_D [eV]	∞	1.3741	∞	0.4003
x_0 [Å]	0.4167	0.4042	0.4113	0.3654
L [Å]	0.3708	0.3453	–	–
ΔW_0 [meV]	0.099 52	0.099 37	0.099 31	0.098 04
$V_0 - W_0^-$ [eV]	0.1476	0.1475	0.1735	0.1997
ν_{QM} [GHz]	24.0173	23.9816	23.9266	23.6601
ν_{SQ} [GHz]	24.0990	24.0625	23.9275	23.6524

6.5.2 Comparison with Other Potentials

In order to verify that the tunneling frequency in the opaque-barrier regime is insensitive to the specific shape of the potential, we compared the values obtained for the ammonia tunneling frequency using the Rosen–Morse potential with those from the three double-well models previously analyzed: the infinite double square well (DSW), the finite-depth double square well (FD-DSW), and the quartic double well. For each potential, the parameters were adjusted so that the energy splitting between the ground and first excited states matches, as close as possible, the experimental ammonia inversion splitting, $\Delta E \approx 0.099$ meV.

Table 2 lists the corresponding potential parameters, together with the resulting tunneling frequencies ν_{QM} and ν_{SQ} for all four models. For the DSW and FD-DSW, the location of the right minimum x_0 is taken to be the center of the right square well. As expected, the values of ν_{QM} and ν_{SQ} exhibit excellent agreement for all potentials considered. This confirms that, once the lowest energy splitting is fixed to the experimental ammonia value, the system indeed operates in the high-barrier regime, where the details of the potential shape become irrelevant for the tunneling dynamics.

7 CONCLUSION

Stochastic quantization, introduced by Edward Nelson in 1966, provides a complete formulation of non-relativistic, spinless quantum mechanics. It offers a complementary point of view and a mathematically robust framework capable of addressing a wide class of quantum-mechanical problems that remain only partially resolved within standard quantum theory. Nelson's postulates—the hypothesis of a universal Brownian motion underlying microscopic dynamics and the corresponding stochastic generalization of Newton's second law—form the foundation of this approach. From these principles, the dynamical equations governing the motion of a quantum particle naturally emerge. In particular, the Madelung hydrodynamic equations, and consequently the Schrödinger equation, arise directly from Nelson's framework.

Beyond Nelson's original formulation, several important developments have strengthened the theoretical structure of stochastic mechanics. The works of Yasue [90, 139], Guerra and Morato [69], and Pavon [15, 68] extended the theory by establishing a variational principle analogous to the classical Hamilton principle, further demonstrating the internal coherence of the stochastic formulation. Moreover, Pavon [72] proved that stochastic quantization is unitarily equivalent to standard quantum mechanics in Hilbert space, placing both descriptions on a formally equal footing.

Thus, quantum mechanics possesses a mathematical structure that mirrors classical mechanics more closely than is often emphasized. Clear correspondences exist between Newtonian, Lagrangian, and Hamiltonian formulations and their stochastic or quantum counterparts. These formulations are not mutually exclusive; instead, they collectively contribute to a more complete description of physical reality. Although neither stochastic mechanics nor the Schrödinger equation is likely the ultimate representation of quantum phenomena, both capture essential aspects of microscopic processes and provide effective descriptions of measurement outcomes.

A striking illustration of this complementarity is the study of tunneling times in double-well systems. In standard quantum mechanics, the tunneling time is associated with half the oscillation period of a localized non-stationary state evolving between the two minima of the potential. In stochastic quantization, by contrast, the tunneling time is defined through first-passage-time theory. Remarkably, these two notions of time are related by a proportionality factor that approaches $\pi/2$ in the opaque-barrier limit, independently of the specific functional form of the potential. This robust correspondence shows that the two approaches describe different but intimately related aspects of a single underlying physical process: stochastic mechanics captures the mean time the particle requires to cross the barrier, while standard quantum mechanics describes the oscillation of the probability

distribution between the wells. This correspondence is further confirmed in the ammonia inversion problem: the experimentally observed inversion frequency of approximately 24 GHz is accurately reproduced by computing the tunneling time within the stochastic quantization framework.

For scattering states, the issue becomes even more intriguing. Standard quantum mechanics does not provide a universally accepted or experimentally accessible definition of tunneling time for transmission through a potential barrier. In contrast, stochastic quantization yields a natural and operational notion of tunneling time for scattering states, recovering the expected physical limits: the classical traversal time when the barrier is negligible and the characteristic exponential growth in the opaque regime. A systematic comparison with other times introduced in the literature—such as those in Refs. [107, 108, 111]—may offer valuable insight into the physical meaning and applicability of the various definitions of quantum tunneling times.

Finally, recent experimental advances continue to stimulate new theoretical questions concerning time in quantum mechanics. In particular, a recent study [140] reports measurements of the time photons spend inside a step-like refractive barrier, enabling an estimate of the effective photon velocity within the classically forbidden region. Stochastic quantization provides a promising framework to reinterpret and complement such experimental findings, potentially offering a unified picture of quantum traversal times across different physical contexts.

In summary, this thesis demonstrates that stochastic quantization not only can reproduce the predictions of conventional quantum mechanics but also offers new insights into quantum temporal phenomena, particularly tunneling. The universality of the relation between the stochastic tunneling time and the quantum oscillation time, the consistency across multiple potential shapes, and the agreement with experimental scales—such as the ammonia inversion frequency—all point to the strength and versatility of the stochastic approach. These findings suggest that stochastic quantization remains a powerful and underexplored tool for understanding quantum dynamics, and that further connections between stochastic mechanics, semiclassical techniques, and experimental observations may uncover even richer aspects of quantum behavior.

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APPENDIX A – BASIC PROBABILITY THEORY

Probability theory is the mathematical branch applied when we do not know exactly what the result of an experiment will be, knowing only the possible outcomes and their respective chances of happening. One of the first and most important works on probability theory was done by Pierre Laplace (1749-1827) and is called *Théorie Analytique des Probabilités* (1812) [141]. Our approach to this theory will follow the axiomatization given by the soviet mathematician Andrei Kolmogorov (1903-1987) based on sets of random events and the application of measure theory on these sets [142]. For a modern treatment of probability theory, see the references [51, 143].

The outcome of a random experiment is represented by ω. The set of all possible elementary outcomes is denoted by Ω. We call an event a set A of outcomes; this means that A is a subset of Ω. We are interested in attributing a probability to the event $A \subset \Omega$. For the case when Ω is countable, we can introduce a probability $P(\omega)$ for each outcome and then the probability of the event A will be just the sum of the probability of each outcome of A, this is

$$P(A) = \sum_{\omega \in A} P(\omega). \tag{A.1}$$

However, this procedure is not applicable when Ω is uncountable, which is the case, e.g., when $\Omega = \mathbb{R}$ or any continuous space. If Ω is uncountable, then a typical event will have uncountably many outcomes. Hence, the formula (A.1) is not useful and we need to define a probability measure.

Before defining a probability measure, we need to specify the class of *observable events* or the subsets of Ω to which a probability measure can be associated. Such a class must be closed under the various set operations, such as union, intersection, complementarity, etc. This is done through the concept of a σ-algebra.

Definition 12 *A family $\mathcal{F}$ of subsets of Ω is a σ-algebra on Ω if the following conditions are fulfilled:*

- $\varnothing \in \mathcal{F}$ *and* $\Omega \in \mathcal{F}$*;*
- $A \in \mathcal{F} \implies A^c \in \mathcal{F}$*, where $A^c = \Omega \backslash A$ is the complement of A in Ω;*
- $A_i \in \mathcal{F},\ i = 1, 2, \ldots \implies \bigcup_{i=1}^{\infty} A_i \in \mathcal{F}$.

The par $(\Omega, \mathcal{F})$ is a measurable space.

It can be verified that the third condition above is equivalent to the requirement

$$A_i \in \mathcal{F},\ i = 1, 2, \ldots \implies \bigcap_{i=1}^{\infty} A_i \in \mathcal{F}. \tag{A.2}$$

The elements $A \subset \mathcal{F}$ are called *measurable sets* or just *events*. For a given outcome ω, it is always possible to say if it belongs or not to A. In this sense, the event A is an observable [37].

The smallest σ-algebra possible is $\mathcal{F}_{\min} = \{\, \varnothing, \Omega \,\}$ and the largest σ-algebra consists of all subsets of Ω and is known as the power set of Ω. It is possible to generate intermediate σ-algebras starting with a family $\mathcal{U}$ of subsets of Ω and form the intersection of all σ-algebras that contain $\mathcal{U}$, this is represented by

$$\mathcal{F}_{\mathcal{U}} = \bigcap \{\, \mathcal{F} \mid \mathcal{F} \supset \mathcal{U} \,\}. \tag{A.3}$$

$\mathcal{F}_{\mathcal{U}}$ is the smallest σ-algebra that contains $\mathcal{U}$ and is called σ-algebra generated by $\mathcal{U}$. It is worth mentioning that an intersection of σ-algebras is always a σ-algebra, but the union of σ-algebras is not necessarily a σ-algebra [143].

Let $\mathcal{I}$ be the class of sub-intervals $(a, b]$ of $\Omega = (0, 1]$. The σ-algebra $\mathcal{B} \equiv \mathcal{F}_{\mathcal{I}}$ generated by $\mathcal{I}$ is known as Borel σ-algebra of the unit interval (after Émile Borel), and its elements are called Borel sets of the unit interval. We can extend the Borel σ-algebra for the case in which $\Omega = \mathbb{R} = (-\infty, \infty)$. This can be done taking the σ-algebra generated by the class of subsets of the form $(-\infty, a]$, $(b, c]$, (d, ∞). This Borel σ-algebra is denoted by $\mathcal{B}^1$. Any reasonable subset of $\mathbb{R}$ is a Borel set, in other words, is an element of $\mathcal{B}^1$. We can extend this construction to the n-dimensional case in which $\Omega = \mathbb{R}^n$, then the respective Borel σ-algebra will be denoted by $\mathcal{B}^n$. The Borel σ-algebra can be defined as the smallest σ-algebra generated by the open sets of the topology in question (in our case, this topology is $\mathbb{R}^n$) [144, 145].

Now we can define a probability measure for any event $A \in \mathcal{F}$ on the measurable space $(\Omega, \mathcal{F})$.

Definition 13 *A probability measure P on the measurable space $(\Omega, \mathcal{F})$ is a function $P : \mathcal{F} \to [0, 1]$ such that*

- *$P(\varnothing) = 0$ and $P(\Omega) = 1$;*
- *If $A_1, A_2, \ldots \in \mathcal{F}$ is a disjoint collection of elements of $\mathcal{F}$, i.e. $A_i \cap A_j = \varnothing$ for $i \neq j$, then $P\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} P(A_i)$.*

The triple $(\Omega, \mathcal{F}, P)$ is known as probability space.

An event is a set $A \in \mathcal{F}$ and the probability for this event is the measure $P(A)$. Consider $\Omega = (0, 1]$ and $\mathcal{F} = \mathcal{B}$ the Borel σ-algebra of the unit interval. For any given sub-interval $A = (a, b] \in \Omega$ we define the probability measure called *Lebesgue measure* (after Henri Lebesgue) [144] and denoted by μ such that

$$\mu(A) = b - a. \tag{A.4}$$

It is easily shown that $P = \mu$ satisfies the two conditions in the definition above. Note that the probability dP of finding an event ω between x and $x + dx$ is

$$dP(\omega) = \mu((x, x + dx]) = dx. \tag{A.5}$$

Hence, for a given set $A \in \mathcal{B}$ its probability can be written as

$$P(A) = \int_{\omega \in A} dP(\omega) = \int_{x \in A} dx. \tag{A.6}$$

This shows the connection between probability theory and integration. Actually, integration can be defined on the measure space $(\mathbb{R}, \mathcal{B}^1, \mu)$. Nevertheless, this is not a proper probability space, since $\mu(\mathbb{R}) = \infty$. The formula (A.6) above is a generalization of the formula (A.1) for the case of an uncountable set of outcomes Ω. Based on that, we can now define what is a random variable or stochastic variable.

A.1 RANDOM VARIABLES

A random variable X is a function that attributes to each outcome ω a real number x. Usually, we can think X as a random number determined by the outcome ω. Let us now give a more formal definition. First, consider the case when X is a discrete random variable, i.e., X can assume a finite number of possible values.

