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# Quantum Monte Carlo study of the continuously monitored two-dimensional dissipative Ising model in a transverse field

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*Ai miei genitori e a mia sorella, per il loro continuo supporto.*

# Abstract

Cold dilute gases represent one of the most powerful platforms for quantum simulation, owing to the unparalleled accuracy and precision with which they can be manipulated via electromagnetic fields. A prominent application is found in optical lattice clocks, where such control enables state-of-the-art metrological performance. The theoretical description of the out-of-equilibrium dynamics of these systems poses a significant computational challenge, which has been recently addressed by the open time-dependent variational Monte Carlo (otVMC) method [arXiv:2506.23928], capable of providing numerically accurate simulations of open many-body quantum dynamics. In this thesis, we extend the otVMC framework to encompass the dynamics of open quantum systems subject to continuous measurement, substantially broadening the class of experimentally relevant regimes accessible to numerical investigation. Continuously monitored quantum systems occupy a central role in modern quantum science, as measurement backaction gives rise to rich phenomenology — including measurement-induced phase transitions and nontrivial entanglement dynamics — that lies beyond the reach of standard Lindbladian descriptions. As a primary testbed, we consider the continuously monitored dissipative two-dimensional transverse-field Ising model. We develop a numerical implementation of the extended algorithm and subject it to systematic benchmarking, with the aim of assessing its accuracy and scalability. The central objective of this work is to extend and validate the otVMC framework for continuously monitored two-dimensional open quantum systems, with particular attention to the accurate estimation of magnetizations, variances, and covariances, which constitute the basic ingredients for future studies of spin squeezing and entanglement dynamics. Particular attention is devoted to the interplay between coherent driving, dissipation, and measurement backaction.

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# Introduction

Quantum mechanics provides an extraordinarily successful framework for describing the behavior of microscopic systems. However, both analytical and numerical studies of quantum systems often become challenging as problem complexity increases. In its original formulation, quantum mechanics describes isolated systems that evolve independently of their surroundings. In practice, however, perfect isolation is rarely achieved, as any realistic quantum system inevitably interacts with its environment. This limitation has motivated the development of the theory of open quantum systems, which explicitly accounts for the influence of environmental degrees of freedom on the system dynamics.

The inclusion of environmental interactions gives rise to physical phenomena that are absent in closed-system dynamics, such as decoherence and dissipation. These effects play a fundamental role in determining the behavior of realistic quantum devices and often represent the main obstacle to preserving genuinely quantum features, including coherence and entanglement. On the other hand, engineered dissipation can also be willingly employed to realize useful quantum states. A thorough understanding of open quantum systems is therefore essential for the development of modern quantum technologies, ranging from quantum computation and quantum simulation to quantum sensing and metrology.

From a computational perspective, the study of many-body quantum systems is hindered by the exponential growth of the Hilbert space with system size. This challenge becomes even more severe in open quantum systems, whose states are described by density matrices rather than pure state vectors, leading to an even larger computational complexity. As a consequence, the investigation of large-scale open quantum systems requires the adoption of efficient approximation techniques capable of balancing accuracy and computational cost.

A promising approach is provided by the combination of variational methods and Monte Carlo techniques. In particular, the framework introduced in Ref. [1, 2]

combines the quantum trajectory formalism with the time-dependent variational Monte Carlo method. This strategy offers several advantages. First, it enables the use of flexible variational ansätze capable of capturing relevant correlations while maintaining a manageable computational cost. Second, it significantly reduces memory requirements by evolving pure-state trajectories instead of the full density matrix. Finally, the statistical independence of different trajectories naturally allows for efficient parallelization, making the method particularly suitable for large-scale simulations on modern high-performance computing architectures.

An additional advantage of the quantum trajectory formalism is its ability to describe conditional dynamics. Such dynamics arise when specific channels of interaction between the system and its environment are continuously monitored, and the acquired measurement information is incorporated into the system description. Conditional dynamics play a central role in many contemporary quantum technologies, including quantum feedback control, state preparation protocols, error-correction schemes, and measurement-based quantum information processing, where monitoring can be exploited to enhance performance and stabilize desired quantum states.

The objective of this thesis is to extend the method proposed in Ref. [3] for solving monitored dynamics with otVMC, to two-dimensional systems and to apply it to the paradigmatic case of a long-range dissipative transverse-field Ising model. This model provides an ideal testbed for investigating the interplay between interactions, quantum fluctuations, and dissipation in many-body systems. By combining variational Monte Carlo techniques with the quantum trajectory approach, this work aims to expand the range of open quantum systems that can be studied efficiently and to provide new insights into their conditional and dissipative dynamics.

## Thesis structure

- **Chapter 1: Open Quantum Systems** This chapter introduces the theoretical framework used to describe open quantum systems. After presenting the Lindblad master equation, the discussion focuses on continuously monitored dynamics, stochastic master equations, quantum trajectories, and the relation between Itô and Stratonovich formulations. This provides the physical background required for the treatment of conditional dynamics.
- **Chapter 2: Quantum Monte Carlo Methods** This chapter reviews the basic Monte Carlo techniques used throughout the thesis. Starting from crude

Monte Carlo and importance sampling, the discussion introduces Markov chains and the Metropolis–Hastings algorithm. This chapter also presents the variational Monte Carlo framework for quantum many-body systems. The variational parametrization of the wave function is introduced together with the local estimators of physical observables. The time-dependent variational Monte Carlo method is then derived.

- **Chapter 3: Open time-dependent Variational Monte Carlo** This chapter extends the variational approach to monitored open quantum systems. The otVMC equations of motion are derived from the stochastic Schrödinger equation in Stratonovich form, leading to a stochastic evolution for the variational parameters. The role of monitored and unmonitored channels is discussed, together with the estimators required to compute observables along individual quantum trajectories.
- **Chapter 4: Numerical Implementation** This chapter describes the numerical implementation of the method. The main components of the code are presented, including the representation of the Hamiltonian and jump operators, the variational wave function, the sampling procedure, and the integration of the stochastic equations of motion. The treatment of numerical stability, regularization, parallelization, and random-number generation is also discussed.
- **Chapter 5: Results** This chapter presents the numerical benchmarks and applications of the method. The otVMC results are compared with exact or reference solutions whenever available, both for unconditional and conditional dynamics. The analysis includes the convergence with respect to the number of trajectories, the study of monitored observables, and the behaviour of nonlinear quantities such as variances and covariances.

# Chapter 1

## Open Quantum Systems

This chapter introduces the theoretical framework of open quantum systems [4, 5], providing the essential concepts and mathematical tools required for the discussion of the numerical methods developed in this thesis. After reviewing the density operator formalism, which extends the standard description of quantum mechanics to systems interacting with an external environment, several key concepts such as entanglement and quantum maps are briefly introduced. These notions naturally lead to the description of Markovian open-system dynamics through the Lindblad master equation, which represents one of the most widely used models for dissipative quantum evolution.

Particular attention is devoted to the stochastic unraveling of the Lindblad equation and to the resulting stochastic Schrödinger equations (SSEs). Rather than pursuing a mathematically rigorous derivation, the presentation aims to provide the physical intuition underlying the stochastic description of open-system dynamics. This perspective directly connects to the quantum trajectory formalism, which constitutes the conceptual foundation of the numerical approach presented in the following chapter.

The discussion is not intended to be exhaustive; instead, it aims to be sufficiently self-contained to provide the necessary background for understanding the methods and results developed throughout the remainder of this thesis.

## 1.1 Introduction

Quantum mechanics provides an extraordinarily successful framework for describing the behavior of microscopic systems. In its standard formulation, however, it primarily addresses idealized isolated systems, whose evolution is governed solely by their intrinsic dynamics. While this assumption is often appropriate for developing fundamental concepts, it is rarely fulfilled in realistic physical situations. Any experimental quantum system inevitably interacts, to some extent, with external degrees of freedom such as measurement devices, electromagnetic fields, thermal reservoirs, or other uncontrolled environmental influences.

The theory of open quantum systems extends the conventional quantum-mechanical description to account for these interactions with the surrounding environment. Rather than treating the system of interest as completely isolated, this framework explicitly incorporates the effects of external degrees of freedom, allowing one to describe phenomena that cannot be captured within the closed-system paradigm. These include dissipation [6], decoherence [7], relaxation processes, and the emergence of non-equilibrium steady states, all of which play a central role in modern quantum technologies and many-body physics.

The study of open quantum systems has become increasingly important across a wide range of disciplines, including quantum optics [8], condensed matter physics, quantum information science [9], and quantum simulation [10, 11]. Beyond its practical relevance for interpreting experimental observations, it also provides a fundamental framework for understanding how quantum systems behave under realistic conditions and how coherent quantum dynamics competes with environmental noise and dissipation.

Given the broad scope and complexity of the subject, the present chapter does not aim to provide a comprehensive review of the theory of open quantum systems. Instead, its purpose is to introduce the essential concepts and formalism required for the discussion developed in the subsequent chapters. In this sense, the chapter is intended to be self-contained, providing the necessary theoretical background for understanding the numerical methods employed throughout this thesis, with particular emphasis on the numerical approach presented in the following chapters.

## 1.2 Mathematical Framework

### 1.2.1 Density Operator

The mathematical description of closed quantum systems is based on the Schrödinger equation,

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad (1.1)$$

where all the information about the state of the system is encoded in the state vector  $|\psi(t)\rangle$ , which belongs to the system Hilbert space  $\mathcal{H}$ . The Hamiltonian operator  $\hat{H}$  is Hermitian and generates a unitary time evolution, ensuring the conservation of the norm of the state vector. Such states are commonly referred to as pure states.

In realistic physical situations, however, a quantum system is rarely completely isolated from its surroundings. Interactions with external degrees of freedom generally lead to non-unitary dynamics, making the state-vector description insufficient. A more general framework is therefore required, which is provided by the density operator formalism. For a pure state, the density operator is defined as

$$\hat{\rho}(t) = |\psi(t)\rangle \langle \psi(t)|$$

while for a statistical ensemble of pure states it takes the form

$$\hat{\rho}(t) = \sum_i p_i(t) |\psi_i(t)\rangle \langle \psi_i(t)|$$

where  $p_i(t) \geq 0$  denotes the probability of finding the system in the pure state  $|\psi_i(t)\rangle$  and  $\sum_i p_i = 1$ . States described by such statistical mixtures are referred to as mixed states.