Definition 14 *Let $(\Omega, \mathcal{F}, P)$ be a probability space and let X be a real-valued function $X : \Omega \to \mathbb{R}$. We say X is a simple (or discrete) random variable if it assumes only finitely many values and if*

$$\{\, \omega \mid X(\omega) = x \,\} \in \mathcal{F},$$

for each real x. (Of course, $\{\, \omega \mid X(\omega) = x \,\} = \varnothing \in \mathcal{F}$ for x outside the range of X).

The point of this definition is to ensure that the probabilities $P(\{\, \omega \mid X(\omega) = x \,\})$ are defined.

Now, we want to consider the case when X is a continuous random variable, i.e., it can assume infinitely many values. In order to proceed, we need the notion of a measurable function.

Definition 15 *Let $(\Omega, \mathcal{F})$ be a measurable space. A function $f : \Omega \to \mathbb{R}$ is measurable with respect to the σ-algebra $\mathcal{F}$, or more compactly, $\mathcal{F}$-measurable, if*

$$f^{-1}(U) \equiv \{\, \omega \mid f(\omega) \in U \,\} \in \mathcal{F},$$

for all Borel sets $U \in \mathcal{B}^1$.

In the probability context, a measurable function is called a random variable. Formally, the definition below holds.

Definition 16 *A random variable X on a probability space $(\Omega, \mathcal{F}, P)$ is a $\mathcal{F}$-measurable function.*

The definition above, in connection with Definition 15, exists to ensure that for any reasonable set U of real numbers (Borel sets) there is a meaningful event $A = X^{-1}(U) = \{\, \omega \mid X(\omega) \in U \,\}$, to which we can assign a probability $P(X(\omega) \in U) = P(A)$. For example, for any interval $(a, b) \subset \mathbb{R}$ we have

$$P(a < X(\omega) < b) = P(\{\, \omega \mid X(\omega) \in (a, b) \,\}). \tag{A.7}$$

Usually, we drop the reference to the random outcomes ω and simply write $P(a < X < b)$.

A random variable X naturally generates a σ-algebra denoted by $\mathcal{F}_X$. This is the σ-algebra generated by the class of sets of the form $\{\, X^{-1}(U) \mid U \in \mathcal{B}^1 \,\}$. $\mathcal{F}_X$ is the smallest σ-algebra with respect to which X is measurable. We can think $\mathcal{F}_X$ as representing the information generated by the random variable X. The σ-algebra $\mathcal{F}_X$ contains the essential information about the structure of the random variable X. In particular, it contains all sets of the form $\{\, \omega \mid a < X(\omega) \leq b \,\}$, meaning that an element of $\mathcal{F}_X$ tell us for which $\omega \in \Omega$ the random variable X assumes values in a given interval $(a, b]$ or a more general Borel set $U \in \mathcal{B}^1$ [37].

A.2 PROBABILITY DISTRIBUTION

Let X be a random variable. The *probability distribution* $F(x)$ of X is defined as

$$F(x) = P(X \leq x), \quad \text{for} \quad x \in \mathbb{R}. \tag{A.8}$$

Probability distributions are defined for discrete and continuous random variables. Sometimes $F(x)$ is called *cumulant probability distribution*. In the case of continuous random variables, there is a particular class of interest, those for which $F(x)$ is differentiable. A distribution function $F(x)$ is said to be *absolutely continuous* if there is a non-negative and integrable function $f(x)$ such that

$$F(x) = \int_{-\infty}^{x} f(x)dx, \tag{A.9}$$

where f is called *probability density function* (pdf) of the random variable X. The existence of a probability density function $f(x)$ allow us to compute the probability of a given event $A = \{\, a \leq X \leq b \,\}$ explicitly through the formula

$$P(A) = \int_a^b f(x)dx. \tag{A.10}$$

As an example, for the Lebesgue measure on the unit interval defined in (A.4), the probability distribution is $F(x) = x$ for $0 < x \leq 1$ and $f(x) = 1$. In other words, the Lebesgue measure represents a uniform distribution on the unit interval.

A.3 EXPECTATION VALUES AND MOMENTS

Let X be an absolutely continuous random variable with probability density function (pdf) given by $p(x)$. The expected (mean) value of the variable X can be defined as

$$\mathbb{E}[X] \equiv \langle X \rangle = \int_{-\infty}^{\infty} xp(x)dx. \tag{A.11}$$

In general, if g is a real-valued function, then

$$\mathbb{E}[g(X)] \equiv \langle g \rangle = \int_{-\infty}^{\infty} g(x)p(x)dx. \tag{A.12}$$

More formally, the expectation value of a general continuous random variable X is defined as

$$\mathbb{E}[X] \coloneqq \int_{\Omega} X(\omega)dP(\omega). \tag{A.13}$$

We say that X is a P-integrable function on the probability space $(\Omega, \mathcal{F}, P)$. The definition (A.13) means that X is in $L^1(\Omega, \mathcal{F}, P)$, i.e., in the space of P-integrable functions on Ω [44, 143]. If X is also in $L^n(\Omega, \mathcal{F}, P)$, we can define the n-th moment of X as

$$\mathbb{E}[X^n] \equiv \langle X^n \rangle \coloneqq \int_{\Omega} X^n(\omega)dP(\omega). \tag{A.14}$$

For an absolutely continuous random variable, making use of the probability density $p(x)$, the n-th moment acquires the form

$$\mathbb{E}[X^n] = \int_{-\infty}^{\infty} x^n p(x)dx. \tag{A.15}$$

The second moment is related to the variance of X. Let its mean value be $\mathbb{E}[X] = m$, the variance is

$$\mathrm{var}[X] = \mathbb{E}[(X-m)^2] = \int_{-\infty}^{\infty} (x-m)^2 p(x)dx = \mathbb{E}[X^2] - m^2. \tag{A.16}$$

The quantity $\sigma_X = \sqrt{\mathrm{var}[X]}$ is the *standard deviation* of the distribution. The variance is a measure of the dispersion of the values of X around the mean. Moreover, the standard deviation σ_X measures the width of the distribution with respect to the mean.

A.4 EQUIVALENT MEASURES

In the section above, we have considered the probability measure in our probability space as being the product of a probability density and the Lebesgue measure, i.e., $dP = p(x)dx$. To formalize this procedure, we will first enounce the following definition [44].

Definition 17 *Let $(\Omega, \mathcal{F}, P)$ be a probability space. The probability measure P is called absolutely continuous with respect to another measure Q (written $P \ll Q$) if for all $A \in \mathcal{F}$ we have $Q(A) = 0 \implies P(A) = 0$. P and Q are equivalent when $P \ll Q$ and $Q \ll P$.*

The definition above means that equivalent probability measures have the same sets of measure zero. Furthermore, equivalent probability measures will also have the same sets of measure unity [44]. This concept is important for the following theorem [44, 144].

Theorem 6 (Radon-Nikodým) *If $P \ll Q$, then there exists an $\mathcal{F}$-measurable function f, such that for every $A \in \mathcal{F}$*

$$P(A) = \int_A f dQ.$$

The function $f = dP/dQ$ is called the Radon-Nikodým derivative of P with respect to Q. If P and Q are equivalent, then

$$\frac{dP}{dQ} = \left(\frac{dQ}{dP}\right)^{-1}. \tag{A.17}$$

As we saw before in Eq. (A.11), $p(x)$ is the Radon-Nikodým derivative of the measure P with respect to the Lebesgue measure. All the probability measures present in this thesis are absolutely continuous with respect to the Lebesgue measure (we say just absolutely continuous). This means that we will always be able to write $dP(x) = p(x)dx$ and most of the time just the probability density p will be used to denote the probability measure.

Therefore, we can translate our probability space of $(\Omega, \mathcal{F}, P)$ by the random variable X into the probability space $(\mathbb{R}, \mathcal{B}^1, p(x)dx)$. This is the structure usually adopted in physical applications. In other words, the sets $A \in \Omega$ are mapped by the random variable X onto open sets (Borel sets) in the Borel σ-algebra of $\mathbb{R}$ [44].

Consider now a group of d real-valued random variables $X_1, X_2, \ldots, X_d$. These random variables are components of a d-dimensional vector $\mathbf{X} \in \mathbb{R}^d$. The probability measure in this case is

$$\begin{aligned} &p(x_1, \ldots, x_d)\, dx_1 \ldots dx_d \\ &\qquad = dP(\omega \in \Omega \mid x_1 \leq X_1(\omega) \leq x_1 + dx_1, \ldots, x_d \leq X_d(\omega) \leq x_d + dx_d), \end{aligned} \tag{A.18}$$

and we transfer the measurable space from $(\Omega, \mathcal{F})$ to $(\mathbb{R}^d, \mathcal{B}^d)$ [44].

A.5 INDEPENDENCE AND CORRELATION

Two events A and B are said to be independent if [146]

$$P(AB) \equiv P(A \cap B) = P(A)P(B). \tag{A.19}$$

This definition is naturally extended to encompass classes of events. Consider a probability space $(\Omega, \mathcal{F}, P)$ and let $\mathcal{A}_1 \subset \mathcal{F}$ and $\mathcal{A}_2 \subset \mathcal{F}$. We say that $\mathcal{A}_1$ and $\mathcal{A}_2$ are independent classes of events if all events of $\mathcal{A}_1$ are independent of all events of $\mathcal{A}_2$. We now define the independence of random variables [37].

Definition 18 *Two random variables X and Y are said to be independent if the σ-algebras $\mathcal{F}_X$ and $\mathcal{F}_Y$ generated by them are independent in the sense above, i.e., if all events in $\mathcal{F}_X$ are independent of all events in $\mathcal{F}_Y$.*

In particular, if X_1 and X_2 are independent random variables with individual densities $p_i(x_i)$, then the joint probability density $p(x_1, x_2)$ is

$$p(x_1, x_2) = p_1(x_1)p_2(x_2), \tag{A.20}$$

which implies in turn that

$$\mathbb{E}[X_1 X_2] = \mathbb{E}[X_1]\mathbb{E}[X_2]. \tag{A.21}$$

The *correlation coefficient* between the random variables X_1 and X_2 is defined to be

$$\rho(X_1, X_2) = \frac{\mathbb{E}[(X_1 - \mathbb{E}[X_1])(X_2 - \mathbb{E}[X_2])]}{\sqrt{\mathrm{var}[X_1]\,\mathrm{var}[X_2]}}. \tag{A.22}$$

The random variables X_1 and X_2 are said to be uncorrelated if $\rho(X_1, X_2) = 0$. In particular, if X_1 and X_2 have zero mean, $\mathbb{E}[X_i] = 0$, then X_1 and X_2 are uncorrelated if

$$\mathbb{E}[X_1 X_2] = 0. \tag{A.23}$$

Independence implies uncorrelation, but the converse needs not to be true.

Suppose a d-dimensional random vector $\mathbf{X} = (X_1, \ldots, X_d)$, where each X_i is a random variable. Its mean value is given by the vector

$$\mathbf{m} = \mathbb{E}[\mathbf{X}] = (\mathbb{E}[X_1], \ldots, \mathbb{E}[X_n]) \tag{A.24}$$

The *covariance matrix* Σ of $\mathbf{X}$ is defined as

$$\begin{aligned} \Sigma_{ij} = \mathrm{cov}(X_i, X_j) &\equiv \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])] \\ &= \mathbb{E}[X_i X_j] - \mathbb{E}[X_i]\mathbb{E}[X_j]. \end{aligned} \tag{A.25}$$

The diagonal element Σ_{ii} is the variance σ_i^2 of the i-th variable, and the element Σ_{ij} is the covariance of X_i and X_j. If $\Sigma_{ij} = 0$ then X_i and X_j are uncorrelated. The matrix Σ is symmetric and positive-definite [143].

It can be easily verified that the variance of the sum of independent random variables is the sum of the variances of each variable [146].

Another important remark concerning independent random variables is that the pdf $p(x)$ of the sum $X = X_1 + X_2$ of two independent random variables X_1 and X_2 is given by the convolution of the original pdfs [143], this is written as

$$p(x) = \int_{-\infty}^{\infty} p_1(s)p_2(x-s)ds, \tag{A.26}$$

where $p_1(x)$ and $p_2(x)$ are the pdfs of the random variables X_1 and X_2, respectively.

Additionally, if two random variables X_1 and X_2 have the same distribution $p(x) = p_1(x) = p_2(x)$, denoted by

$$X_1 \overset{\mathrm{d}}{=} X_2, \tag{A.27}$$

where the symbol $\overset{\mathrm{d}}{=}$ denotes equality in the distribution sense, then we say they are *identically distributed*. Independent and identically distributed random variables are denoted as i.i.d. variables.

Suppose that two random variables are not independent. Yet, there is some information we can get about the distribution of one variable based on the measurement of the other variable. Considering the joint distribution of two random variables, $p(x_1, x_2)$, we define their *marginal distributions*

$$p_1(x_1) = \int_{-\infty}^{\infty} p(x_1, x_2)dx_2, \tag{A.28}$$

$$p_2(x_2) = \int_{-\infty}^{\infty} p(x_1, x_2)dx_1. \tag{A.29}$$

The *conditional probability* density function of the random variable X_1 given X_2 is defined as

$$p(x_1|x_2) = \frac{p(x_1, x_2)}{p_2(x_2)}, \tag{A.30}$$

where we are assuming $p_2(x_2) \neq 0$. This is the pdf of a measurement of the variable X_1 given that a measurement of the variable X_2 resulted in x_2. The conditional expectation is given by

$$\mathbb{E}[x_1|x_2] = \int_{-\infty}^{\infty} x_1\, p(x_1|x_2)\, dx_1. \tag{A.31}$$

The conditional expectation (A.31) is itself a random variable due to its dependence on x_2. We can calculate its expectation value by

$$\mathbb{E}[\mathbb{E}[x_1|x_2]] = \mathbb{E}[x_1] = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x_1\, p(x_1, x_2)\, dx_1 dx_2. \tag{A.32}$$

The result above can be easily proved using the previous definitions [44].

A.6 THE GAUSSIAN DISTRIBUTION

A Gaussian, or normal distribution, with mean m and standard deviation σ is denoted by $\mathcal{N}(m, \sigma)$ and has the following pdf:

$$p_{\mathcal{N}}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-m)^2}{2\sigma^2}\right]. \tag{A.33}$$

Remember that σ^2 is the variance of the distribution. Without loss of generality, we can suppose that $m = 0$; in this case, the nonzero moments of the Gaussian distribution are

$$\mathbb{E}[X^2] = \sigma^2, \tag{A.34}$$

$$\mathbb{E}[X^{2n}] = 1 \cdot 3 \cdot 5 \cdot \ldots \cdot (2n-1)\sigma^{2n}. \tag{A.35}$$

Furthermore, all the odd moments vanish since $p_{\mathcal{N}}$ is an even function of x.

The Gaussian distribution has two properties that make it a special distribution. The first one is that it is a *stable distribution*, which means that the sum of two independent Gaussian random variables is also a Gaussian random variable. The second important property is the Central Limit Theorem. This theorem states that adding up infinitely many independent random variables, X_i, with finite variance (or equivalently, with finite mean and second moment), the sum will be distributed according to a Gaussian distribution [37, 44, 45, 147]. The Central Limit Theorem is enounced as follows.

Theorem 7 *Suppose* $\{ X_i \}$ *is an infinite sequence of independent random variables with zero mean,* $\mathbb{E}[X_i] = 0$*, and finite variance,* $\mathrm{var}[X_i] = \sigma_i^2$*. Define*

$$S_n = \sum_{i=1}^{n} X_i$$

and

$$s_n^2 = \mathrm{var}[S_n] = \sum_{i=1}^{n} \sigma_i^2.$$

If the following requirement, known as Lindberg condition, holds,

$$\lim_{n\to\infty} \left[\frac{1}{s_n^2} \sum_{i=1}^{n} \int_{|x|>ts_n} x^2\, p_i(x)\, dx\right] = 0,$$

for any $t > 0$*, then the probability distribution of the random variable*

$$Y_n = \frac{S_n}{s_n}$$

approaches the normal distribution $\mathcal{N}(0, 1)$ *as* $n \to \infty$*.*

The existence of this theorem is what makes the appearance of Gaussian distributions so frequent in statistical physics.

APPENDIX B – BASICS OF STOCHASTIC PROCESSES

Stochastic processes can be understood as time-dependent probabilistic phenomena. This concept can be mathematically defined as follows [44, 45].

Definition 19 *A stochastic process is a collection of random variables*

$$\{ X_t \}_{t \in I},$$

defined on some probability space $(\Omega, \mathcal{F}, P)$ *and parametrized by the variable* t.

The index t usually is time. The index set I can be discrete, in this case $I = \mathbb{N}$, and we will have a *discrete time stochastic process*. Otherwise, I can be continuous, in this case $I = \mathbb{R}$ and we will have a *continuous time stochastic process*. For most cases, $I = [0, \infty)$.

A stochastic process is a function of two variables, the parameter t and the random variable ω,

$$\begin{aligned} X : I \times \Omega &\to \mathbb{R}^d \\ (t, \omega) &\mapsto X(t, \omega) = X_t(\omega). \end{aligned} \tag{B.1}$$

For a fixed random outcome ω, X_t is a function of time and is called a *realization*, *path*, or *trajectory* of the stochastic process. In Fig. 39, we can see an example of three different realizations of a stochastic process $X(t, \omega)$ represented by a standard Brownian motion.

For a fixed t, the stochastic process X_t is a random variable and can be described by a probability distribution and a probability density. The finite dimensional probability distribution of the stochastic process X_t are the joint probability distribution of the random variables $X_{t_1}, \ldots, X_{t_n}$, that is

$$F(x_1, t_1; \ldots; x_n, t_n) = P(X_{t_1} \leq x_{t_1}, \ldots, X_{t_n} \leq x_{t_n}), \tag{B.2}$$

for all possible choices of times $t_1, \ldots, t_n \in I$ and $n \geq 1$. Kolmogorov's theorem asserts that if $\mathcal{P}$ is a family of finite-dimensional distributions,

$$\mathcal{P} = \{ F(x_1, t_1; \ldots; x_n, t_n) \mid \ n \geq 1, \ t_1, \ldots, t_n \in I, \ x_1 \ldots, x_n \in \mathbb{R} \} \tag{B.3}$$

satisfying proper conditions, then there exists a probability space $(\Omega, \mathcal{F}, P)$ with a stochastic process $\{ X_t \}_{t \in I}$ [142].

Theorem 8 (Kolmogorov) *Let* I *be an arbitrary index set. For each non-empty, finite subset* $J = \{t_1, \ldots, t_n\} \subset I$, *let* μ_J *be a probability measure on the Euclidean space* $(\mathbb{R}^n, \mathcal{B}^n)$, *where* $\mathcal{B}^n$ *is the Borel* σ*-algebra on* $\mathbb{R}^n$.

Suppose this family of measures $\{\mu_J\}$ *satisfies the following two consistency conditions:*

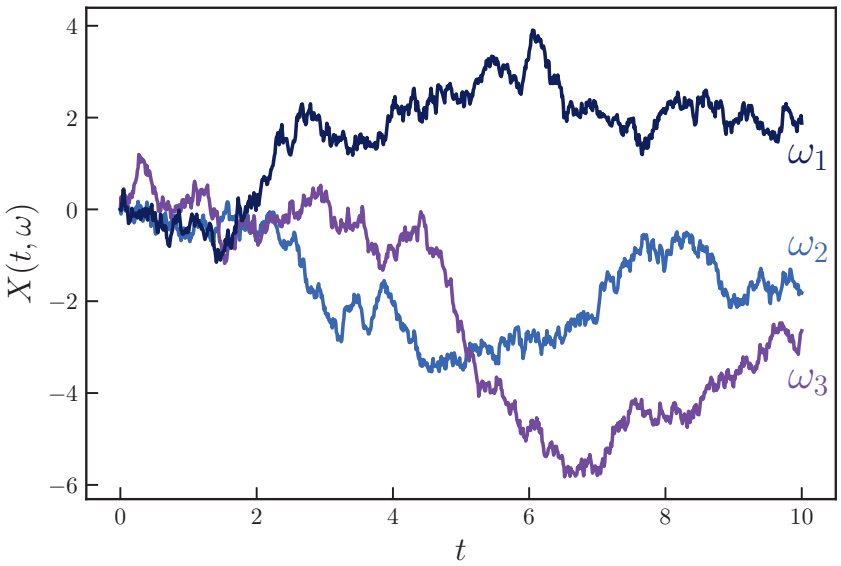


FIGURE 39 – Three different realizations of one-dimensional Brownian motion as example of a stochastic process $X(t,\omega)$ in function of the parameter t, they are: $X(t,\omega_1)$, $X(t,\omega_2)$ and $X(t,\omega_3)$.

1. ***Permutation Invariance:*** *For any finite subset $J = \{t_1, \ldots, t_n\} \subset I$ and any permutation π of $\{1, \ldots, n\}$, the measure is invariant under the reordering of coordinates. If $B_1, \ldots, B_n \subset \mathbb{R}$, where B_i is a Borel set, then*

$$\mu_{\{t_1,\ldots,t_n\}}(B_1 \times \cdots \times B_n) = \mu_{\{t_{\pi(1)},\ldots,t_{\pi(n)}\}}(B_{\pi(1)} \times \cdots \times B_{\pi(n)}).$$

2. ***Marginalization Consistency:*** *For any finite subset $J = \{t_1, \ldots, t_n\} \subset I$ with $m < n$, let $K = \{t_1, \ldots, t_m\}$. The measure μ_K must be the marginal distribution of μ_J. For any set $A \in \mathcal{B}^m$, this means:*

$$\mu_K(A) = \mu_J(A \times \mathbb{R}^{n-m}).$$

In other words, if we "project" the measure from $\mathbb{R}^n$ down to $\mathbb{R}^m$ by ignoring the last $n - m$ coordinates, we recover the measure for the smaller set of indices.

Then, there exists a probability space $(\Omega, \mathcal{F}, P)$ and a real-valued stochastic process $X = \{X_t\}_{t\in I}$ defined on this space, such that for any finite subset $J = \{t_1, \ldots, t_n\} \subset I$, the joint probability measure of the random vector $(X_{t_1}, \ldots, X_{t_n})$ is given by the measure μ_J.

$$P((X_{t_1}, \ldots, X_{t_n}) \in A) = \mu_J(A) \quad \forall\ A \in \mathcal{B}^n.$$

A stochastic process is said to be absolutely continuous if the random variables X_{t_i} for all $t_i \in I$ are absolutely continuous. For an absolutely continuous stochastic process, the probability density associated with the joint distribution (B.2) can be defined by [44]

$$p(x_1, t_1; \ldots; x_n, t_n) = \int_\Omega \delta\Big(x_1 - X_{t_1}(\omega)\Big) \ldots \delta\Big(x_n - X_{t_n}(\omega)\Big) dP(\omega). \tag{B.4}$$

The measure $p(x,t)dx$ is the probability of finding a value of the stochastic process X_t between x and $x+dx$ at time t, while $p(x_1,t_1;\ldots;x_n,t_n)dx_1\ldots dx_n$ is the probability of a stochastic process pass through $[x_1, x_1+dx_1]$ at time t_1 and $\ldots$ $[x_n, x_n+dx_n]$ at time t_n. From Eq. (B.4) we can write

$$F(x_1,t_1;\ldots;x_n,t_n) = \int_{-\infty}^{x_1}\cdots\int_{-\infty}^{x_n} p(x_1,t_1;\ldots;x_n,t_n)dx_1\ldots dx_n. \tag{B.5}$$

Now, the two consistency conditions of the Kolmogorov's theorem can be rewritten in terms of the pdf $p_n(x_1,t_1;\ldots;x_n,t_n)$ [44]:

1. Permutation invariance (or symmetry)

$$p_n(\ldots;x_k,t_k;\ldots;x_l,t_l;\ldots) = p_n(\ldots;x_l,t_l;\ldots;x_k,t_k;\ldots); \tag{B.6}$$

2. Marginalization consistency (or completeness)

$$\int p_n(x_1,t_1;\ldots;x_n,t_n)dx_n = p_{n-1}(x_1,t_1;\ldots;x_{n-1},t_{n-1}). \tag{B.7}$$

The joint distribution in (B.2), and consequently the pdf in (B.4), determines many but not all relevant properties of a stochastic process. We should impose additional requirements, such as the continuity of the paths, which is reasonable on physical grounds [37].

In many cases, for a time long enough, the stochastic process reaches a steady state where its properties no longer depend on time. Thus, let us define *stationary processes*.

Definition 20 *A stochastic process is said to be stationary if all its finite-dimensional distributions are invariant under a time translation, that is*

$$F(x_1,t_1;\ldots;x_n,t_n) = F(x_1,t_1+\tau;\ldots;x_n,t_n+\tau)$$

for all choices of the indices $t_1,\ldots,t_n \in I$, $n \geq 1$, *and* τ *with* $t_1+\tau,\ldots,t_n+\tau \in I$.