The density operator possesses several fundamental properties that guarantee its physical interpretation. First, its **trace is equal to one**,

$$\text{Tr}[\hat{\rho}] = 1$$

which reflects the conservation of total probability. Furthermore, **it is Hermitian**,

$$\hat{\rho} = \hat{\rho}^\dagger$$

and **positive semidefinite**, implying that all its eigenvalues are non-negative. Finally, the density operator allows the computation of expectation values of observables through the relation

$$\langle \hat{A} \rangle = \text{Tr}[\hat{A}\hat{\rho}]$$

The density matrix formalism naturally generalizes the Schrödinger description and provides a convenient framework for both closed and open quantum systems. In particular, for isolated systems the evolution of the density operator is governed by the von Neumann equation,

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] \quad (1.2)$$

which is completely equivalent to the Schrödinger equation.

## 1.2.2 Entanglement

Entanglement is one of the most distinctive features of quantum mechanics and plays a central role in the theory of open quantum systems. Although a comprehensive discussion is beyond the scope of this thesis, it is useful to briefly introduce the concept and its relevance.

Consider a bipartite quantum system composed of two subsystems A and B, with Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$  respectively. A pure state  $|\psi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$  is said to be separable if it can be expressed as the tensor product of two subsystem states,

$$|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\phi\rangle_B$$

If such a decomposition does not exist, the state is said to be entangled.

The notion of separability can be extended to mixed states described by a density operator. A bipartite density matrix is separable if it can be written as a convex combination of product states,

$$\hat{\rho}_{AB} = \sum_k p_k \hat{\rho}_A^k \otimes \hat{\rho}_B^k$$

where  $p_k \geq 0$ . States that cannot be expressed in this form are entangled.

Entanglement is of fundamental importance not only in quantum information theory but also in the study of open quantum systems. Interactions between a system and its environment generally generate correlations that can be understood in terms of

entanglement. As a consequence, entanglement plays a crucial role in phenomena such as decoherence, dissipation, and information exchange between the system and its surroundings.

### 1.2.3 Quantum Maps

In closed quantum systems, the evolution of the state is described by unitary transformations generated by the system Hamiltonian. The presence of an environment, however, requires a more general description capable of accounting for non-unitary processes. In this context, the dynamics of quantum states are described by quantum maps, also known as quantum operations.

A physically admissible quantum map must be linear, completely positive, and trace non-increasing. Complete positivity represents a fundamental requirement that extends the notion of ordinary positivity. While a positive map sends positive operators into positive operators, complete positivity ensures that positivity is preserved even when the map acts on only a part of a larger composite system.

More precisely, let  $\phi$  be a map acting on the states of a quantum system. Complete positivity requires that, for every integer  $n$ , the extended map  $\phi \otimes \mathbb{I}_{\mathbb{C}^n}$  remains positive. This condition guarantees that the evolution of a subsystem does not lead to unphysical states when the subsystem is entangled with additional degrees of freedom. Since open quantum systems are naturally embedded in larger environments, complete positivity is an essential requirement for any physically meaningful dynamical description.

The second important property concerns the trace of the density operator. Quantum maps are generally required to be trace non-increasing, allowing the description of probabilistic processes such as measurements, post-selection procedures, or loss mechanisms. When the trace is preserved for all input states, the map describes a deterministic physical evolution and is referred to as a quantum channel.

Quantum maps provide the most general framework for describing the evolution of open quantum systems and constitute the foundation upon which master equations and stochastic unraveling are built.

### 1.2.4 Open quantum evolution

The starting point in the description of an open quantum system is the decomposition of the total Hilbert space into a system and an environment,

$$\mathcal{H}_{\text{tot}} = \mathcal{H}_S \otimes \mathcal{H}_E$$

The dynamics of the combined system is assumed to be unitary and generated by the total Hamiltonian

$$\hat{H}_T = \hat{H}_S \otimes \hat{\mathbb{I}}_E + \hat{\mathbb{I}}_S \otimes \hat{H}_E + \hat{V}$$

where  $\hat{H}_S$  and  $\hat{H}_E$  describe the free evolution of the system and environment respectively, while  $\hat{V}$  accounts for their interaction.

In principle, the state of the composite system is described by a density operator  $\rho_T$  evolving according to the von Neumann equation (1.2). However, the environmental degrees of freedom are typically inaccessible and one is interested only in the state of the system. The latter is obtained through the partial trace over the environment,

$$\hat{\rho}_S = \text{Tr}_E [\hat{\rho}_T]$$

The reduced dynamics of  $\hat{\rho}_S$  is generally non-unitary and depends on the properties of the environment and its interaction with the system. Under suitable assumptions, discussed below, it can be described by the Lindblad master equation.

## 1.3 The Lindblad Master Equation

A central result in the theory of open quantum systems is the Lindblad master equation, which provides a general description of the dynamics of Markovian quantum systems. As discussed in the previous section, the interaction between a quantum system and its environment prevents, in general, a description based solely on the Schrödinger equation for a pure state. Instead, the state of the system must be represented by a density operator whose evolution accounts for both coherent and incoherent processes.

Under suitable assumptions, namely weak coupling between the system and the environment, negligible memory effects in the bath, and a clear separation of timescales between system and environment dynamics, the reduced dynamics of the system can be shown to form a quantum dynamical semigroup. The most general generator of

such dynamics that preserves positivity, complete positivity, and trace conservation is given by the Lindblad equation. A rigorous derivation is beyond the scope of the present work. The interested reader is referred to the standard literature on open quantum systems, particularly Refs. [4, 12]. In the following, only the main assumptions and physical interpretation of the equation are discussed.

The evolution of the density matrix is therefore governed by

$$\frac{d\hat{\rho}(t)}{dt} = -i[\hat{H}, \hat{\rho}(t)] + \sum_k \left( \hat{L}_k \hat{\rho}(t) \hat{L}_k^\dagger - \frac{1}{2} \{ \hat{L}_k^\dagger \hat{L}_k, \hat{\rho}(t) \} \right) \quad (1.3)$$

Here and in the following we consider units for which  $\hbar = 1$ . The Hamiltonian  $\hat{H}$  in the first term is called the effective Hamiltonian. In general, other than the free evolution Hamiltonian of the system  $\hat{H}_S$ , it contains additional terms due to the interaction with the environment. The term  $-i[\hat{H}, \hat{\rho}]$  therefore describes the coherent evolution in accordance with von Neumann equation (1.2). On the other hand,  $\hat{L}_k$  is a set of operators commonly referred to as Lindblad operators or jump operators. Each Lindblad operator represents a specific dissipation channel through which the system exchanges information or energy with the environment. Depending on the physical context, these processes may correspond to spontaneous emission, particle losses, dephasing, or other irreversible mechanisms.

An important feature of the Lindblad equation is that it guarantees the physical consistency of the density matrix throughout the evolution. In particular, the trace of the density matrix remains conserved, while positivity and complete positivity are preserved at all times. These properties are essential for maintaining a valid probabilistic interpretation of the quantum state.

The Lindblad formalism also provides a clear physical picture of open-system dynamics. The coherent evolution generated by the Hamiltonian competes with stochastic environmental processes described by the jump operators. This interplay gives rise to phenomena that are absent in isolated systems, such as decoherence and dissipation. Decoherence suppresses quantum superpositions through the loss of phase information to the environment, while dissipative processes lead to irreversible energy exchange and relaxation toward stationary states.

## 1.4 Stochastic Master Equations

An alternative and particularly insightful description of open quantum systems is provided by the framework of *Stochastic Master Equations (SMEs)*. While the Lindblad master equation describes the average evolution of an ensemble of identically prepared systems, SMEs aim at describing the evolution of an individual realization of the dynamics conditioned on the information extracted from the environment.

A useful distinction can therefore be made between two different levels of description:

- **Unconditional dynamics**, where no information about the environment is available. In this case the state of the system is described by the reduced density matrix and evolves according to the Lindblad master equation.
- **Conditional dynamics**, where the environment is continuously monitored and the measurement outcomes are recorded. The state of the system is then conditioned on the observed measurement record and evolves according to a stochastic equation.

### 1.4.1 Derivation

The derivation employed here follows Ref. [13], for a more rigorous derivation, one may refer to Ref. [4]. As in the previous section, the total Hilbert space is assumed to be the tensor product of the system and environment Hilbert spaces. The total Hamiltonian can therefore be written as

$$\hat{H}_T = \hat{H}_S \otimes \hat{\mathbb{I}}_E + \hat{\mathbb{I}}_S \otimes \hat{H}_E + \hat{V}$$

where  $\hat{H}_S$  describes the system,  $\hat{H}_E$  the environment, and  $\hat{V}$  their interaction.

The environment is modelled as a continuum of bosonic modes characterized by their frequency  $\omega$ . Its free Hamiltonian is

$$\hat{H}_E = \int d\omega \, \omega \, \hat{b}_\omega^\dagger \hat{b}_\omega$$

where  $\hat{b}_\omega$  and  $\hat{b}_\omega^\dagger$  are bosonic operators that satisfy the canonical commutation relations  $[\hat{b}_\omega, \hat{b}_{\omega'}^\dagger] = \delta(\omega - \omega')$ .

The interaction is assumed to be linear in the bosonic field operators,

$$\hat{V} = i \int_0^\infty d\omega \sqrt{\frac{\kappa(\omega)}{2\pi}} (\hat{c} \otimes \hat{b}_\omega^\dagger - \hat{c}^\dagger \otimes \hat{b}_\omega) \quad (1.4)$$

where  $\hat{c}$  is a system operator and  $\kappa(\omega)$  determines the coupling strength between the system and the environmental mode of frequency  $\omega$ .