Alternatively to the definition above, we can say that a stochastic process is stationary if the collection of random variables $\{ X_{t_i} \}$ and $\{ X_{t_i+\tau} \}$ are identically distributed, i.e.,

$$(X_{t_1},\ldots,X_{t_n}) \overset{\mathrm{d}}{=} (X_{t_1+\tau},\ldots,X_{t_n+\tau}). \tag{B.8}$$

We can define stationarity for the increments of a stochastic process as follows.

Definition 21 *A stochastic process* $\{ X_t \}_{t\in I}$ *is said to have stationary increments if*

$$X_t - X_s \overset{d}{=} X_{t+\tau} - X_{s+\tau},$$

$\forall$ $s < t \in I$, *and* τ *with* $t+\tau$, $s+\tau \in I$. *The process* X_t *is said to have independent increments if*

$$X_{t_2} - X_{t_1},\ldots,X_{t_n} - X_{t_{n-1}}$$

are independent random variables for all choices of times $t_1 < t_2 < \ldots < t_n$.

Some types of stochastic processes that are non-stationary can have stationary increments; an example of such a process is the random walk [37, 44].

We can also generalize the definition of conditional probability (A.30) for a stochastic process, i.e.,

$$p_2(x_1,t_1;x_2,t_2) = p_{1|1}(x_2,t_2|x_1,t_1)p_1(x_1,t_1), \tag{B.9}$$

and due to the completeness of p_2, see Eq. (B.7), we have a normalization for the conditional probability:

$$\int dx_2\ p_{1|1}(x_2,t_2|x_1,t_1) = 1. \tag{B.10}$$

B.1 CORRELATION FUNCTION

The mean of a stochastic process $X_t = X(t)$ with pdf $p_n(x_1,t_1;\ldots;x_n,t_n)$ at time t_1 can be calculated by

$$\langle X(t_1)\rangle = \int_{\mathbb{R}^n} dx_1\ldots dx_n\ x_1\ p_n(x_1,t_1;\ldots;x_n,t_n), \tag{B.11}$$

and in the same way for the other moments

$$\langle X(t_1)\ldots X(t_i)\rangle = \int_{\mathbb{R}^n} dx_1\ldots dx_n\ x_1\ldots x_i\ p_n(x_1,t_1;\ldots;x_n,t_n). \tag{B.12}$$

The two-point correlations between two stochastic processes $X_i(t)$ and $X_j(t)$ is defined through the time-dependent covariance matrix

$$\begin{aligned}\Sigma_{ij}(t_1,t_2) = \mathrm{cov}[X_i(t_1),X_j(t_2)] &= \Big\langle \Big(X_i(t_1) - \langle X_i(t_1)\rangle\Big)\Big(X_j(t_2) - \langle X_j(t_2)\rangle\Big)\Big\rangle \\ &= \langle X_i(t_1)X_j(t_2)\rangle - \langle X_i(t_1)\rangle\langle X_j(t_2)\rangle,\end{aligned} \tag{B.13}$$

where the diagonal elements $\sigma^2(t_1,t_2) \equiv \Sigma_{ii}(t_1,t_2)$ are called *autocorrelation functions* (or just correlation functions) and the off-diagonal elements $\Sigma_{ij}(t_1,t_2)$ for $i \neq j$ are called *cross-correlation functions*. If the process is stationary, then its correlation function depends only on the time difference $t_2 - t_1$:

$$\sigma^2(t_1,t_2) = \sigma^2(t_2 - t_1). \tag{B.14}$$

If the process is stationary and additionally has zero mean, $\langle X_t\rangle = 0$, for all t, then the correlation function can be written as

$$\sigma^2(t) = \langle X(t_0)X(t_0+t)\rangle, \tag{B.15}$$

for any t_0.

B.2 MARTINGALE PROCESSES

The martingale processes are a special class of stochastic processes with important applications in the financial market and many physical phenomena. Let us start defining the concept of a *fair game* [44].

Definition 22 *A sequence* $\{ X_n \}_{n\in\mathbb{N}}$ *is called absolutely fair when for all* $n = 1, 2, \ldots$ *we have*

$$\mathbb{E}[X_1] = 0$$

and

$$\mathbb{E}[X_{n+1}|X_1, \ldots, X_n] = 0.$$

Consider now another sequence of random variables $\{ Y_n \}_{n\in\mathbb{N}}$ defined by

$$Y_n = \mathbb{E}[Y_1] + X_1 + \ldots + X_n. \tag{B.16}$$

Based on the definition above, it is possible to show that

$$\mathbb{E}[Y_{n+1}|Y_1, \ldots, Y_n] = \mathbb{E}[Y_{n+1}|X_1, \ldots, X_n] = Y_n. \tag{B.17}$$

Then, we define the martingale processes [44].

Definition 23 *A sequence* $\{ Y_n \}_{n\in\mathbb{N}}$ *is a martingale if and only if*

$$\mathbb{E}[Y_{n+1}|Y_1, \ldots, Y_n] = Y_n.$$

It is a submartingale if and only if

$$\mathbb{E}[Y_{n+1}|Y_1, \ldots, Y_n] \geq Y_n,$$

and is a supermartingale if and only if

$$\mathbb{E}[Y_{n+1}|Y_1, \ldots, Y_n] \leq Y_n.$$

For a martingale, the best estimate we can get for the next value is the present value. If the process is a martingale, its increments are a fair game, meaning that the mean value of the increments is zero. The random walk is an example of a martingale, since its position process is the sum of fair game increments [37, 44].

This process is related to another kind of stochastic processes called *Markov processes* named after the russian mathematician Andrei Markov (1856-1922).

B.3 MARKOV PROCESSES

In a few words, we can define Markov processes as processes without memory, meaning that the past of a trajectory is not important for the future, and the future will only be determined by the present result [44, 148].

Definition 24 *For a Markov process, we have for all n and all $t_1 < \ldots < t_n$*

$$p(x_n, t_n|x_1, t_1; \ldots; x_{n-1}, t_{n-1}) = p(x_n, t_n|x_{n-1}, t_{n-1}).$$

Therefore, we only need to know the actual state of the system, (x_{n-1}, t_{n-1}), in order to calculate the probability of the system changing to (x_n, t_n). Consequently, we have

$$p_n(x_1, t_1; \ldots; x_n, t_n) = \prod_{i=2}^{n} p_{1|1}(x_i, t_i|x_{i-1}, t_{i-1}) p_1(x_1, t_1). \tag{B.18}$$

Equation (B.18) is the property of Markov processes responsible for introducing an enormous simplification in the calculation of $p_n(x_1, t_1; \ldots; x_n, t_n)$. It means that, in order to describe the stochastic process completely, we just need to know $p_1(x_1, t_1)$ and the transition probability $p_{1|1}(x_i, t_i|x_{i-1}, t_{i-1})$.

Let us consider the case when $n = 3$, i.e.,

$$p_3(x_1, t_1; x_2, t_2; x_3, t_3) = p_{1|1}(x_3, t_3|x_2, t_2) p_{1|1}(x_2, t_2|x_1, t_1) p_1(x_1, t_1). \tag{B.19}$$

If we integrate over x_2 and apply the completeness property (B.7), we get

$$p_2(x_1, t_1; x_3, t_3) = p_1(x_1, t_1) \int dx_2 \; p_{1|1}(x_3, t_3|x_2, t_2) p_{1|1}(x_2, t_2|x_1, t_1). \tag{B.20}$$

Considering the conditional probability definition for stochastic processes in Eq. (B.9), we arrive at the result

$$p_{1|1}(x_3, t_3|x_1, t_1) = \int dx_2 \; p_{1|1}(x_3, t_3|x_2, t_2) p_{1|1}(x_2, t_2|x_1, t_1), \tag{B.21}$$

for $t_3 \geq t_2 \geq t_1$. Equation (B.21) is known as the *Chapman-Kolmogorov equation* and is a consistency equation for the conditional probabilities of a Markov process. Considering now $n = 2$, i.e.,

$$p_2(x_2, t_2; x_1, t_1) = p_{1|1}(x_2, t_2|x_1, t_1) p_1(x_1, t_1), \tag{B.22}$$

integrating it over x_1 and applying again the completeness property (B.7), we find

$$p_1(x_2, t_2) = \int dx_1 \; p_{1|1}(x_2, t_2|x_1, t_1) p_1(x_1, t_1). \tag{B.23}$$

In fact, the following theorem can be stated [44].

Theorem 9 *Two positive, normalized functions p_1 and $p_{1|1}$ which fulfill the Chapman-Kolmogorov equation*

$$p_{1|1}(x_3,t_3|x_1,t_1) = \int dx_2\ p_{1|1}(x_3,t_3|x_2,t_2)p_{1|1}(x_2,t_2|x_1,t_1)$$

and

$$p_1(x_2,t_2) = \int dx_1\ p_{1|1}(x_2,t_2|x_1,t_1)p_1(x_1,t_1),$$

completely and uniquely define a Markov process.

B.4 MASTER EQUATION AND FOKKER-PLANCK EQUATION

From the Chapman-Kolmogorov equation, one can derive the evolution equations for Markov processes. Consider now a Markov process with a stationary transition probability defined by

$$p_{1|1}(x_i,t_i|x_{i-1},t_{i-1}) = p_{1|1}(x_i,t_i+\Delta t|x_{i-1},t_{i-1}+\Delta t) \overset{\Delta t=-t_{i-1}}{=} p_t(x_i|x_{i-1}), \tag{B.24}$$

where $p_t(x_i,x_{i-1})$ denotes a *transition probability* from x_{i-1} at time t_0 to x_i at time t_0+t ($t=t_i-t_{i-1}$) for any t_0. Here, stationarity means that the function in question only depends on time differences, which is often called time homogeneity. Using the Chapman-Kolmogorov equation (B.21) yields

$$p_{t+t'}(x_{i+1}|x_{i-1}) = \int dx_i\ p_{t'}(x_{i+1}|x_i)\, p_t(x_i|x_{i-1}). \tag{B.25}$$

In the discrete case, the Chapman-Kolmogorov equation above takes the form of a matrix multiplication:

$$p_{t+t'}(x_{n+1}|x_{n-1}) = \sum_n p_{t'}(x_{n+1}|x_n)\, p_t(x_n|x_{n-1}). \tag{B.26}$$

Considering small times interval t' in Eq. (B.25), we can express the transition probability $p_{t'}(x_{i+1}|x_i)$ in the form

$$p_{t'}(x_{i+1}|x_i) = (1-w_{tot}(x_i)t')\delta(x_{i+1}-x_i) + t'w(x_{i+1}|x_i) + \mathcal{O}(t'^2) \tag{B.27}$$

Where $w(x_{i+1}|x_i)$ is the *transition rate*—transition probability per unity time—from x_i to x_{i+1}, note that $w(x_i|x_i)=0$. The factor $(1-w_{tot}(x_i)t')$ is the probability to remain in x_i until an additional time t'. Applying the normalization condition in (B.10) for $p_{t'}(x_{i+1}|x_i)$, we find

$$w_{tot}(x_i) = \int dx_{i+1}\ w(x_{i+1}|x_i). \tag{B.28}$$

Substituting Eq. (B.27) in the Chapman-Kolmogorov equation (B.25) leads to

$$p_{t+t'}(x_{i+1}|x_{i-1}) = (1-w_{tot}(x_{i+1})t')p_t(x_{i+1}|x_{i-1}) + t'\int dx_i\ w(x_{i+1}|x_i)p_t(x_i|x_{i-1}). \tag{B.29}$$

Rearranging the terms,

$$\begin{aligned}&\frac{p_{t+t'}(x_{i+1}|x_{i-1}) - p_t(x_{i+1}|x_{i-1})}{t'} \\ &= \int dx_i\ w(x_{i+1}|x_i)p_t(x_i|x_{i-1}) - \int dx_i\ w(x_i|x_{i+1})p_t(x_{i+1}|x_{i-1}),\end{aligned} \tag{B.30}$$

where we have used the Eq. (B.28) for w_{tot}. Now, taking the limit $t' \to 0$ we arrive at

$$\frac{\partial}{\partial t}p_t(x_{i+1}|x_{i-1}) = \int dx_i\ w(x_{i+1}|x_i)p_t(x_i|x_{i-1}) - \int dx_i\ w(x_i|x_{i+1})p_t(x_{i+1}|x_{i-1}). \tag{B.31}$$

The equation above is an integro-differential version of the Chapman-Kolmogorov equation. Multiplying it by $p_1(x_{i-1}, t_0)$ and integrating over x_{i-1}, yields

$$\frac{\partial}{\partial t}p_1(x_{i+1}, t) = \int dx_i\ w(x_{i+1}|x_i)p_1(x_i, t) - \int dx_i\ w(x_i|x_{i+1})p_1(x_{i+1}, t), \tag{B.32}$$

where we have used the formula (B.23). Equation (B.32) is the *master equation*, which describes the time evolution of the probability density of a Markov process with stationary transition probability. In order to simplify the notation, let us make the changes $p_1 \to p$, $x_{i+1} \to x$ and $x_i \to x'$:

$$\frac{\partial}{\partial t}p(x, t) = \int dx'\ w(x|x')p(x', t) - \int dx'\ w(x'|x)p(x, t). \tag{B.33}$$

In the discrete case, this equation takes the form

$$\frac{\partial}{\partial t}p(n, t) = \sum_{n'} \left[w(n|n')p(n', t) - w(n'|n)p(n, t)\right]. \tag{B.34}$$

The master equation can be interpreted as a balance between an inward flux of probability and an outward flux of probability. The first term describes the probability increase due to the tax of transitions from any x' to x. Otherwise, the second term describes the probability decrease due to the tax of transitions from x to any x' [44].

Studied by Adriaan Fokker (1887-1972) and Max Planck (1858-1947), the Fokker-Planck equation was first introduced by Kolmogorov in 1931, and it is a second-order partial differential equation that describes the time evolution of the probability density for a Markovian process [38, 45]. In order to derive this equation, consider the master equation in (B.33) and let us make the following assumptions [44]:

1. We write $w(x|x') = w(x|x-r) =: w(x-r; r)$, where the "jump distance" is $r := x - x'$. Similarly, $w(x'|x) = w(x - r, x) =: w(x; -r)$;

2. Only small jumps occur, i.e., $w(x - r; r)$ as a function of r is sharply peaked around $r = 0$,

$$\exists \delta > 0 \quad \text{such that} \quad w(x - r; r) \approx 0, \quad |r| > \delta;$$

3. $w(x-r;r)$ is a slowly varying function of its first argument,

$$\exists \delta' > 0 \quad \text{such that} \quad w(x-r;r) \approx w(x;r), \quad |r| < \delta'$$

this assumption also holds for $p(x,t)$;

4. The functions w and p are sufficiently smooth in both arguments.

Thus, we rewrite Eq. (B.33) as

$$\frac{\partial}{\partial t}p(x,t) = \int_{-\infty}^{+\infty} w(x-r;r)\, p(x-r,t)\, dr - p(x,t)\int_{-\infty}^{+\infty} w(x;-r)\, dr. \tag{B.35}$$

Performing a Taylor series expansion on the integrand of the first integral, $w(x-r;r)\, p(x-r,t)$, for small r, follows

$$\begin{aligned}\frac{\partial}{\partial t}p(x,t) = {} & p(x,t)\int_{-\infty}^{+\infty} w(x;r)\, dr - p(x,t)\int_{-\infty}^{+\infty} w(x;-r)\, dr \\ & - \int_{-\infty}^{+\infty} r\frac{\partial}{\partial x}[w(x;r)p(x,t)]dr + \frac{1}{2}\int_{-\infty}^{+\infty} r^2\frac{\partial^2}{\partial x^2}[w(x;r)p(x,t)]dr - \ldots,\end{aligned} \tag{B.36}$$

yielding

$$\begin{aligned}\frac{\partial}{\partial t}p(x,t) &= \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}[a_n(x)p(x,t)], \\ a_n(x) &= \int_{\infty}^{\infty} r^n w(x;r)dr.\end{aligned} \tag{B.37}$$

Equation (B.37) is known as the *Kramers-Moyal expansion* of the master equation. This equation transforms the integro-differential equation (B.33) into a partial differential equation of infinite order. Since we have assumed that both the transition rate $w(x;r)$ and the probability density $p(x,t)$ are slowly varying functions with respect to the first argument, we can truncate this series at a certain order. Keeping only the terms up to the second order in the Kramers-Moyal expansion, we obtain the one-dimensional Fokker-Planck equation:

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}[a_1(x)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[a_2(x)p(x,t)], \tag{B.38}$$

where $a_1(x)$ is called *drift coefficient* and $a_2(x)/2$ is called *diffusion coefficient*. Recall that we have made use of this equation in Sec. 2.1.1, see Eq. (2.17), to find the probability density of a Brownian particle. For the three-dimensional case, the Fokker-Planck equation takes the form

$$\begin{aligned}\frac{\partial}{\partial t}p(\mathbf{x},t) &= \frac{1}{2}\nabla^2[a_2(\mathbf{x})p(\mathbf{x},t)] - \nabla\cdot[a_1(\mathbf{x})p(\mathbf{x},t)] \\ &= \nabla\cdot\left\{\frac{1}{2}\nabla[a_2(\mathbf{x})p(\mathbf{x},t)] - a_1(\mathbf{x})p(\mathbf{x},t)\right\}.\end{aligned} \tag{B.39}$$

The Fokker-Planck equation can be rewritten for the conditional probability $p(x,t|x_0,t_0)$ as

$$\frac{\partial}{\partial t}p(x,t|x_0,t_0) = -\frac{\partial}{\partial x}[a_1(x)p(x,t|x_0,t_0)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[a_2(x)p(x,t|x_0,t_0)]. \tag{B.40}$$

Since this equation involves derivatives with respect to time t, we call it the *forward Fokker-Planck equation*, and to solve it we need to specify the initial conditions at time t_0. We will now derive the corresponding *backward Fokker-Planck equation*. To do this, we start with a simple relation:

$$\frac{\partial}{\partial s}p(x,t|x_0,t_0) = 0, \tag{B.41}$$

which can be rewritten as

$$\begin{aligned}
0 &= \frac{\partial}{\partial s}\int dz\, p(x,t|z,s)\, p(z,s|x_0,t_0) \\
&= \int dz \left[p(z,s|x_0,t_0)\frac{\partial}{\partial s}p(x,t|z,s) + p(x,t|z,s)\frac{\partial}{\partial s}p(z,s|x_0,t_0)\right] \\
&= \int dz p(z,s|x_0,t_0)\frac{\partial}{\partial s}p(x,t|z,s) + \int dz \left\{ p(x,t|z,s)\left(-\frac{\partial}{\partial z}[a_1(z)p(z,s|x_0,t_0)]\right.\right. \\
&\quad \left.\left. +\frac{1}{2}\frac{\partial^2}{\partial z^2}[a_2(z)p(z,s|x_0,t_0)]\right)\right\},
\end{aligned} \tag{B.42}$$

where we have inserted the forward Fokker-Planck equation (B.40) in the last term. Performing integration by parts and assuming that all boundary terms are zero, we have

$$\begin{aligned}
\int dz\, p(z,s|x_0,t_0) \Bigg[&\frac{\partial}{\partial s}p(x,t|z,s) + a_1(z)\frac{\partial}{\partial z}p(x,t|z,s) \\
&+a_2(z)\frac{1}{2}\frac{\partial^2}{\partial z^2}p(x,t|z,s)\Bigg] = 0.
\end{aligned} \tag{B.43}$$

Since this equation must be valid for any and all $p(z,s|x_0,t_0)$, then we have

$$\frac{\partial}{\partial s}p(x,t|z,s) = -a_1(z)\frac{\partial}{\partial z}p(x,t|z,s) - \frac{1}{2}a_2(z)\frac{\partial^2}{\partial z^2}p(x,t|z,s). \tag{B.44}$$

This is the *Kolmogorov backward equation*, also known as the backward Fokker-Planck equation, where the derivatives are taken with respect to the initial coordinates $(z,\, s)$. To solve this equation in the interval $[t_0,T]$, we need to specify the final conditions at time $t=T$.

We will now use the forward Fokker-Planck equation to estimate the moments $\langle X^n(t)\rangle$ of the stochastic variable for short times t. First, let us calculate the mean value.

$$\begin{aligned}
\langle X(t)\rangle &= \int_0^t dt' \frac{d}{dt'}\langle X(t')\rangle = \int_0^t dt' \int_\Omega dx\; x\; \frac{\partial}{\partial t'}p(x,t') \\
&= -\int_0^t dt' \int_\Omega dx\; x\; \frac{\partial}{\partial x}[a_1(x)p(x,t')] + \frac{1}{2}\int_0^t dt' \int_\Omega dx\; x\; \frac{\partial^2}{\partial x^2}[a_2(x)p(x,t')] \\
&= -\int_0^t dt'[x a_1(x)p(x,t')]_{\partial\Omega} + \int_0^t dt' \int_\Omega dx\; a_1(x)p(x,t') \\
&\quad + \frac{1}{2}\int_0^t dt' \left[x\frac{\partial}{\partial x}(a_2(x)p(x,t')) - a_2(x)p(x,t')\right]_{\partial\Omega}.
\end{aligned} \tag{B.45}$$

Assuming that the boundary terms are zero and using the initial condition $p(x,0) = \delta(x)$, we have

$$\begin{aligned}\langle X(t)\rangle &= \int_\Omega dx \int_0^t dt'\ a_1(x)p(x,t') \overset{t\to 0}{=} \int_\Omega dx\ a_1(x)\delta(x)\int_0^t dt' \\ &= a_1(0)t + \mathcal{O}(t).\end{aligned} \tag{B.46}$$

Similarly, we can calculate the second moment, for which we obtain

$$\begin{aligned}\langle X^2(t)\rangle &= \int_0^t dt' \int_\Omega dx\ x^2\ \frac{\partial}{\partial t'}p(x,t') \\ &= -\int_0^t dt' \int_\Omega dx\ x^2\ \frac{\partial}{\partial x}[a_1(x)p(x,t')] + \frac{1}{2}\int_0^t dt' \int_\Omega dx\ x^2\ \frac{\partial^2}{\partial x^2}[a_2(x)p(x,t')] \\ &= -\int_0^t dt'[x^2 a_1(x)p(x,t')]_{\partial\Omega} + 2\int_0^t dt' \int_\Omega dx\ x a_1(x)p(x,t') \\ &+ \frac{1}{2}\int_0^t dt' \left[x^2\frac{\partial}{\partial x}(a_2(x)p(x,t'))\right]_{\partial\Omega} - \int_0^t dt' \int_\Omega dx\ x\frac{\partial}{\partial x}[a_2(x)p(x,t')].\end{aligned} \tag{B.47}$$

Canceling out the boundary terms and applying one more integration by parts in the last term, we get

$$\begin{aligned}\langle X^2(t)\rangle &= 2\int_0^t dt' \int_\Omega dx\ x a_1(x)p(x,t') + \int_0^t dt' \int_\Omega dx\ a_2(x)p(x,t') \\ &= \int_\Omega dx\,[2x a_1(x) + a_2(x)]\int_0^t dt'\ p(x,t') \\ &\overset{t\to 0}{=} \int_\Omega dx\,[2x a_1(x) + a_2(x)]\,\delta(x)t = a_2(0)t + \mathcal{O}(t),\end{aligned} \tag{B.48}$$

and for the remaining moments is easy to see that

$$\langle X^n(t)\rangle = \mathcal{O}(t) \quad \text{for } n \geq 3. \tag{B.49}$$

Notice that in both the results obtained in the introductory example for the diffusion of a Brownian particle, see Eq. (2.23), and in Eq. (B.48), the position second moment is proportional to t. That is, stochastic processes with probability density evolution described by the Fokker-Planck equation have a characteristic diffusion behavior of the form $\langle x^2\rangle \propto t$ [38, 44].

APPENDIX C – DEDUCTION OF THE SCHRÖDINGER EQUATION FROM HAMILTON'S PRINCIPLE IN STOCHASTIC MECHANICS AND THE QUANTUM EXTENSION OF THE SECOND NEWTON'S LAW

In the classical setting, Hamilton's principle states that the actual trajectory of a system extremizes the action functional. In Nelson's stochastic mechanics, the particle trajectory $\mathbf{x}(t)$ is a diffusion process driven by a Wiener noise of strength $\sigma^2 = \hbar/m$. Then, the notion of a deterministic path must be replaced in the formulation of a stochastic-based quantum Hamilton principle.

Nelson's formulation introduces two velocity fields: the *current velocity* $\mathbf{v}(\mathbf{x}, t)$, which is the mean forward drift of the diffusion, and the *osmotic velocity* $\mathbf{u}(\mathbf{x}, t)$, which encodes the gradient of the probability density. The combination

$$\mathbf{v}_q(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}, t) - i\mathbf{u}(\mathbf{x}, t) \tag{C.1}$$

defines a complex *quantum velocity*. Its real part v governs the mean motion, while the imaginary part $-u$ encodes the diffusion-induced spread of the probability cloud. In the classical limit $\hbar \to 0$, the diffusion vanishes, and the quantum velocity reduces to the ordinary classical velocity.