To simplify the dynamics it is convenient to move to the interaction picture with respect to the free Hamiltonian given by  $\hat{H}_S$  and  $\hat{H}_E$ . Assuming that the dominant system dynamics is characterized by a frequency  $\omega_0$ , the operators evolve approximately as

$$\hat{c}_{\text{int}}(t) = \hat{c} e^{-i\omega_0 t} \quad \hat{b}_{\omega, \text{int}}(t) = \hat{b}_\omega e^{-i\omega t}$$

The interaction Hamiltonian (1.4) then becomes

$$\hat{V} = i \int_0^\infty d\omega \sqrt{\frac{\kappa(\omega)}{2\pi}} (\hat{c} \otimes \hat{b}_\omega^\dagger e^{i(\omega-\omega_0)t} - \hat{c}^\dagger \otimes \hat{b}_\omega e^{-i(\omega-\omega_0)t})$$

At this stage the first Markov approximation is introduced. Physically, it corresponds to assuming that the reservoir possesses a very broad and almost flat spectrum around the characteristic system frequency  $\omega_0$ . This means approximating  $\kappa(\omega) = \kappa$  for  $\omega \in [\omega_0 - \theta, \omega_0 + \theta]$ , while 0 elsewhere. This motivates the introduction of the time-domain field operators

$$\hat{b}_t = \frac{1}{\sqrt{2\pi}} \int_{\omega_0 - \theta}^{\omega_0 + \theta} d\omega \hat{b}_\omega e^{-i(\omega - \omega_0)t}$$

which satisfy the commutation relation

$$[\hat{b}_t, \hat{b}_{t'}^\dagger] = \delta(t - t') \quad (1.5)$$

The interaction Hamiltonian finally acquires the compact form

$$\hat{V}_{\text{int}}(t) = i\sqrt{\kappa}(\hat{c} \otimes \hat{b}_t^\dagger - \hat{c}^\dagger \otimes \hat{b}_t)$$

It is important to note that the commutation relation (1.5) is ill-defined at equal times. To obtain well-defined quantities, one introduces the field increment over a finite time interval  $\delta t$ ,

$$\delta \hat{b}_t = \int_t^{t+\delta t} \hat{b}_s(s) ds.$$

Taking the infinitesimal limit  $\delta t \rightarrow dt$ , the new operator satisfies

$$[\delta \hat{b}_t, \delta \hat{b}_t^\dagger] = \hat{\mathbb{I}} dt \quad (1.6)$$

Finally, it is convenient to introduce a normalized bosonic operator  $\hat{B}_t$  through  $\delta \hat{b}_t = \hat{B}_t \sqrt{dt}$ . The commutation relation then takes the canonical form  $[\hat{B}_t, \hat{B}_t^\dagger] = \hat{\mathbb{I}}$ . Physically,  $\hat{B}_t$  can be interpreted as the annihilation operator associated with the infinitesimal temporal mode of the field contained in the interval  $[t, t + dt]$ . In this picture, the environment can be viewed as a sequence of independent temporal modes, each interacting with the system during an infinitesimal time step  $dt$ .

To derive the effective evolution of the system, we now invoke the Born-Markov approximation. Under this assumption, the interaction between the system and each infinitesimal temporal mode of the environment is sufficiently weak that correlations do not build up over time. Consequently, at any instant, the total state can be approximated as a product state,

$$R(t) = \rho(t) \otimes \mu_t \quad (1.7)$$

where  $\rho(t)$  denotes the reduced state of the system and  $\mu_t$  is the state of the environmental mode interacting with the system. Throughout this derivation, the environment is assumed to be in the vacuum state,  $\mu_t = |0\rangle \langle 0|$ . The evolution of the total density operator is governed by the von Neumann equation (1.2). Equivalently, in the interaction picture, the state after an infinitesimal time interval  $dt$  can be written as

$$R(t + dt) = \hat{U}(t + dt, t) R(t) \hat{U}^\dagger(t + dt, t) \quad (1.8)$$

where the infinitesimal propagator is generated by the interaction Hamiltonian,

$$\hat{U}(t + dt, t) = e^{-i\hat{V}_{\text{int}}(t)dt} = e^{\sqrt{\kappa dt}(\hat{c} \otimes \hat{B}_t^\dagger - \hat{c}^\dagger \otimes \hat{B}_t)}$$

Expanding the exponential up to second order and retaining only contributions of order  $dt$ , one obtains

$$\begin{aligned} \hat{U}(t + dt, t) = & \hat{\mathbb{I}} \otimes \hat{\mathbb{I}} + \sqrt{\kappa dt} (\hat{c} \hat{B}_t^\dagger - \hat{c}^\dagger \hat{B}_t) \\ & + \frac{\kappa}{2} dt (\hat{c}^2 \hat{B}_t^{\dagger 2} + \hat{c}^{\dagger 2} \hat{B}_t^2 - \hat{c} \hat{c}^\dagger \hat{B}_t^\dagger \hat{B}_t - \hat{c}^\dagger \hat{c} \hat{B}_t \hat{B}_t^\dagger) \end{aligned} \quad (1.9)$$

Substituting this expansion into the evolution equation for  $R(t)$  (1.8) together with

the Born-Markov approximation (1.7) yields

$$\begin{aligned}
 R(t + dt) = & \rho(t) \otimes |0\rangle \langle 0| + \sqrt{\kappa} \left( \hat{c} \rho(t) \otimes |1\rangle \langle 0| + \rho(t) \hat{c}^\dagger \otimes |0\rangle \langle 1| \right) \sqrt{dt} \\
 & + \kappa \left( \hat{c} \rho(t) \hat{c}^\dagger \otimes |1\rangle \langle 1| \right) dt \\
 & + \frac{\kappa}{2} \left( \sqrt{2} \hat{c}^2 \rho(t) \otimes |2\rangle \langle 0| - \hat{c}^\dagger \hat{c} \rho(t) \otimes |0\rangle \langle 0| + \text{h.c.} \right) dt
 \end{aligned} \tag{1.10}$$

which represents the infinitesimal evolution of the combined system-environment state.

At this stage the distinction between unconditional and conditional dynamics naturally emerges.

### Unconditional Dynamics

If no measurement is performed on the environment, all information carried away by the bath is discarded. Mathematically, this corresponds to tracing over the environmental degrees of freedom. Performing the partial trace over the bath in the previous equation (1.10) gives

$$\rho(t + dt) = \rho(t) + \kappa \hat{c} \rho(t) \hat{c}^\dagger - \frac{\kappa}{2} \left( \hat{c}^\dagger \hat{c} \rho(t) + \rho(t) \hat{c}^\dagger \hat{c} \right) dt$$

which can be rearranged into the form

$$\frac{d\rho(t)}{dt} = \kappa \mathcal{D}[\hat{c}] \rho(t)$$

where the dissipative superoperator is defined as

$$\mathcal{D}[\hat{c}] \rho = \hat{c} \rho \hat{c}^\dagger - \frac{1}{2} \{ \hat{c}^\dagger \hat{c}, \rho \}$$

This is precisely the Lindblad master equation previously introduced. Therefore, the Lindblad equation can be interpreted as the effective evolution obtained after averaging over all possible environmental outcomes.

The previous derivation can be straightforwardly generalized by including an evolution of the system under a Hamiltonian  $\hat{H}$ . To preserve consistency with the Markov approximation, the characteristic timescale associated with this Hamiltonian evolution should be much longer than the correlation time of the environment. Physically, this ensures that the environmental modes interact with the system

instantaneously compared to the intrinsic evolution generated by  $\hat{H}$ . Furthermore, multiple independent dissipation channels can be incorporated by introducing a set of system operators  $\hat{c}_j$ , each coupled to an independent environmental field and characterized by a decay rate  $\kappa_j$ . In this case, the master equation assumes the general Lindblad form

$$\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t) = -\frac{i}{\hbar}[\hat{H}, \rho(t)] + \sum_j \kappa_j \mathcal{D}[\hat{c}_j]\rho(t)$$

### Conditional Dynamics

The situation changes significantly when the environment is continuously monitored. In this case, the information extracted from the bath is retained rather than discarded, and the state of the system becomes conditioned on the sequence of measurement outcomes. As a consequence, after each infinitesimal interaction the environmental mode associated with the operator  $\hat{B}_t$  is measured. We consider the idealized case of projective measurements on the bath, described by the set of projectors  $\hat{\Pi}_j = |j\rangle\langle j|$ . At each timestep, the conditional reduced state  $\rho_c(t)$  of the system is obtained by projecting the total state  $R(t)$  onto the corresponding environmental outcome  $|j\rangle\langle j|$  and subsequently normalizing the result,

$$\rho_c(t+dt) = \frac{\langle j|R(t+dt)|j\rangle}{p_j(t+dt)} = \frac{\langle j|R(t+dt)|j\rangle}{\text{Tr}[R(t+dt)(\mathbb{I}_S \otimes |j\rangle\langle j|)]} \quad (1.11)$$

Different choices of measurement basis, more generally described by different positive operator-valued measures (POVMs) acting on the environmental mode, lead to different stochastic master equations. Positive operator-valued measures generalize the notion of quantum measurement beyond the case of ideal projective measurements. They associate each possible measurement outcome with a positive operator, with the condition that the sum of all these operators is equal to the identity, so that the total probability of all possible outcomes is normalized. This formalism is particularly useful when the measurement is not described as a direct projection onto orthogonal states, but rather as the result of a more general detection process, possibly involving auxiliary degrees of freedom or an incomplete description of the measuring apparatus. In this sense, a POVM can be understood as an effective description of how information is extracted from the system or from the environment. In the following sections, two important and widely used measurement schemes will be discussed.

### 1.4.2 Photo-Detection Stochastic Master Equation

A possible choice of environmental measurement is obtained by monitoring the bath through a photon detector. In this case the measurement record is not continuous, but consists of a sequence of detection events. This unraveling is known as the *photo-detection* or *quantum-jump* stochastic master equation.

We consider the case in which the environment is continuously monitored by projecting (1.10) onto the Fock basis. Since the interaction is treated over an infinitesimal time interval  $dt$ , only two outcomes are relevant: either no photon is detected, corresponding to the projection onto  $|0\rangle\langle 0|$ , or one photon is detected, corresponding to the projection onto  $|1\rangle\langle 1|$ .

**Measurement result: 0** For the no-detection outcome, the conditional state is obtained by projecting the total density matrix onto the vacuum state of the environment (with the tilde symbol to highlight that this state is not normalized),

$$\tilde{\rho}_0^{(c)}(t+dt) = \langle 0|R(t+dt)|0\rangle = \rho^{(c)}(t) - \frac{\kappa}{2} \left\{ \hat{c}^\dagger \hat{c}, \rho^{(c)}(t) \right\} dt \quad (1.12)$$

The probability associated with this outcome is given by the trace of the unnormalized state,

$$p_0(t+dt) = \text{Tr} \left[ \tilde{\rho}_0^{(c)}(t+dt) \right] = 1 - \kappa \left\langle \hat{c}^\dagger \hat{c} \right\rangle_t dt \quad (1.13)$$

where

$$\left\langle \hat{c}^\dagger \hat{c} \right\rangle_t = \text{Tr} \left[ \rho^{(c)}(t) \hat{c}^\dagger \hat{c} \right] \quad (1.14)$$

The normalized conditional state is therefore, by expanding the denominator and truncating to first order

$$\begin{aligned} \rho_0^{(c)}(t+dt) &= \frac{\tilde{\rho}_0^{(c)}(t+dt)}{p_0(t+dt)} \\ &\approx \left( \rho^{(c)}(t) - \frac{\kappa}{2} \left\{ \hat{c}^\dagger \hat{c}, \rho^{(c)}(t) \right\} dt \right) \left( 1 + \kappa \left\langle \hat{c}^\dagger \hat{c} \right\rangle_t dt \right) \\ &\approx \hat{\rho}^{(c)} - \frac{\kappa}{2} \mathcal{H}[\hat{c}^\dagger \hat{c}] \rho^{(c)} dt \end{aligned} \quad (1.15)$$

where:

$$\mathcal{H}[\hat{A}] \bullet = \hat{A} \bullet + \bullet \hat{A}^\dagger - \left\langle \hat{A} + \hat{A}^\dagger \right\rangle_t \bullet$$

**Measurement result: 1** On the other hand, if one photon is detected, the environment is projected onto the one-photon base. The corresponding unnormalized state is

$$\tilde{\rho}_1^{(c)}(t + dt) = \langle 1 | R(t + dt) | 1 \rangle = \kappa \hat{c} \rho^{(c)}(t) \hat{c}^\dagger dt \quad (1.16)$$

The probability of this event is

$$p_1(t + dt) = \text{Tr} [\tilde{\rho}_1^{(c)}(t + dt)] = \kappa \langle \hat{c}^\dagger \hat{c} \rangle_t dt \quad (1.17)$$

After normalization, the conditional state following a detection event becomes

$$\rho_1^{(c)}(t + dt) = \frac{\hat{c} \rho^{(c)}(t) \hat{c}^\dagger}{\langle \hat{c}^\dagger \hat{c} \rangle_t} \quad (1.18)$$

The measurement result, on an interval  $dt$ , can be represented as a random variable taking values 0 or 1 with probabilities (1.13) and (1.17), respectively. Then, a Poisson increment  $dN_t$  can be introduced, which takes values

$$dN_t = \begin{cases} 1 & \text{if a photon is detected} \\ 0 & \text{otherwise} \end{cases} \quad (1.19)$$

and has a mean value of

$$\mathbb{E}[dN_t] = 0 p_0(t + dt) + 1 p_1(t + dt) = \kappa \langle \hat{c}^\dagger \hat{c} \rangle_t dt \quad (1.20)$$

The conditional variation of the state can then be written by distinguishing the two possible outcomes,

$$\begin{aligned} d\rho^{(c)}(t) &= \rho^{(c)}(t + dt) - \rho^{(c)}(t) \\ &= dN_t \left( \rho_1^{(c)}(t + dt) - \rho^{(c)}(t) \right) + (1 - dN_t) \left( \rho_0^{(c)}(t + dt) - \rho^{(c)}(t) \right) \end{aligned} \quad (1.21)$$

Substituting the expressions (1.15)-(1.18) derived above and retaining only terms up to first order in  $dt$ , one obtains

$$d\rho^{(c)} = dN_t \left( \frac{\hat{c} \rho^{(c)} \hat{c}^\dagger}{\langle \hat{c}^\dagger \hat{c} \rangle_t} - \rho^{(c)} \right) + (1 - dN_t) \left[ -\frac{\kappa}{2} \{ \hat{c}^\dagger \hat{c}, \rho^{(c)} \} dt + \kappa \langle \hat{c}^\dagger \hat{c} \rangle_c \rho^{(c)} dt \right] \quad (1.22)$$

Restoring the unitary evolution generated by the system Hamiltonian  $\hat{H}$ , the photo-

detection stochastic master equation becomes

$$\begin{aligned}
 d\rho^{(c)} = & -i [\hat{H}, \rho^{(c)}] dt - \frac{\kappa}{2} \{ \hat{c}^\dagger \hat{c}, \rho^{(c)} \} dt + \kappa \langle \hat{c}^\dagger \hat{c} \rangle_t \rho^{(c)} dt \\
 & + \left( \frac{\hat{c} \rho^{(c)} \hat{c}^\dagger}{\langle \hat{c}^\dagger \hat{c} \rangle_t} - \rho^{(c)} \right) dN_t
 \end{aligned} \tag{1.23}$$

This nonlinear equation in the state describes a piecewise deterministic evolution. Between two detection events, the state evolves according to a non-unitary deterministic dynamics, conditioned on the absence of emitted photons. Whenever  $dN_t = 1$ , the state undergoes a discontinuous jump induced by the action of the operator  $\hat{c}$ . By averaging over all possible realizations of the counting process  $\rho(t) = \mathbb{E}[\rho^{(c)}(t)]$ , the unconditional Lindblad master equation is recovered.

### 1.4.3 Homodyne Detection Stochastic Master Equation

A second important measurement scheme is obtained by continuously monitoring a field quadrature of the output mode. In contrast to photon counting, where the measurement outcomes are discrete, homodyne detection produces a continuous measurement record and therefore leads to a diffusive stochastic evolution.

The measured quadrature observable is represented by the operator

$$\hat{x}_\theta = \frac{1}{\sqrt{2}} \left( e^{i\theta} \hat{B}_t + e^{-i\theta} \hat{B}_t^\dagger \right) \tag{1.24}$$

where the phase  $\theta$  is fixed and is an arbitrary parameter of the measurement scheme. Since  $\hat{x}_\theta$  is Hermitian, its eigenvalues form a continuous spectrum. The conditional state of the system is therefore obtained by projecting the total state onto the corresponding quadrature eigenstates,

$$\rho^{(c)}(t + dt) = \frac{\tilde{\rho}^{(c)}(t + dt)}{p_{x_\theta}(t + dt)} = \frac{\langle x_\theta | R(t + dt) | x_\theta \rangle}{\text{Tr} [\langle x_\theta | R(t + dt) | x_\theta \rangle]} \tag{1.25}$$

where the tilde denotes an unnormalized conditional state.

Assuming that the environmental mode is initially in the vacuum state, the probability distribution of the measurement outcome is Gaussian,

$$p(x_\theta) = |\langle x_\theta | 0 \rangle|^2 = \frac{1}{\sqrt{\pi}} e^{-x_\theta^2} \tag{1.26}$$

By expanding both the numerator and the denominator up to order  $\sqrt{\kappa dt}$ , one obtains for the unnormalized conditional state

$$\begin{aligned}
 \tilde{\rho}^{(c)}(t+dt) &= |\langle x_\theta|0\rangle|^2 \rho^{(c)}(t) \\
 &\quad + \left( \hat{c}\rho^{(c)}(t) \langle x_\theta|1\rangle \langle 0|x_\theta\rangle + \rho^{(c)}(t) \hat{c}^\dagger \langle x_\theta|0\rangle \langle 1|x_\theta\rangle \right) \sqrt{\kappa dt} + o(\sqrt{\kappa dt}) \\
 &= p_{x_\theta}(t) \left[ \rho^{(c)}(t) + \left( \hat{c}\rho^{(c)}(t)e^{i\theta} + \rho^{(c)}(t)\hat{c}^\dagger e^{-i\theta} \right) x_\theta \sqrt{\kappa dt} \right] + o(\sqrt{\kappa dt})
 \end{aligned} \tag{1.27}$$

where the identity

$$\langle x_\theta|1\rangle = \sqrt{2} x_\theta e^{i\theta} \langle x_\theta|0\rangle$$

has been used to obtain the second expression. Similarly, for the probability distribution one obtains

$$\begin{aligned}
 p_{x_\theta}(t+dt) &= \text{Tr} [\tilde{\rho}^{(c)}(t+dt)] \\
 &= p_{x_\theta}(t) \left( 1 + \sqrt{2\kappa dt} x_\theta \langle \hat{c}e^{i\theta} + \hat{c}^\dagger e^{-i\theta} \rangle_t \right) + o(\sqrt{\kappa dt}) \\
 &\approx \frac{1}{\sqrt{\pi}} \exp \left[ - \left( x_\theta - \sqrt{\frac{\kappa dt}{2}} \langle \hat{c}e^{i\theta} + \hat{c}^\dagger e^{-i\theta} \rangle_t \right)^2 \right]
 \end{aligned} \tag{1.28}$$

From the last expression, it follows that, up to order  $\sqrt{dt}$ , the probability distribution is equivalent to a Gaussian with variance  $1/2$  and mean value  $\sqrt{\frac{\kappa dt}{2}} \langle \hat{c}e^{i\theta} + \hat{c}^\dagger e^{-i\theta} \rangle_t$ . It is therefore convenient to introduce the stochastic increment

$$dy_t = I(t)dt = \sqrt{\kappa} \langle \hat{c}e^{i\theta} + \hat{c}^\dagger e^{-i\theta} \rangle_t dt + dW_t \tag{1.29}$$

where  $dW_t$  is a Gaussian random variable with vanishing mean and variance  $dt$ . In the theory of stochastic processes,  $dW_t$  is called a Wiener increment and satisfies the Ito relation  $dW_t^2 = dt$ . The quantity  $I(t)$  is usually referred to as the homodyne photocurrent.

By substituting Eqs. (1.27), (1.28), and (1.29) into the expression for the conditional state, one obtains

$$d\rho^{(c)}(t) = \sqrt{\kappa} \mathcal{H} [\hat{c}e^{i\theta}] \rho^{(c)}(t) dW_t + o(\sqrt{\kappa dt}) \tag{1.30}$$

Since averaging over all possible measurement outcomes must reproduce the unconditional Lindblad master equation (1.3), the missing contributions of order  $dt$  can be

immediately identified, yielding

$$d\rho^{(c)}(t) = -i[\hat{H}, \rho^{(c)}(t)]dt + \kappa\mathcal{D}[\hat{c}]\rho^{(c)}(t)dt + \sqrt{\kappa}\mathcal{H}[\hat{c}e^{i\theta}]\rho^{(c)}(t)dW_t \quad (1.31)$$

where the superoperators,

$$\mathcal{D}[\hat{A}]\rho = \hat{A}\rho\hat{A}^\dagger - \frac{1}{2}\{\hat{A}^\dagger\hat{A}, \rho\} \quad (1.32)$$

$$\mathcal{H}[\hat{A}]\rho = \hat{A}\rho + \rho\hat{A}^\dagger - \text{Tr}[(\hat{A} + \hat{A}^\dagger)\rho]\rho \quad (1.33)$$

already introduced, have the following meaning: the superoperator  $\mathcal{D}$  describes the dissipative evolution induced by the coupling to the environment, whereas  $\mathcal{H}$  accounts for the stochastic back-action associated with the continuous measurement process.

The stochastic contribution is responsible for the continuous update of the system state according to the measurement record. Averaging over all realizations of the Wiener process removes the stochastic term, since  $\mathbb{E}[dW_t] = 0$ , and immediately recovers the unconditional Lindblad master equation. For this reason, Eq. (1.31) is often referred to as a *diffusive stochastic master equation*. As in the case of the photodetection SME, this equation is non-linear in the conditional state because it explicitly depends on the expectation value  $\langle \hat{c}e^{i\theta} + \hat{c}^\dagger e^{-i\theta} \rangle_t$ .