A variational principle that treats $\mathbf{v}_q$ as the fundamental dynamical variable leads to a unified description of the action and the entropy production, often called the *quantum Hamilton principle* [15, 68].

C.1 QUANTUM MECHANICS FROM HAMILTON'S PRINCIPLE IN STOCHASTIC MECHANICS

The quantum action functional is defined as [15, 18]

$$I_Q[\mathbf{x}, \mathbf{v}_q] = \mathbb{E}\left[\int_{t_0}^{t_1} \left(\frac{m}{2}\,\mathbf{v}_q(t)\cdot\mathbf{v}_q(t) - V\Big(\mathbf{x}(t)\Big)\right) dt + \phi_0(\mathbf{x}(t_0))\right], \tag{C.2}$$

where $V(\mathbf{x})$ is the external potential and $\mathbb{E}[\cdot]$ denotes the expectation over the stochastic process. The functional is subject to the dynamical constraint that the diffusion satisfies the generalized Itô's formula for a complex-valued function $\phi(\mathbf{x}, t)$:

$$d\phi\Big(\mathbf{x}(t), t\Big) = \left(\partial_t\phi + \mathbf{v}_q(t)\cdot\nabla\phi - i\frac{\hbar}{2m}\nabla^2\phi\right) dt + \nabla\phi\Big(\mathbf{x}(t), t\Big)\cdot d\mathbf{W}_q(t), \tag{C.3}$$

where $d\mathbf{W}_q$ is the quantum noise, see Eq. (3.103). The constraint enforces consistency between the stochastic dynamics and the chosen phase function ϕ.

The original constrained problem is to "extremize" the quantum action I_Q under the drift constraint. The quantum Hamilton principle can be regarded as a *saddle-point*

extremum in terms of the underlying real variables $(\mathbf{v}, \mathbf{u})$, as it unifies the saddle-point action principle (minimizing with respect to $\mathbf{v}$, maximizing with respect to $\mathbf{u}$) and the saddle-point entropy production principle (maximizing with respect to $\mathbf{v}$, minimizing with respect to $\mathbf{u}$). However, when expressed in terms of the single complex quantum velocity $\mathbf{v}_q = \mathbf{v} - i\mathbf{u}$, the resulting functional possesses a single stationary point that simultaneously encodes these two opposite variational tendencies, appearing as a pure extremum.

To enforce the dynamical constraint, we introduce a Lagrange functional $\Lambda^\phi(\mathbf{x}, \mathbf{v}_q)$ associated with a complex-valued function $\phi(\mathbf{x}, t)$, twice continuously differentiable in $\mathbf{x}$, once in t, and satisfying $\mathbb{E}[\int_{t_0}^t |\nabla\phi(\mathbf{x}(s), s)|^2 ds] < \infty$, where Λ^ϕ is defined as

$$\Lambda^\phi[\mathbf{x}, \mathbf{v}_q] = \mathbb{E}\Bigg[\int_{t_0}^{t_1}\Big(-\partial_t\phi - \mathbf{v}_q(t)\cdot\nabla\phi + i\frac{\hbar}{2m}\nabla^2\phi\Big)\,dt \\ +\phi(\mathbf{x}(t_1), t_1) - \phi(\mathbf{x}(t_0), t_0)\Bigg]. \tag{C.4}$$

When the pair $(\mathbf{x}, \mathbf{v}_q)$ satisfies the dynamical constraint, i.e., $\mathbf{v}_q$ is the quantum drift of $\mathbf{x}$, the generalized Itô formula (C.3) implies that $\Lambda^\phi = 0$. This is because the expectation of the stochastic integral term, $\mathbb{E}[\int_{t_0}^{t_1} \nabla\phi(\mathbf{x}(t), t)\cdot d\mathbf{W}_q(t)]$, vanishes.

The variational problem is now to extremize the unconstrained functional $(I_Q + \Lambda^\phi)$. The integrand of $(I_Q + \Lambda^\phi)$ is given by:

$$\mathcal{L}(\mathbf{x}, \mathbf{v}_q, t) = \frac{m}{2}\mathbf{v}_q(t)\cdot\mathbf{v}_q(t) - V(\mathbf{x}(t)) - \partial_t\phi(\mathbf{x}(t), t) - \mathbf{v}_q(t)\cdot\nabla\phi(\mathbf{x}(t), t) \\ + i\frac{\hbar}{2m}\nabla^2\phi(\mathbf{x}(t), t). \tag{C.5}$$

For a fixed path $\mathbf{x}(t)$ and time t, we perform a pointwise extremization of $\mathcal{L}$ with respect to $\mathbf{v}_q(t)$. Since $\mathbf{v}_q$ is a complex vector, we can treat its real and imaginary parts as independent real variables. As $\mathcal{L}$ is holomorphic in $\mathbf{v}_q$ (it depends on $\mathbf{v}_q$ but not on its complex conjugate $\bar{\mathbf{v}}_q$), the standard derivative with respect to $\mathbf{v}_q$ applies. Setting

$$\frac{\partial\mathcal{L}}{\partial\mathbf{v}_q} = 0, \tag{C.6}$$

yields

$$m\mathbf{v}_q^*(t) - \nabla\phi\Big(\mathbf{x}(t), t\Big) = 0 \quad\Longrightarrow\quad \mathbf{v}_q^*(t) = \frac{1}{m}\,\nabla\phi\Big(\mathbf{x}(t), t\Big). \tag{C.7}$$

This gives the optimal quantum velocity $\mathbf{v}_q^*(t)$.

Substituting the optimal quantum velocity $\mathbf{v}_q^*(t)$ from Eq. (C.7) back into the

integrand $\mathcal{L}$:

$$\begin{aligned}\mathcal{L}\Big(\mathbf{x},\mathbf{v}_q^*,t\Big) &= \frac{1}{2}m\left(\frac{1}{m}\nabla\phi\right)\cdot\left(\frac{1}{m}\nabla\phi\right) - V(\mathbf{x}(t)) - \partial_t\phi(\mathbf{x}(t),t) - \left(\frac{1}{m}\nabla\phi\right)\cdot\nabla\phi(\mathbf{x}(t),t)\\ &\quad + i\frac{\hbar}{2m}\nabla^2\phi(\mathbf{x}(t),t)\\ &= \frac{1}{2m}(\nabla\phi)\cdot(\nabla\phi) - V(\mathbf{x}(t)) - \partial_t\phi(\mathbf{x}(t),t) - \frac{1}{m}(\nabla\phi)\cdot(\nabla\phi)\\ &\quad + i\frac{\hbar}{2m}\nabla^2\phi(\mathbf{x}(t),t)\\ &= -\frac{1}{2m}(\nabla\phi)\cdot(\nabla\phi) - V(\mathbf{x}(t)) - \partial_t\phi(\mathbf{x}(t),t) + i\frac{\hbar}{2m}\nabla^2\phi(\mathbf{x}(t),t).\end{aligned}$$

For the unconstrained functional $(I_Q + \Lambda^\phi)$ to be constant (or extremized independently of $\mathbf{x}$), the integrand $\mathcal{L}(\mathbf{x},\mathbf{v}_q^*,t)$ must be identically zero. Setting $\mathcal{L}(\mathbf{x},\mathbf{v}_q^*,t) = 0$ and rearranging the terms, we obtain the Hamilton-Jacobi-like equation:

$$\partial_t\phi + \frac{1}{2m}(\nabla\phi)\cdot(\nabla\phi) + V(\mathbf{x}) - i\,\frac{\hbar}{2m}\,\nabla^2\phi = 0\,. \tag{C.8}$$

The imaginary and real parts of Eq. (C.8) correspond, respectively, to the first and second Madelung equations.

The complex-valued function $\phi(\mathbf{x},t)$ that emerges as the "principal function" in the quantum Hamilton principle is directly related to the logarithm of the quantum wave function $\psi(\mathbf{x},t)$. If we write the wave function in polar form, $\psi(\mathbf{x},t) = \exp\Big[R(\mathbf{x},t) + \frac{i}{\hbar}S(\mathbf{x},t)\Big]$, where $R(\mathbf{x},t)$ is related to the amplitude and $S(\mathbf{x},t)$ to the phase, then:

$$\phi(\mathbf{x},t) = \frac{\hbar}{i}\ln\psi(\mathbf{x},t) = S(\mathbf{x},t) - i\hbar R(\mathbf{x},t). \tag{C.9}$$

Thus, the real part of ϕ is $S(\mathbf{x},t)$, and the imaginary part is $-\hbar R(\mathbf{x},t)$. The gradients of R and S are directly linked to the current and osmotic velocities:

$$\mathbf{v} = \frac{1}{m}\nabla S \quad \text{and} \quad \mathbf{u} = \frac{\hbar}{m}\nabla R. \tag{C.10}$$

This connection shows how the complex wave function, typically seen as a mathematical construct, naturally arises from the real-valued stochastic processes and their associated velocities.

The Hamilton–Jacobi-like equation (C.8) is precisely the Schrödinger equation when $\phi(\mathbf{x},t) = (\hbar/i)\ln\psi(\mathbf{x},t)$. Substituting this relation into (C.8) results in

$$\begin{aligned}&\partial_t\left(\frac{\hbar}{i}\ln\psi\right) + \frac{1}{2m}\left(\nabla\left(\frac{\hbar}{i}\ln\psi\right)\right)\cdot\left(\nabla\left(\frac{\hbar}{i}\ln\psi\right)\right) + V(\mathbf{x}) - i\frac{\hbar}{2m}\nabla^2\left(\frac{\hbar}{i}\ln\psi\right) = 0\\ &\frac{\hbar}{i}\frac{\partial_t\psi}{\psi} + \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\nabla\psi}{\psi}\right)\cdot\left(\frac{\hbar}{i}\frac{\nabla\psi}{\psi}\right) + V(\mathbf{x}) - i\frac{\hbar}{2m}\left(\frac{\hbar}{i}\frac{\nabla^2\psi}{\psi} - \frac{\hbar}{i}\frac{(\nabla\psi)\cdot(\nabla\psi)}{\psi^2}\right) = 0.\end{aligned}$$

Multiplying by ψ, yields

$$\begin{aligned}\frac{\hbar}{i}\partial_t\psi + \frac{1}{2m}\left(\frac{\hbar}{i}\right)^2\frac{(\nabla\psi)\cdot(\nabla\psi)}{\psi} + V(\mathbf{x})\psi - i\frac{\hbar}{2m}\left(\frac{\hbar}{i}\nabla^2\psi - \frac{\hbar}{i}\frac{(\nabla\psi)\cdot(\nabla\psi)}{\psi}\right) &= 0\\ \frac{\hbar}{i}\partial_t\psi - \frac{\hbar^2}{2m}\frac{(\nabla\psi)\cdot(\nabla\psi)}{\psi} + V(\mathbf{x})\psi - \frac{\hbar^2}{2m}\nabla^2\psi + \frac{\hbar^2}{2m}\frac{(\nabla\psi)\cdot(\nabla\psi)}{\psi} &= 0\\ \frac{\hbar}{i}\partial_t\psi + V(\mathbf{x})\psi - \frac{\hbar^2}{2m}\nabla^2\psi &= 0.\end{aligned}$$

This is nothing but the Schrödinger equation

$$i\hbar\,\partial_t\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{x})\psi. \tag{C.11}$$

This equivalence is a profound result, demonstrating that the fundamental equation of quantum mechanics can be derived from a variational principle within stochastic mechanics.

The variational problem requires an initial specification $\phi(\mathbf{x}, t_0) = \phi_0(\mathbf{x})$. Through the relation $\phi = (\hbar/i)\ln\psi$, this translates into an initial wave function:

$$\psi(\mathbf{x}, t_0) = \exp\Big[\tfrac{i}{\hbar}\phi_0(\mathbf{x})\Big]. \tag{C.12}$$

The real part of ϕ_0 gives the initial phase $S(\mathbf{x}, t_0)$, while the imaginary part determines the initial amplitude $\exp[R(\mathbf{x}, t_0)]$ via $R = -\frac{1}{\hbar}\operatorname{Im}\phi_0$. Consequently, the initial probability density $p(\mathbf{x}, t_0) = |\psi(x, t_0)|^2$ and the initial drift fields $\mathbf{v}(\mathbf{x}, t_0)$ and $\mathbf{u}(\mathbf{x}, t_0)$ are fully specified. In the stochastic picture, this fixes both the initial distribution of diffusion paths and the initial drift fields.