In Eq. (1.31) a unit measurement efficiency has been implicitly assumed. This corresponds to the ideal situation in which all the information carried away by the environmental output field is collected by the detector [13]. In other words, the rate at which information is acquired from the measurement is maximal and matches the rate at which the system is decohered by its coupling to the monitored channel. In realistic situations, losses in the detection apparatus or unobserved environmental modes reduce the amount of information available in the measurement record. This effect is described by introducing a measurement efficiency  $0 \leq \eta \leq 1$ .

The inefficient homodyne SME can be written as

$$d\rho^{(c)}(t) = -i[\hat{H}, \rho^{(c)}(t)]dt + \kappa\mathcal{D}[\hat{c}]\rho^{(c)}(t)dt + \sqrt{\eta\kappa}\mathcal{H}[\hat{c}e^{i\theta}]\rho^{(c)}(t)dW_t \quad (1.34)$$

Equivalently, the dissipative contribution can be split into a monitored and an unmonitored part,

$$\kappa\mathcal{D}[\hat{c}] = \eta\kappa\mathcal{D}[\hat{c}] + (1 - \eta)\kappa\mathcal{D}[\hat{c}] \quad (1.35)$$

Only the first contribution is associated with an observed measurement record

and therefore contributes to the innovation term, while the second one represents information lost to the environment and produces dissipation without conditioning the state. Thus, inefficient detection leaves the total Lindblad dissipation unchanged, but reduces the stochastic back-action by the factor  $\sqrt{\eta}$ . The ideal equation (1.31) is recovered for  $\eta = 1$ , whereas for  $\eta = 0$  no information is extracted and the conditional dynamics reduces to the unconditional Lindblad evolution. Throughout this thesis, ideal detection is assumed, and therefore the measurement efficiency is set to  $\eta = 1$  in all monitored dynamics considered.

## 1.5 Quantum Trajectories Formalism

As discussed in the previous section, continuously monitoring the environment conditions the evolution of an open quantum system on the obtained measurement record. The resulting dynamics is no longer described by a deterministic master equation but by a stochastic evolution, whose form depends on the specific measurement scheme.

An important feature of the stochastic master equations (1.23) (1.31) introduced above is that, when the initial state is pure, the conditioned evolution preserves the purity of the state. The conditional density matrix can therefore be written as

$$\rho^{(c)}(t) = |\psi^{(c)}(t)\rangle \langle \psi^{(c)}(t)| \quad (1.36)$$

where the conditioned state vector  $|\psi^{(c)}(t)\rangle$  obeys a *stochastic Schrödinger equation* (SSE). Individual realizations of these stochastic evolutions are known as *quantum trajectories* [14, 15].

From a physical perspective, each trajectory represents the evolution of a single continuously monitored quantum system conditioned on a particular measurement record. Averaging over all trajectories recovers the unconditional dynamics described by the Lindblad master equation,

$$\rho(t) = \mathbb{E}[|\psi^{(c)}(t)\rangle \langle \psi^{(c)}(t)|] \quad (1.37)$$

where  $\mathbb{E}[\cdot]$  denotes the average over all stochastic realizations. In many applications, including the present work, the primary object of interest is the conditioned dynamics itself rather than its ensemble average. The quantum trajectories formalism therefore provides both a natural description of continuously monitored open quantum systems and the theoretical framework underlying the numerical method developed in the

following chapter.

Starting from a stochastic master equation, the corresponding SSE can be obtained by differentiating

$$\rho^{(c)}(t) = |\psi^{(c)}(t)\rangle \langle \psi^{(c)}(t)|, \quad (1.38)$$

and applying Itô's product rule,

$$d\rho^{(c)} = d|\psi^{(c)}\rangle \langle \psi^{(c)}| + |\psi^{(c)}\rangle d\langle \psi^{(c)}| + d|\psi^{(c)}\rangle d\langle \psi^{(c)}| \quad (1.39)$$

By comparing this expression with the corresponding SME, one obtains the stochastic equations governing the conditioned pure states.

**Quantum jump unraveling** In the photon-counting case, the environment is monitored by detecting the emitted quanta. The corresponding stochastic evolution is discontinuous: most of the time the state evolves smoothly under an effective non-Hermitian Hamiltonian, while random detection events produce instantaneous jumps. The normalized nonlinear stochastic Schrödinger equation is

$$d|\psi^{(c)}(t)\rangle = \left[ -i\hat{H} - \frac{1}{2}(\hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger \hat{c} \rangle_t) \right] |\psi^{(c)}(t)\rangle dt + \left[ \frac{\hat{c}}{\sqrt{\langle \hat{c}^\dagger \hat{c} \rangle_t}} - \mathbb{I} \right] |\psi^{(c)}(t)\rangle dN_t \quad (1.40)$$

Here and in the following for simplicity the dissipation rate  $\kappa$  for each jump operator is meant to be included in the jump operator  $\hat{c}$  itself. The term  $dN_t$  is a Poisson increment, taking values 0 or 1, with statistical mean  $\mathbb{E}[dN_t] = \langle \hat{c}^\dagger \hat{c} \rangle_t dt$ , where

$$\langle \hat{O} \rangle_t = \langle \psi^{(c)}(t) | \hat{O} | \psi^{(c)}(t) \rangle \quad (1.41)$$

The term proportional to  $dt$  describes the deterministic evolution between two detection events, while the term proportional to  $dN_t$  describes the stochastic jumps induced by photon detections.

**Diffusive unraveling** In this case the measurement record is continuous and the corresponding stochastic evolution is diffusive. The normalized nonlinear diffusive SSE can be written as [13]

$$d|\psi^{(c)}(t)\rangle = \left[ -i\hat{H} - \frac{1}{2} \left( \hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger + \hat{c} \rangle_t \hat{c} + \frac{1}{4} \langle \hat{c}^\dagger + \hat{c} \rangle_t^2 \right) \right] |\psi^{(c)}(t)\rangle dt + \left[ \hat{c} - \frac{1}{2} \langle \hat{c}^\dagger + \hat{c} \rangle_t \right] |\psi^{(c)}(t)\rangle dW_t \quad (1.42)$$

Here  $dW_t$  is a Wiener increment satisfying  $\mathbb{E}[dW_t] = 0$  and  $\mathbb{E}[dW_t^2] = dt$ . Unlike the quantum jump case, the stochastic evolution is continuous in time. The noise term represents the random fluctuations of the homodyne measurement record, while the nonlinear drift terms ensure the normalization of the conditioned state.

The quantum jump and diffusive equations describe two different classes of conditioned dynamics associated with distinct measurement schemes. While their ensemble averages reproduce the same Lindblad evolution, individual trajectories retain the information acquired through continuous monitoring and therefore provide access to the physics of single experimental realizations. In the following chapter, these stochastic pure-state evolutions will constitute the starting point for the variational numerical approach presented in this work.

### 1.5.1 Itô and Stratonovich Formulations

The stochastic Schrödinger equations introduced in the previous sections belong to the broader class of stochastic differential equations (SDEs). In contrast to ordinary differential equations, SDEs involve stochastic increments, whose trajectories are nowhere differentiable. As a consequence, the stochastic integral is not uniquely defined, and different mathematical interpretations can be adopted.

The two most commonly used formulations are the *Itô* and *Stratonovich* interpretations. In the Itô formalism the stochastic increment is evaluated at the beginning of each time interval, leading to a non-anticipating stochastic process with particularly convenient mathematical properties. In the Stratonovich interpretation the stochastic increment is instead evaluated at the midpoint of the interval, allowing the use of the ordinary rules of differential calculus, such as the standard chain rule.

While the two descriptions converge to different integrals, and therefore it is important to explicitly declare which one is in use, they are mathematically equivalent and can always be transformed into one another by appropriately modifying the deterministic drift term. In general, an SDE written in Stratonovich form as

$$dX_t = f(X_t, t) dt + \sigma(X_t, t) \circ dW_t \quad (1.43)$$

admits the equivalent Itô representation

$$dX_t = \left[ f(X_t, t) + \frac{1}{2} \sigma(X_t, t) \frac{\partial \sigma(X_t, t)}{\partial X} \right] dt + \sigma(X_t, t) dW_t \quad (1.44)$$

Unless explicitly stated otherwise, all stochastic master equations and stochastic Schrödinger equations introduced so far are understood in the Itô sense. Stratonovich convention is recognized when the symbol  $\circ$  is used in the diffusion term.

### Diffusive Stochastic Schrödinger Equation

The diffusive SSE, already introduced in the previous sections, can be written in the Itô formalism and the multiple noise channels case as

$$d|\psi^{(c)}\rangle = \left[ -\frac{i}{\hbar} \hat{H} - \frac{1}{2} \sum_n \left( \hat{c}_n^\dagger \hat{c}_n - \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \hat{c}_n + \frac{1}{4} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle^2 \right) \right] |\psi^{(c)}\rangle dt + \sum_n \left( \hat{c}_n - \frac{1}{2} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) |\psi^{(c)}\rangle dW_n \quad (1.45)$$

The equation can be rewritten in a more compact form defining,

$$\hat{H}_{\text{eff}} = \hat{H} - \frac{i\hbar}{2} \sum_n \left( \hat{c}_n^\dagger \hat{c}_n - \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \hat{c}_n + \frac{1}{4} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle^2 \right) \quad (1.46)$$

obtaining

$$d|\psi^{(c)}\rangle = \left\{ -\frac{i}{\hbar} \hat{H}_{\text{eff}} dt + \sum_n \left( \hat{c}_n - \frac{1}{2} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) dW_n \right\} |\psi^{(c)}\rangle \quad (1.47)$$

For practical purposes, and in particular for the variational formulation [2] developed in the following chapters (which requires the chain rule to determine the stochastic evolution of variational parameters), it is often convenient to recast the evolution in the Stratonovich form, yielding

$$d|\psi^{(c)}\rangle = \left\{ -\frac{i}{\hbar} \hat{H}_{\text{eff}}^{\text{Strat}} dt + \sum_n \left( \hat{c}_n - \frac{1}{2} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) \circ dW_n \right\} |\psi^{(c)}\rangle \quad (1.48)$$

where

$$\hat{H}_{\text{eff}}^{\text{Strat}} = \hat{H} - \frac{i\hbar}{2} \sum_n \left( \hat{c}_n^\dagger \hat{c}_n - 2 \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \hat{c}_n + \hat{c}_n^2 + \langle \hat{c}_n + \hat{c}_n^\dagger \rangle^2 - \frac{1}{2} \langle \hat{c}_n^2 + 2 \hat{c}_n^\dagger \hat{c}_n + \hat{c}_n^{\dagger 2} \rangle \right) \quad (1.49)$$

In particular, the Stratonovich formulation will prove advantageous when deriving the variational equations of motion, since it allows manipulations analogous to those employed in deterministic differential equations.