The derivation clarifies how the current and osmotic velocities combine into a complex quantum velocity whose extremization of the quantum functional action unifies the action principle with the entropy-production principle.

The analysis rests on several assumptions: the particle is non-relativistic, spinless, and subject to a smooth external potential; the diffusion coefficient is constant $\sigma^2 = \hbar/m$; and the probability density remains sufficiently regular to permit the use of Itô calculus. Within this framework, the quantum Hamilton principle provides a compact and conceptually transparent route from stochastic dynamics to quantum mechanics.

C.2 QUANTUM NEWTON LAW

From the quantum Hamilton principle, a "quantum Newton law" can also be derived [15]. Define the quantum acceleration $\mathbf{a}_q(\mathbf{x}, t)$ as a substantial time derivative of the quantum velocity $\mathbf{v}_q^*(\mathbf{x}, t)$:

$$\mathbf{a}_q(\mathbf{x}, t) = \left(\partial_t + \mathbf{v}_q^*(x, t) \cdot \nabla - i\frac{\hbar}{2m}\nabla^2\right) \mathbf{v}_q^*(\mathbf{x}, t). \tag{C.13}$$

This definition can be justified by taking the mean of the complex Itô's formula (C.3) with ϕ replaced by $\mathbf{v}_q^*$. Taking the gradient of both sides of (C.8) and using the definition of $\mathbf{v}_q^*$, Eq. (C.7), one finds:

$$\mathbf{a}_q(\mathbf{x}, t) = -\frac{1}{m}\nabla V(\mathbf{x}). \tag{C.14}$$

This equation is a direct analogue of Newton's second law, but formulated for the quantum acceleration (C.13) and the classical potential force.

APPENDIX D – PROOFS OF THE UNITARY EQUIVALENCE THEOREM FOR NELSON'S STOCHASTIC QUANTIZATION AND ITS REMARK

Here are presented the proofs for the unitary equivalence theorem and its remark concerning the spectre of eigenstates, establishing the equivalence between Nelson's stochastic quantization and the standard quantum mechanics formulated in Hilbert space. Both results were presented in Sec. 3.4.

Proof of the Theorem 5 (Unitary Equivalence)

Let $g(\mathbf{x},t)$ be a function in $L^{2,1}(|\psi|^2)$. We first apply the right-hand side of relation (3.194) to the function g, yielding

$$M_\psi^{-1}\left(\frac{\partial}{\partial t}+\frac{i}{\hbar}H\right)M_\psi\, g = M_\psi^{-1}\left(\frac{\partial(\psi g)}{\partial t}+\frac{i}{\hbar}H(\psi g)\right)$$
$$= \frac{\partial g}{\partial t}+\psi^{-1}\frac{\partial \psi}{\partial t}\, g+\frac{i}{\hbar}\,\psi^{-1}H(\psi g). \tag{D.1}$$

Because ψ satisfies the Schrödinger equation,

$$i\hbar\,\frac{\partial\psi}{\partial t}=H\psi,$$

we have $\dfrac{\partial\psi}{\partial t}=-\dfrac{i}{\hbar}H\psi$. Substituting this into (D.1) gives

$$M_\psi^{-1}\left(\frac{\partial}{\partial t}+\frac{i}{\hbar}H\right)M_\psi\, g = \frac{\partial g}{\partial t}-\frac{i}{\hbar}\psi^{-1}(H\psi)\, g+\frac{i}{\hbar}\psi^{-1}H(\psi g)$$
$$= \frac{\partial g}{\partial t}+\frac{i}{\hbar}\psi^{-1}(H(\psi g)-(H\psi)g)\,. \tag{D.2}$$

Next, we shall expand $H(\psi g)$, using $H=-\dfrac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})$. Consider

$$\nabla^2(\psi g)=\psi\,\nabla^2 g+2\nabla\psi\cdot\nabla g+g\,\nabla^2\psi.$$

Hence,

$$H(\psi g)=-\frac{\hbar^2}{2m}\Big(\psi\,\nabla^2 g+2\nabla\psi\cdot\nabla g+g\,\nabla^2\psi\Big)+V\psi g, \tag{D.3}$$

and

$$(H\psi)\, g=-\frac{\hbar^2}{2m}g\nabla^2\psi+V\psi g. \tag{D.4}$$

Subtracting Eq. (D.4) from (D.3) gives

$$H(\psi g)-(H\psi)\, g=-\frac{\hbar^2}{2m}\Big(\psi\,\nabla^2 g+2\nabla\psi\cdot\nabla g\Big). \tag{D.5}$$

Substituting Eq. (D.5) into (D.2) yields

$$M_\psi^{-1}\left(\frac{\partial}{\partial t}+\frac{i}{\hbar}H\right)M_\psi\, g=\frac{\partial g}{\partial t}+\frac{i}{\hbar}\psi^{-1}\left[-\frac{\hbar^2}{2m}\Big(\psi\,\nabla^2 g+2\nabla\psi\cdot\nabla g\Big)\right] \tag{D.6}$$

$$=\frac{\partial g}{\partial t}-\frac{i\hbar}{2m}\,\nabla^2 g-\frac{i\hbar}{m}\,\frac{\nabla\psi}{\psi}\cdot\nabla g. \tag{D.7}$$

The operator acting on g on the right-hand side of Eq. (D.7) is precisely the bi-directional generator L_b of the Nelson process with $\mathbf{v}_q=-\dfrac{i\hbar}{m}\nabla\ln\psi$, i.e.,

$$L_b g=-\frac{i\hbar}{m}\,\frac{\nabla\psi}{\psi}\cdot\nabla g-\frac{i\hbar}{2m}\,\nabla^2 g,$$

so that

$$M_\psi^{-1}\left(\frac{\partial}{\partial t}+\frac{i}{\hbar}H\right)M_\psi=\frac{\partial}{\partial t}+L_b,$$

which establishes (3.194).

Finally, by the definition of the norm

$$\|g\|_{L^{2,1}(|\psi|^2)}\coloneqq\|\psi g\|_{L^{2,1}},$$

the multiplication operator M_ψ is an isometry from $L^{2,1}(|\psi|^2)$ onto $L^{2,1}$. Since ψ never vanishes, M_ψ^{-1} (multiplication by ψ^{-1}) is well defined and M_ψ is bijective. Therefore, the two operators are unitarily equivalent.

Proof of the Remark 2

Let $\phi(\mathbf{x},t)$ be any solution of the Schrödinger equation. Define $f=\phi/\psi$. Then $\phi=M_\psi f$, and because ϕ satisfies

$$\left(\frac{\partial}{\partial t}+\frac{i}{\hbar}H\right)\phi=0,$$

apply M_ψ^{-1} on the left and use the unitary equivalence identity to obtain

$$\left(\frac{\partial}{\partial t}+L_b(\psi)\right)f=M_\psi^{-1}\left(\frac{\partial}{\partial t}+\frac{i}{\hbar}H\right)M_\psi f=M_\psi^{-1}\left(\frac{\partial}{\partial t}+\frac{i}{\hbar}H\right)\phi=0.$$

Thus, every Schrödinger solution ϕ produces a solution $f=\phi/\psi$ of the stochastic evolution equation $\Big(\partial_t+L_b(\psi)\Big)f=0$.

Finally, consider the stationary eigenbasis case. Suppose $H\phi_n=E_n\phi_n$ and take a stationary, nodeless reference state $\psi(\mathbf{x},t)=\psi_0(\mathbf{x})e^{-iE_0t/\hbar}$ (for instance the ground state). Then

$$\phi_n(\mathbf{x},t)=\phi_n(\mathbf{x})e^{-iE_nt/\hbar},$$

and their ratio is

$$f_n(\mathbf{x},t) = \frac{\phi_n(\mathbf{x},t)}{\psi(\mathbf{x},t)} = \frac{\phi_n(\mathbf{x})}{\psi_0(\mathbf{x})}\, e^{-i(E_n-E_0)t/\hbar}.$$

Since ϕ_n satisfies the Schrödinger equation, the same argument above yields

$$\left(\frac{\partial}{\partial t} + L_b(\psi)\right) f_n = 0.$$

Hence, the eigenvalue/eigenfunction data (E_n, ϕ_n) of H are carried into the L_b-representation as the time-harmonic stochastic modes f_n by the unitary map M_ψ. No additional state-dependent family of transformations is needed, the single multiplication operator M_ψ is responsible for the unitary transport of spectral information.

APPENDIX E – NUMERICAL SOLUTION OF THE QUANTUM HAMILTON EQUATIONS

Here we describe the numerical procedure used to solve the quantum Hamilton equations for stationary states (i.e., with vanishing current velocity $\mathbf{v} = 0$), presented in Sec. 3.3.3.1. These equations take the form

$$dx(t) = u(x(t))dt + \sigma dW(t), \qquad x(0) = x_0, \tag{E.1}$$

$$du(x(t)) = \frac{1}{m}\frac{dV(x(t))}{dx}dt + \frac{q(x(t))}{m}dW_*(t), \qquad u(x(T)) = 0, \tag{E.2}$$

where $\sigma^2 = \hbar/m$,

$$q(x(t)) = \sqrt{\hbar m}\ \left.\frac{du(x)}{dx}\right|_{x=x(t)},$$

and $u(x)$ denotes the osmotic velocity and $V(x)$ the potential acting on the particle. Equation (E.2) constitutes a system of coupled forward–backward stochastic differential equations (FBSDEs). Solving this system provides the osmotic velocity $u(x)$ directly, and the resulting solution is equivalent to the osmotic velocity obtained from the stationary wavefunction solving the Schrödinger equation. A full derivation and mathematical justification of the method can be found in Refs. [17, 83, 149].

The numerical method is iterative. Assume that an approximation $u^{j-1}(x)$ has been obtained at iteration step $j-1$. Iteration j proceeds as follows. The spatial domain $[x_{\min}, x_{\max}]$ is partitioned into L subintervals, $D_l \coloneqq [x_{\min} + (l-1)\delta,\ \ x_{\min} + l\delta]$ for $l = 1, \ldots, L$, where the grid spacing δ is given by

$$\delta = \frac{x_{\max} - x_{\mathrm{mim}}}{L}. \tag{E.3}$$

We first generate a forward trajectory for the process $x(t)$ using the Heun method for SDEs [124]. We discretize the time interval as $\Delta t_i \coloneqq t_{i+1} - t_i$, for $i = 0, \ldots, N-1$, with $t_0 = 0$ and $t_N = T$. After nondimensionalizing the forward equation for $x(t)$, the Heun scheme reads

$$\begin{aligned} x^j(0) &= x_0, \\ \tilde{x}^j(t_{i+1}) &= x^j(t_i) + \Delta t_i\, u^{j-1}(x^j(t_i)) + \Delta W_i^j, \\ x^j(t_{i+1}) &= x^j(t_i) + \frac{\Delta t_i}{2}\left[u^{j-1}(x^j(t_i)) + u^{j-1}(\tilde{x}^j(t_{i+1}))\right] + \Delta W_i^j, \end{aligned} \tag{E.4}$$

for $i = 0, \ldots, N-1$ and $j = 1, \ldots, N_{\mathrm{iter}}$, where N_{iter} is the number of iterations. The terms $\Delta W_i^j = W^j(t_{i+1}) - W^j(t_i)$ are increments of a Wiener process, sampled as Gaussian random variables with mean zero and variance Δt_i for each iteration j.