## 1.6 Long-range dissipative transverse-field Ising model

Spin models provide a convenient description of quantum many-body systems whose local Hilbert space can be restricted to two relevant states. This is the case, for instance, for ensembles of effective two-level atoms, where the two internal states can be denoted by  $|\uparrow\rangle$  and  $|\downarrow\rangle$ . In this representation, each atom is mapped onto a spin-1/2 degree of freedom and the dynamics can be expressed in terms of Pauli operators. The standard pseudospin representation is defined as

$$\hat{\sigma}^x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| \quad (1.50)$$

$$\hat{\sigma}^y = i(|\downarrow\rangle\langle\uparrow| - |\uparrow\rangle\langle\downarrow|) \quad (1.51)$$

$$\hat{\sigma}^z = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow| \quad (1.52)$$

With this convention,  $|\uparrow\rangle$  and  $|\downarrow\rangle$  are eigenstates of  $\hat{\sigma}^z$  with eigenvalues  $+1$  and  $-1$ , respectively. The collective spin operator along the  $z$  direction is therefore

$$\hat{J}_z = \frac{1}{2} \sum_{i=1}^N \hat{\sigma}_i^z = \frac{\hat{N}_\uparrow - \hat{N}_\downarrow}{2} \quad (1.53)$$

Thus, it has a direct interpretation of the population difference between the two internal atomic states.

The physical system considered in this thesis is a two-dimensional long-range transverse-field Ising model subject to local dissipation and continuous monitoring of a collective spin observable. This model provides a paradigmatic setting for the study of open many-body quantum dynamics, since it combines coherent long-range interactions, coupling to an environment, and measurement backaction [16, 17, 18, 19].

The coherent part of the dynamics is governed by the Hamiltonian

$$\hat{H} = -\frac{J}{\mathcal{K}_\beta} \sum_{i < j} \frac{\hat{\sigma}_i^z \hat{\sigma}_j^z}{r_{ij}^\beta} - h \sum_i \hat{\sigma}_i^x - l \sum_i \hat{\sigma}_i^z \quad (1.54)$$

Here,  $J$  denotes the interaction strength,  $h$  is the transverse magnetic field,  $\beta$  controls the range of the interaction, and  $l$  is a longitudinal magnetic field. The operators  $\hat{\sigma}_i^\alpha$ , with  $\alpha = x, y, z$ , are Pauli matrices acting on the spin located at site  $i$ . The distance  $r_{ij}$  is defined as the minimum distance between lattice sites  $i$  and  $j$  under periodic

boundary conditions. These conditions are imposed along both spatial directions in order to preserve translational invariance and reduce finite-size effects.

The factor  $\mathcal{K}_\beta$  is the Kac normalization,

$$\mathcal{K}_\beta = \frac{1}{N-1} \sum_{i < j} \frac{1}{r_{ij}^\beta} \quad (1.55)$$

which rescales the interaction energy and ensures a well-defined thermodynamic limit in the presence of long-range couplings. Throughout this thesis, the longitudinal field is set to zero, namely  $l = 0$ .

Dissipation is introduced through local jump operators

$$\hat{c}_n = \sqrt{\kappa} \hat{\sigma}_n^- \quad (1.56)$$

where  $\kappa$  is the local decay rate and  $\hat{\sigma}_n^-$  is the lowering operator acting on site  $n$ . These operators describe irreversible spin relaxation processes induced by the coupling to an external environment.

In addition to local dissipation, the system is continuously monitored through the collective operator

$$\hat{c}_{\text{mon}} = \sqrt{\Gamma} \hat{J}_z = \frac{\sqrt{\Gamma}}{2} \sum_i \hat{\sigma}_i^z \quad (1.57)$$

where  $\Gamma$  is the measurement strength and

$$\hat{J}_z = \frac{1}{2} \sum_i \hat{\sigma}_i^z \quad (1.58)$$

is the collective spin component along the  $z$  direction.

The above Hamiltonian encompasses many relevant interaction regimes, with varying  $\beta$ :  $\beta = 0$  corresponds to the all-to-all Ising model, also called the One-Axis Twisting Hamiltonian [20] which has relevance in cavity-enhanced atomic clocks [21]; the limit  $\beta \rightarrow \infty$  corresponds to the standard nearest-neighbour Ising model; values  $1 \leq \beta \leq 6$  are instead relevant for several atomic and ion platforms. We focus on the case  $\beta = 2$ , which is the marginal case between mean-field and short-range physics in two-dimensional systems [22].

Retaining the measurement record associated with the collective observable  $\hat{J}_z$  leads to conditional stochastic dynamics. The monitored channel contributes both through a deterministic Lindblad term,  $\Gamma \mathcal{D}[\hat{J}_z]$ , corresponding to global dephasing, and

through a stochastic innovation term describing measurement backaction. If the measurement outcomes are averaged over, the stochastic contribution vanishes and only the unconditional global-dephasing channel remains. Including also the local dissipative channels, the conditional density matrix (1.31) obeys

$$d\rho^{(c)}(t) = -i[\hat{H}, \rho^{(c)}(t)]dt + \sum_i \kappa_i \mathcal{D}[\hat{\sigma}_i^-] \rho^{(c)}(t)dt + \Gamma \mathcal{D}[\hat{J}_z] \rho^{(c)}(t)dt + \sqrt{\Gamma} \mathcal{H}[\hat{J}_z] \rho^{(c)}(t)dW_t \quad (1.59)$$

with operators  $\mathcal{D}[\bullet]$  and  $\mathcal{H}[\bullet]$  defined by equations (1.32) and (1.33).

Long-range interacting spin systems are relevant in several modern quantum simulation platforms, including trapped ions, Rydberg atom arrays, and dipolar quantum gases. In these systems, tunable interactions and controlled dissipation make it possible to investigate non-equilibrium many-body phenomena beyond the reach of closed-system descriptions. The presence of continuous monitoring further enriches the dynamics, since information extraction from the environment competes with coherent evolution and dissipation. This competition can generate collective effects, non-trivial correlations, and measurement-induced dynamical behavior, making the model a useful benchmark for variational approaches to open quantum many-body systems.

### 1.6.1 Observables and spin squeezing

Spin squeezing is one of the most relevant manifestations of useful quantum correlations in collective spin systems [23, 20, 24, 25]. Its definition is not unique, since the concept has been introduced in different contexts, ranging from the characterization of multipartite entanglement to the improvement of precision measurements. In this thesis, the relevant notion is the metrological one, in which spin squeezing quantifies the enhancement of phase sensitivity with respect to a coherent spin state.

For an ensemble of  $N$  spin-1/2 particles, the collective spin operators are defined as

$$\hat{J}_\alpha = \frac{1}{2} \sum_{i=1}^N \hat{\sigma}_i^\alpha \quad \alpha = x, y, z \quad (1.60)$$

The mean collective spin vector is

$$\langle \hat{\mathbf{J}} \rangle = (\langle \hat{J}_x \rangle, \langle \hat{J}_y \rangle, \langle \hat{J}_z \rangle) \quad (1.61)$$

It defines the average orientation of the collective spin on the Bloch sphere. A coherent spin state is a product state in which all spins point in the same direction. For a direction specified by the angles  $(\theta, \varphi)$ , it can be written as

$$|\text{CSS}\rangle = \bigotimes_{i=1}^N \left[ \cos\left(\frac{\theta}{2}\right) |\downarrow\rangle_i + e^{i\varphi} \sin\left(\frac{\theta}{2}\right) |\uparrow\rangle_i \right] \quad (1.62)$$

Such a state is uncorrelated and represents the natural classical reference state for an ensemble of spins. Its collective spin has maximal length,  $|\langle \hat{\mathbf{J}} \rangle| = \frac{N}{2}$ , and its fluctuations are isotropic in the plane perpendicular to the mean spin direction,  $(\Delta J_{\perp})_{\text{CSS}}^2 = \frac{N}{4}$ .

The standard quantum limit follows from the phase sensitivity of a coherent spin state. If a small phase rotation is estimated from the displacement of the collective spin, the uncertainty can be written as

$$\Delta\phi = \frac{\Delta J_{\perp}}{|\langle \hat{\mathbf{J}} \rangle|} \quad (1.63)$$

where  $\hat{J}_{\perp}$  is a spin component orthogonal to the mean spin direction. For a coherent spin state this gives

$$\Delta\phi_{\text{CSS}} = \frac{1}{\sqrt{N}} \quad (1.64)$$

which is the standard quantum limit. This limit represents the best scaling achievable with independent, uncorrelated particles.

A spin-squeezed state is characterized by a reduction of the fluctuation of one collective spin component below the coherent-state value. However, for metrological purposes, it is not sufficient to consider the variance of an arbitrary fixed component, such as  $\hat{J}_z$ . The relevant fluctuation is the one along a direction perpendicular to the mean spin vector. This is because a phase shift corresponds to a small rotation of the collective spin, and the sensitivity to this rotation is determined by the noise in the transverse plane around the average spin direction.

The geometrical construction is the following. The vector  $\langle \hat{\mathbf{J}} \rangle$  identifies the direction in which the collective spin is, on average, pointing. This direction defines a local longitudinal axis on the Bloch sphere. The two-dimensional plane perpendicular to it is the tangent plane relevant for small rotations. Fluctuations inside this plane determine how precisely a phase rotation can be resolved. If the quantum state is squeezed, the noise distribution in this transverse plane is not circular, as in a coherent spin state, but becomes anisotropic: one transverse direction has reduced

variance, while the orthogonal transverse direction has increased variance.

The metrologically relevant variance is therefore the smallest variance among all possible directions in this transverse plane. This quantity is denoted by  $(\Delta J_{\perp,\min})^2$ . The corresponding Wineland spin-squeezing parameter [24, 25] is

$$\xi^2 = \frac{N(\Delta J_{\perp,\min})^2}{|\langle \hat{\mathbf{J}} \rangle|^2} \quad (1.65)$$

Equivalently, it can be interpreted as the ratio between the phase uncertainty of the considered state and that of a coherent spin state,

$$\xi^2 = \frac{(\Delta\phi)^2}{(\Delta\phi_{\text{CSS}})^2}. \quad (1.66)$$

A coherent spin state has  $\xi^2 = 1$ , while  $\xi^2 < 1$  signals metrologically useful spin squeezing, namely a phase sensitivity below the standard quantum limit. The condition  $\xi^2 < 1$  also has an important interpretation in terms of quantum correlations. For an ensemble of pseudo spin-1/2 particles, metrological spin squeezing below the standard quantum limit provides a sufficient criterion for multipartite entanglement [24, 23].

In order to determine the minimum transverse variance, the covariance matrix of the collective spin components is introduced:

$$\Gamma_{\alpha\beta} = \frac{1}{2} \langle \hat{J}_\alpha \hat{J}_\beta + \hat{J}_\beta \hat{J}_\alpha \rangle - \langle \hat{J}_\alpha \rangle \langle \hat{J}_\beta \rangle \quad \alpha, \beta = x, y, z \quad (1.67)$$

The diagonal elements of this matrix are the variances of the collective spin components, while the off-diagonal elements describe their covariances. The covariance matrix therefore contains the full information on the shape and orientation of the collective-spin noise distribution.

Operationally, the direction of the mean spin is first identified. Then, the covariance matrix is restricted to the plane perpendicular to this direction. The two eigenvalues of the resulting transverse covariance matrix give the variances along the two principal noise axes in the tangent plane. The smaller of these two eigenvalues is  $(\Delta J_{\perp,\min})^2$ , and it is the quantity entering the spin-squeezing parameter. This procedure makes explicit that spin squeezing is a geometrical property of the noise distribution around the mean collective spin, rather than simply the reduction of fluctuations along a fixed laboratory axis.

The same collective quantities can be expressed in terms of normalized magnetizations.

In this thesis, the magnetization components are related to the collective spin operators by

$$\hat{M}_\alpha = \frac{2}{N} \hat{J}_\alpha \quad \alpha = x, y, z \quad (1.68)$$

Therefore, the magnetizations are proportional to the collective spin components, and their variances and covariances contain the same information up to the corresponding normalization factors.

In the numerical analysis presented in this thesis, the spin-squeezing parameter is not computed explicitly. Instead, the focus is placed on the accurate evaluation of the quantities from which it can be constructed, namely the magnetizations and their variances and covariances. This is a necessary preliminary step because, while magnetizations are linear observables, variances and covariances are nonlinear functions of expectation values and require a careful statistical treatment, especially in conditional dynamics. Establishing reliable estimators for these quantities is therefore essential before performing a systematic analysis of metrological spin squeezing.

## Chapter 2

# Quantum Monte Carlo Methods

Quantum many-body systems constitute one of the major challenges of modern theoretical physics. Although the fundamental laws governing their dynamics are well established, the dimensionality of the associated Hilbert space grows exponentially with the number of degrees of freedom, making exact analytical and numerical treatments rapidly impractical. This complexity is particularly evident when evaluating expectation values, solving equations of motion, or determining equilibrium properties, all of which generally involve multidimensional integrals over high-dimensional configuration spaces.

Monte Carlo methods provide a powerful framework to address these difficulties [26, 27]. Their central idea is to replace the deterministic evaluation of multidimensional integrals with a stochastic estimation based on random sampling. By interpreting physical quantities as expectation values with respect to suitable probability distributions, Monte Carlo techniques make it possible to extract accurate information about quantum systems while avoiding the full exploration of a multidimensional grid of the exponentially large configuration space.

The flexibility and efficiency of Monte Carlo approaches have made them indispensable tools across many areas of physics, ranging from condensed matter and quantum chemistry to statistical mechanics and quantum information. Depending on the specific problem under consideration, different variants of Quantum Monte Carlo (QMC) methods have been developed, each combining stochastic sampling with additional approximations or variational principles to address particular classes of quantum systems.

A comprehensive review of the numerous QMC techniques available in the literature

lies beyond the scope of this thesis. Instead, the purpose of this chapter is to introduce only the concepts and methods that are directly relevant for the developments presented in the following chapters. We begin by discussing the general principles of Monte Carlo integration and the construction of Markov chains through the Metropolis algorithm. Building upon these foundations, we introduce Variational Monte Carlo (VMC) and its time-dependent extension, the Time-Dependent Variational Monte Carlo (tVMC) method for closed quantum systems. These techniques will constitute the essential numerical ingredients for the formulation of the open time-dependent Variational Monte Carlo (otVMC) approach developed later in Chapter 3, where they are combined with the quantum trajectory formalism introduced in Chapter 1.

## 2.1 Monte Carlo Method

Multidimensional integrals naturally arise in the computation of expectation values, partition functions, and in the solution of equations governing the dynamics of quantum systems. While analytical treatments are possible in a limited number of cases, the complexity of these integrals generally increases rapidly with the number of degrees of freedom, making exact calculations impractical for realistic many-body systems.

Numerical approaches therefore become indispensable. However, conventional deterministic integration methods struggle as their computational cost typically grows significantly with the dimensionality of the integration domain. Monte Carlo methods provide an effective alternative by replacing the deterministic evaluation of integrals with a statistical estimation based on random sampling.

The central idea of Monte Carlo integration is to interpret an integral as an expectation value with respect to a suitably chosen probability distribution. The desired quantity can then be estimated by generating a finite set of configurations and averaging the corresponding values of the integrand over the sampled configurations. Owing to their stochastic nature, Monte Carlo estimates are affected by statistical uncertainties, which can be systematically quantified and reduced through more efficient sampling strategies and longer simulations.

### 2.1.1 Basic Monte Carlo Methods

The simplest Monte Carlo approach, commonly referred to as *crude Monte Carlo*, provides a stochastic estimate of definite integrals. Let  $h(x)$  be a continuous function defined on the interval  $[a, b]$ . Its integral can be written as

$$\int_a^b h(x)dx = (b-a) \int_a^b h(x) \frac{1}{b-a} dx$$

The second term can be interpreted as the expectation value of  $h(x)$  with respect to the uniform probability distribution over the interval, denoted by  $\mathcal{U}[a, b]$ . Therefore,

$$\begin{aligned} \int_a^b h(x)dx &= (b-a) \int_a^b h(x) \frac{1}{b-a} dx \\ &= (b-a) \mathbb{E}_{\mathcal{U}}[h(x)] = (b-a) \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N h(x_i) \quad \text{with } x_i \sim \mathcal{U}[a, b] \end{aligned}$$

In practice, the expectation value is approximated from a finite sample of  $N$  independent random variables  $x_i$ . This leads to the Monte Carlo estimator

$$\hat{I} = \frac{b-a}{N} \sum_{i=1}^N h(x_i) \quad \text{with } x_i \in \mathcal{U}[a, b]$$

which is an unbiased estimator of the exact integral. Its variance is given by

$$\text{Var}[\hat{I}] = \frac{(b-a)^2}{N} \text{Var}[h(x_i)]$$

demonstrating that the statistical uncertainty decreases as the inverse of the number of samples. Consequently, the standard error of the estimate scales as  $1/\sqrt{N}$ .

The above construction can be straightforwardly generalized to multivariate functions by replacing the integration interval with an arbitrary multidimensional domain and sampling points uniformly over it. An important feature of Monte Carlo integration is that the convergence rate, proportional to  $1/\sqrt{N}$ , is independent of the dimensionality of the problem. For this reason, Monte Carlo techniques are particularly well suited for the study of many-body systems and other problems involving high-dimensional integrals.

The crude Monte Carlo approach can be generalized by replacing uniform sampling with an arbitrary probability density function  $p(x)$ . This technique, known as *importance sampling*, is based on the observation that the integral of interest can be

rewritten as

$$\langle h \rangle = \int_{\mathcal{D}} h(x) dx = \int_{\mathcal{D}} \frac{h(x)}{p(x)} p(x) dx$$

As in the previous case, the right-hand side can be interpreted as the expectation value of the function  $h(x)/p(x)$  with respect to the probability distribution  $p(x)$ . The integral can therefore be estimated as

$$\int_{\mathcal{D}} h(x) dx \approx \frac{1}{N} \sum_i \frac{h(x_i)}{p(x_i)} \quad \text{with } x_i \sim p(x)$$

which again constitutes an unbiased estimator of the exact integral. The corresponding variance is

$$\sigma^2 = \int_{\mathcal{D}} \left( \frac{h(x)}{p(x)} \right)^2 p(x) dx - \langle h \rangle^2$$

By selecting an appropriate probability density, one can substantially reduce the variance of the estimator, improving the accuracy of the calculation without increasing the number of samples.

The practical implementation of importance sampling, therefore, relies on the ability to generate random configurations distributed according to an arbitrary target probability density. A possible approach is to construct a stochastic process whose stationary distribution coincides with the desired probability density. This naturally leads to the concepts of Markov chains and the Metropolis-Hastings algorithm, which constitute the foundation of most Quantum Monte Carlo methods.

### 2.1.2 Markov Chains and the Metropolis–Hastings Algorithm

As discussed in the previous section, the effectiveness of importance sampling strongly depends on the ability to generate random samples with an arbitrary probability density function. In many practical applications, directly drawing independent samples from a given distribution is either difficult or computationally prohibitive. A powerful alternative is provided by *Markov Chain Monte Carlo* (MCMC) methods, which generate correlated samples by constructing a stochastic process whose stationary distribution matches the desired distribution.

A *Markov chain* is a stochastic process in which the probability of reaching a new state depends only on the present state and not on the previous history of the process. Denoting by  $X_n$  the state of the system at the  $n$ -th step, for a discrete state space,

the dynamic of the chain is entirely specified by the transition matrix

$$T_{ij} = P(X_{n+1} = j | X_n = i) \quad (2.1)$$

hence,  $T_{ij}$  is the probability of transition from state  $i$  to state  $j$  and whose elements satisfy

$$0 \leq T_{ij} \leq 1 \quad \sum_j T_{ij} = 1 \quad (2.2)$$

For continuous state spaces, the transition matrix is replaced by a transition probability density, or kernel,

$$T(x \rightarrow x') \quad (2.3)$$

such that

$$T(x \rightarrow x') \geq 0 \quad \int dx' T(x \rightarrow x') = 1 \quad (2.4)$$

The central idea of MCMC methods is to construct a Markov chain whose stationary distribution coincides with a target probability density  $p(x)$ . Under suitable conditions, such as irreducibility and aperiodicity, the chain converges asymptotically to this stationary distribution, so that samples generated after an initial equilibration period can be regarded as distributed according to  $p(x)$ .