The backward equation in Eq. (E.2) is discretized using the Euler-Maruyama method (see Sec. 5.1.2). The resulting scheme reads

$$u^j(t_N) = u^{j-1}(x^j(t_N)), \quad q^j(t_N) = 0, \tag{E.5}$$

$$u^j(t_i) = u^j(t_{i+1}) - \Delta\, t_i \frac{dV(x)}{dx}\bigg|_{x=x^j(t_i)} - q^j(t_i)\Delta W_i^j, \tag{E.6}$$

Equation (E.6) cannot be solved uniquely because both $u^j(t_i)$ and $q^j(t_i)$ are unknown at each discrete time step [150]. Nevertheless, the process $q(t)$ must guarantee the adaptation of $u(t)$—a functional of the forward process $x(t)$—to the filtration generated by x (see Sec. 2.2.3 for the definition of filtration). To extract $q^j(t_i)$, we multiply Eq. (E.6) by ΔW_i^j and take the conditional expectation with respect to the filtration $\mathcal{F}_i$ generated by the forward process up to time t_i. Using the property $(\Delta W)^2 \sim \Delta t$ and the fact that $\mathbb{E}[\Delta W_i^j|\mathcal{F}_i] = 0$, we obtain

$$\begin{aligned} q^j(x^j(t_i)) &= \frac{1}{\Delta t_i}\mathbb{E}\left[u^j(x^j(t_{i+1}))\Delta W_i^j \middle| \mathcal{F}_i\right] \\ &= \frac{1}{\Delta t_i}\mathbb{E}\left[u^j(x^j(t_{i+1}))\Delta W_i^j \middle| x^j(t_i)\right], \end{aligned} \tag{E.7}$$

which expresses q^j as a conditional expectation conditioned only on the current forward position, once the process $x(t)$ is Markovian. To approximate this conditional expectation numerically, we generate an ensemble of M forward trajectories in the j-th iteration, denoted by $x^{j,m}(t_i)$ with $m = 1, \ldots, M$. For each sample trajectory, we define

$$q^{j,m}(t_i) = q^j(x^{j,m}(t_i)), \tag{E.8}$$

as the m-th realization of $q^j(t_i)$. The conditional expectation satisfies the property $\mathbb{E}[Y|X] = f(X)$, where the function $f(X)$ is characterized as the minimizer of the mean-square error,

$$f = \arg\min_{\nu}\, \mathbb{E}[\,|\nu(X) - Y|^2], \tag{E.9}$$

with the minimization taken over all measurable functions ν such that $\mathbb{E}[\,|\nu(X)|^2\,] < \infty$ [149]. Following this regression approach for conditional expectations, and adopting a least-squares approximation scheme [149], the quantity $q^{j,m}(t_i)$ is estimated as

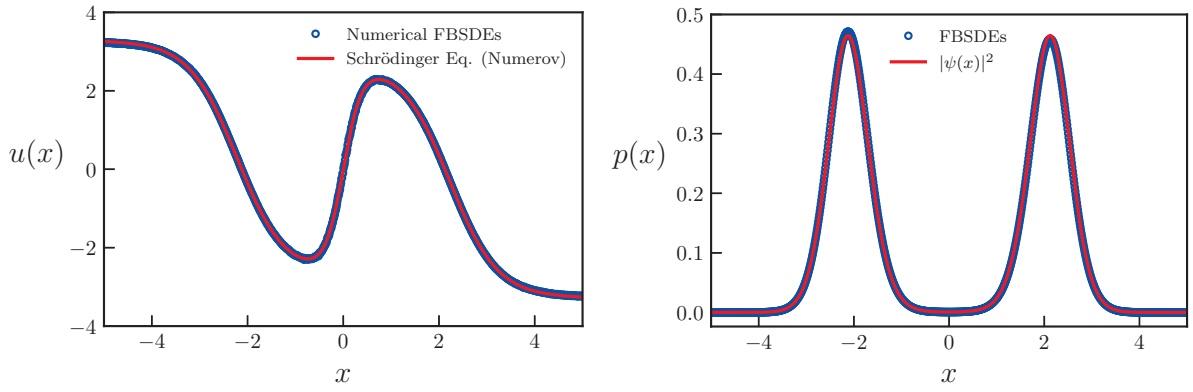
$$q^{j,m}(t_i) = \frac{1}{\Delta t_i}\alpha_i^j\, \eta(x^{j,m}(t_i)), \tag{E.10}$$

where the coefficient

$$\alpha_i^j = \frac{1}{M}\sum_{m=1}^{M} \eta(x^{j,m}(t_i))\, u^{j,m}(t_{i+1})\, \Delta W_i^{j,m} \tag{E.11}$$

is computed through a sample average, and $\eta(x)$ is an indicator function of the partition of the spatial domain defined as

$$\eta(\cdot) = \left(\mathbb{1}_{D_l}(\cdot)\right)_{l=1,\ldots,L}, \tag{E.12}$$



(a) (b)

FIGURE 40 – Left: osmotic velocity of the ground state of the Rosen–Morse potential with parameters $A = 400$ cm^{-1}, $B = 2800$ cm^{-1}, $d = 17$ pm, and $k = 2.22$. The result obtained from the numerical solution of the FBSDEs, defining the quantum Hamilton equations (blue circles), is shown together with the osmotic velocity computed directly from the ground-state wave function obtained via the Numerov method applied to the Schrödinger equation (red line). Right: corresponding probability distributions, calculated either from $p(x) = |\psi(x)|^2$ (red line) or by integrating the numerically evaluated osmotic velocity (blue circles). Values in dimensionless units ($\hbar = m = d = 1$).

where

$$\mathbb{1}_{D_l}(x) = \begin{cases} 1, & x \in D_l, \\ 0, & \text{otherwise.} \end{cases} \tag{E.13}$$

Thus, $\eta(x^{j,m}(t_i))$ singles out the interval D_l to which the forward position belongs at time t_i. With this approximation for $q^{j,m}(t_i)$, the backward integration scheme for the m-th trajectory becomes

$$\begin{aligned} u^{j,m}(t_N) &= u^{j-1}(x^{j,m}(t_N)), \quad q^{j,m}(t_N) = 0, \\ u^{j,m}(t_i) &= u^{j,m}(t_{i+1}) - \Delta t_i \left.\frac{dV(x)}{dx}\right|_{x=x^{j,m}(t_i)} - q^{j,m}(t_i)\Delta W_i^{j,m}, \\ i &= N-1,\ldots,0, \quad m = 1,\ldots,M, \quad j = 1,\ldots,N_{\text{iter}}. \end{aligned} \tag{E.14}$$

After finishing the backward sweep of iteration j, the updated approximation of the osmotic velocity is obtained by averaging all values $u^{j,m}(t_i)$ that fall within the same spatial subinterval D_l. As noted in Ref. [149], reliable estimation of the conditional expectation requires a large number of sample paths. In particular, the number of trajectories should scale at least quadratically with the number of time steps, $M = \mathcal{O}(N^2)$.

This iterative forward–backward scheme yields the osmotic velocity corresponding to the ground-state solution associated with the potential $V(x)$ and is fully equivalent to the solution obtained from the stationary Schrödinger equation.

We present in Fig. 40(a) the result for the osmotic velocity of the ground state of the Rosen-Morse potential defined in Eq. (6.86), with parameters $A = 400\ \mathrm{cm}^{-1}$, $B = 2800\ \mathrm{cm}^{-1}$, $d = 17$ pm and $k = 2.22$, as discussed in Sec. 6.5.1. The osmotic velocity was obtained by applying the numerical procedure introduced here to solve the FBSDEs of the quantum Hamilton equations. The parameters were set as $N = 10^2$, $M = 10^6$, and $L = 3 \times 10^3$. A number of 10 iterations were enough for the convergence of the method. The result exhibits excellent agreement with the corresponding quantity computed directly from the ground-state wavefunction obtained via the Numerov solution [130, 131] of the stationary Schrödinger equation. The probability density can be reconstructed directly from the osmotic velocity through the relation

$$p(x) = C \exp\left(\frac{2m}{\hbar}\int_{-\infty}^{x} u(x')dx'\right), \tag{E.15}$$

where the normalization constant C is determined from

$$\int_{-\infty}^{\infty} p(x)dx = 1. \tag{E.16}$$

Figure 40(b) compares the ground-state probability density obtained from the wavefunction, $p(x) = |\psi(x)|^2$, with the probability density reconstructed from the osmotic velocity, computed numerically with the method presented here, using Eq. (E.15). Once again, the level of agreement is remarkably good. The excellent agreement between the two approaches validates the numerical scheme for solving the FBSDEs in this potential.

Applying the SUSY formalism presented in Sec. 3.5, the same numerical method can be extended to solve the FBSDEs associated with the excited states. Having obtained the ground-state osmotic velocity $u_0(x)$ for the potential $V(x)$, we construct the SUSY partner potential

$$V_1(x) = V(x) - \hbar\frac{du_0(x)}{dx}, \tag{E.17}$$

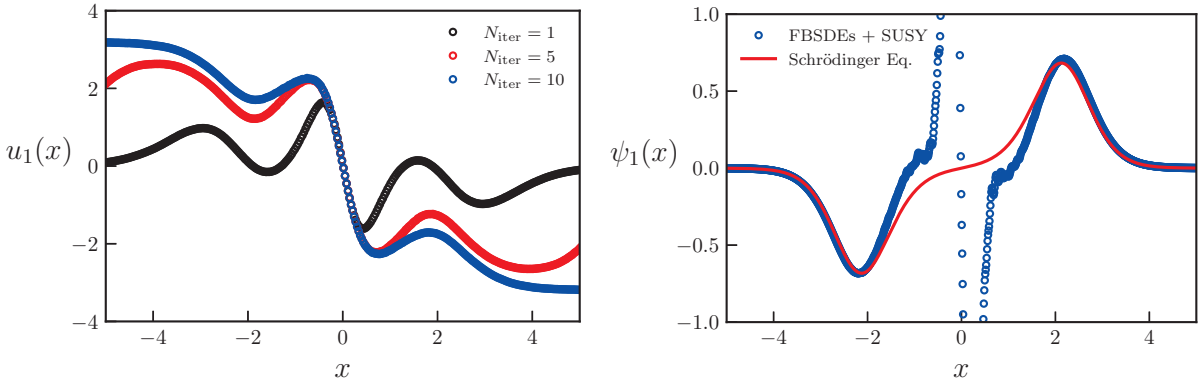
where $u_0(x)$ is computed numerically as described above. Applying the same forward-backward scheme to the potential $V_1(x)$ yields the osmotic velocity $u_1(x)$ associated with the ground state of the SUSY partner Hamiltonian. From $u_1(x)$, the ground-state wavefunction of the SUSY partner system, $\varphi_0^1(x)$, follows from

$$\varphi_0^1(x) = c_0 \exp\left(\frac{m}{\hbar}\int_{-\infty}^{x} u_1(x')dx'\right), \tag{E.18}$$

with normalization constant c_0. Using the standard SUSY relation, the first excited state of the original Hamiltonian is then reconstructed as

$$\psi_1(x) = \sqrt{\frac{m}{2(E_1 - E_0)}}\left(u_0(x) + \frac{\hbar}{m}\frac{d}{dx}\right)\varphi_0^1(x). \tag{E.19}$$

The associated eigenenergies are obtained from the averaging procedure described in Eq. (3.209).



(a) (b)

FIGURE 41 – Left: osmotic velocity $u_1(x)$ associated with the ground state of the SUSY partner potential $V_1(x)$, obtained from the numerical solution of the FBSDEs. Results for three different values of the iteration number are displayed, illustrating the convergence behavior of the numerical scheme. Right: wave function of the first excited state of the original Hamiltonian for the Rosen-Morse potential, reconstructed from the SUSY formalism using the numerically evaluated osmotic velocity $u_1(x)$ (blue circles), and compared with the corresponding solution obtained from the direct numerical integration of the Schrödinger equation via the Numerov method (red line). The comparison highlights both the accuracy and the limitations of the SUSY–FBSDE approach, particularly near the node of the excited state. Values in dimensionless units ($\hbar = m = d = 1$).

Considering $V(x)$ as the Rosen-Morse potential as above, Fig. 41(a) shows the convergence of the osmotic velocity $u_1(x)$ as the number of iterations in the FBSDEs scheme is increased. Additionally, Fig. 41(b) shows the first excited-state wavefunction obtained through the SUSY-based FBSDEs approach, together with the corresponding wave function obtained by solving the Schrödinger equation via the Numerov method [130, 131]. The parameters were set as $N = 10^2$, $M = 10^6$, and $L = 10^3$. For the first excited state, we observe that the FBSDEs solution exhibits a divergence near the node at $x = 0$. This behavior arises from the sensitivity of the SUSY reconstruction to the choice of numerical parameters, particularly in the vicinity of the nodes of excited states, where small numerical deviations in the osmotic velocity are amplified upon integration. This scheme can be further extended to higher excited states by iteratively applying the SUSY construction.

A numerical method for solving the nonlinear differential equation (3.148) satisfied by the osmotic velocity $u(x)$ was introduced in Ref. [83]. However, in our tests, that method showed slow or difficult convergence. Applications of the FBSDEs-based approach to the harmonic oscillator, the quartic double-well potential, and the Hydrogen atom are discussed in Refs. [14, 17, 89]. A comparable numerical algorithm for solving the quantum Hamilton equations in the non-stationary case ($\mathbf{v} \neq 0$) is, to date, not yet feasible [83].