One of the most widely used algorithms to achieve this goal is the *Metropolis–Hastings algorithm* [28, 29]. From the current state  $x$ , a candidate configuration  $x'$  is generated according to a proposal distribution  $q(x' | x)$  that specifies the probability density of proposing a move from  $x$  to  $x'$ . In general, such proposal distribution can be arbitrary and determines how quickly the method converges. Usually,  $q(x' | x)$  is taken as a uniform or Gaussian distribution. The proposed move is then accepted with probability

$$A(x \rightarrow x') = \min \left[ 1, \frac{p(x') q(x | x')}{p(x) q(x' | x)} \right] \quad (2.5)$$

If the move is accepted, the new state of the chain becomes  $x_{n+1} = x'$ ; otherwise, the proposal is rejected, and the chain remains in the current state, namely  $x_{n+1} = x$ .

The acceptance rule is constructed so that the resulting transition kernel satisfies the detailed balance condition,

$$p(x) T(x \rightarrow x') = p(x') T(x' \rightarrow x) \quad (2.6)$$

which guarantees that  $p(x)$  is a stationary distribution of the Markov process.

From an implementation perspective, the algorithm only requires the repeated

execution of three elementary steps: generation of a candidate configuration according to  $q(x'|x)$ , evaluation of the acceptance probability, and update of the chain depending on whether the proposal is accepted or rejected. The procedure is then iterated until the desired number of samples is obtained.

An important advantage of the Metropolis–Hastings algorithm is that the target distribution does not need to be normalized. Since the acceptance probability only depends on ratios of probabilities, any unknown normalization constant cancels identically. This feature makes the method particularly suitable for high-dimensional problems, where the normalization of the target distribution is often inaccessible.

A drawback of MCMC methods is that successive samples are generally correlated, since each configuration is generated from the previous one through the Markov dynamics. Consequently, standard estimators based on independent samples underestimate the statistical uncertainty. In practical calculations, the effects of autocorrelation must therefore be taken into account, and dedicated techniques, such as blocking or binning analyses, are commonly employed to obtain reliable estimates of statistical errors.

## 2.2 Variational Monte Carlo

Variational Monte Carlo (VMC) is a computational method that combines the variational principle with stochastic sampling techniques to approximate the ground-state properties of quantum many-body systems [30]. The method relies on the introduction of a parametrized trial wavefunction  $\Psi_\theta(x)$  where  $x$  denotes a configuration of the system and  $\theta$  is a set of variational parameters.

According to the variational principle, for any normalized trial state the expectation value of the Hamiltonian provides an upper bound to the exact ground- or excited-state energy  $E_0$ ,

$$E_0 \leq \frac{\langle \Psi_\theta | \hat{H} | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} \equiv E_{\text{var}}$$

The central idea of VMC is therefore to optimize the parameters  $\theta$  so as to minimize the variational energy  $E_{\text{var}}$ .

More generally, the expectation value of an arbitrary observable  $\hat{O}$  can be written as

$$\langle \hat{O} \rangle = \frac{\langle \Psi_\theta | \hat{O} | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle}. \quad (2.7)$$

By inserting the resolution of the identity in the configuration basis,  $\mathbb{I} = \sum_x |x\rangle\langle x|$  (or the corresponding integral in continuous systems), the expectation value becomes

$$\langle \hat{O} \rangle = \sum_x \frac{|\Psi_\theta(x)|^2}{\langle \Psi_\theta | \Psi_\theta \rangle} O_{\text{loc}}(x) \quad (2.8)$$

where

$$O_{\text{loc}}(x) \equiv \frac{\langle x | \hat{O} | \Psi_\theta \rangle}{\langle x | \Psi_\theta \rangle} \quad (2.9)$$

is usually referred to as the local estimator of the observable.

The previous expression has the form of an expectation value with respect to the probability distribution

$$p_\theta(x) = \frac{|\Psi_\theta(x)|^2}{\langle \Psi_\theta | \Psi_\theta \rangle}. \quad (2.10)$$

Consequently, if a set of configurations  $\{x_i\}_{i=1}^N$  is sampled according to  $p_\theta(x)$ , the expectation value can be estimated as

$$\langle \hat{O} \rangle \approx \frac{1}{N} \sum_{i=1}^N O_{\text{loc}}(x_i) \quad (2.11)$$

Configurations  $x_i$  can be sampled from the probability distribution  $p_\theta(x)$  using the previously discussed Metropolis–Hastings algorithm. Importantly, the normalization constant of the wavefunction cancels out in the acceptance ratio and therefore does not need to be evaluated explicitly.

The quantity of primary interest in VMC is the variational energy, obtained by choosing  $\hat{O} = \hat{H}$ . The corresponding local estimator is the local energy,

$$E_{\text{loc}}(x) = \frac{\langle x | \hat{H} | \Psi_\theta \rangle}{\langle x | \Psi_\theta \rangle} \quad (2.12)$$

and the variational energy is estimated as

$$E_{\text{var}} \approx \frac{1}{N} \sum_{i=1}^N E_{\text{loc}}(x_i) \quad (2.13)$$

By iteratively updating the variational parameters so as to minimize  $E_{\text{var}}$ , one obtains increasingly accurate approximations of the ground- or excited-state. The flexibility in the choice of the variational ansatz, together with the favorable scaling of Monte Carlo sampling in high-dimensional spaces and the possibility of using various optimization algorithms [31], makes VMC particularly attractive for the

study of strongly correlated quantum many-body systems.

## 2.3 Time-dependent Variational Monte Carlo

While Variational Monte Carlo is primarily formulated as a method for approximating ground-state properties, many problems of physical interest require the description of the dynamics of quantum many-body systems. Examples include non-equilibrium phenomena, quantum quenches, and dissipative processes.

The central idea of Time-Dependent Variational Monte Carlo (tVMC) is to extend the variational approach to dynamical problems by promoting the variational parameters to time-dependent quantities. As a result, the wavefunction evolves within a restricted manifold of parametrized states rather than exploring the full Hilbert space, whose dimension generally grows exponentially with system size [32, 33, 34, 35].

The exact time evolution generated by the Schrödinger equation cannot, in general, be represented exactly within a finite variational manifold. The dynamics is therefore approximated by determining, at each instant of time, the evolution of the variational parameters that best reproduces the exact quantum dynamics while remaining inside the chosen variational subspace. In this way, the many-body problem is reduced to solving a set of coupled equations for a comparatively small number of parameters.

As in conventional VMC, the quantities entering the equations of motion can be expressed as expectation values over the probability distribution induced by the variational state and are therefore efficiently evaluated through Monte Carlo sampling. This combination of variational principles and stochastic sampling allows tVMC to address the dynamics of systems that would otherwise be inaccessible to exact numerical methods, while hopefully describing accurate dynamics when sufficiently expressive ansätze are employed.

### 2.3.1 Equations of Motion

Consider a variational state  $|\Psi(\boldsymbol{\alpha}(t))\rangle$ , where the variational parameters  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_M) \in \mathbb{C}^M$  are complex values allowed to depend on time. The exact dynamics is generated by the Schrödinger equation,

$$\left( \frac{d}{dt} |\Psi\rangle \right)_{\text{ex}} = -\frac{i}{\hbar} \hat{H} |\Psi\rangle \quad (2.14)$$

whereas the variational evolution is constrained to remain on the manifold of parametrized states. The chain rule yields,

$$\left( \frac{d}{dt} |\Psi\rangle \right)_{\text{var}} = \sum_k \dot{\alpha}_k \frac{\partial}{\partial \alpha_k} |\Psi\rangle \quad (2.15)$$

Following the time-dependent variational principle, the optimal evolution is obtained by minimizing the distance between the two tangent vectors in Hilbert space,

$$\Delta^2(t) = \frac{1}{\langle \Psi | \Psi \rangle} \left\| \left( \frac{d}{dt} |\Psi\rangle \right)_{\text{var}} - \left( \frac{d}{dt} |\Psi\rangle \right)_{\text{ex}} \right\|^2 \quad (2.16)$$

Substituting the expressions above gives

$$\Delta^2(t) = \frac{1}{\langle \Psi | \Psi \rangle} \left\| \sum_k \dot{\alpha}_k \frac{\partial |\Psi\rangle}{\partial \alpha_k} + \frac{i}{\hbar} \hat{H} |\Psi\rangle \right\|^2 \quad (2.17)$$

Introducing the configuration basis  $\mathbb{I} = \sum_x |x\rangle \langle x|$  and multiplying and dividing by  $|\langle x | \Psi \rangle|^2$ , the distance can be rewritten as

$$\Delta^2(t) = \sum_x \frac{|\langle x | \Psi(\alpha) \rangle|^2}{\langle \Psi(\alpha) | \Psi(\alpha) \rangle} \left| \sum_k \frac{1}{\langle x | \Psi(\alpha) \rangle} \frac{\partial \langle x | \Psi(\alpha) \rangle}{\partial \alpha_k} \dot{\alpha}_k + \frac{i}{\hbar} \frac{\langle x | \hat{H} | \Psi(\alpha) \rangle}{\langle x | \Psi(\alpha) \rangle} \right|^2 \quad (2.18)$$

This expression can be interpreted as an expectation value over the probability distribution  $p(x) = \frac{|\langle x | \Psi \rangle|^2}{\langle \Psi | \Psi \rangle}$ . It is therefore convenient to define the *local energy*

$$E_{\text{loc}}(x) = \frac{\langle x | \hat{H} | \Psi \rangle}{\langle x | \Psi \rangle} \quad (2.19)$$

and the *local operators*

$$O_k(x, \alpha) = \frac{1}{\langle x | \Psi \rangle} \frac{\partial \langle x | \Psi \rangle}{\partial \alpha_k} = \frac{\partial}{\partial \alpha_k} \log \langle x | \Psi \rangle \quad (2.20)$$

The quantity to be minimized then becomes

$$\Delta^2(t) = \left\langle \left| \sum_k O_k(x) \dot{\alpha}_k + \frac{i}{\hbar} E_{\text{loc}}(x) \right|^2 \right\rangle \quad (2.21)$$

where  $\langle \bullet \rangle$  denotes the expectation value with respect to  $p(x)$ .

The equations of motion are obtained by requiring stationarity of  $\Delta^2(t)$  with respect to the complex variables  $\dot{\alpha}_k$ , thus imposing:

$$\frac{\partial \Delta^2(t)}{\partial \dot{\alpha}_k^R} = 2 \operatorname{Re} \left\langle \sum_{k'} O_k^*(x, \alpha) O_{k'}(x, \alpha) \dot{\alpha}_{k'} + \frac{i}{\hbar} O_k^*(x; \alpha) \mathcal{E}(x; \alpha) \right\rangle = 0 \quad (2.22)$$

$$\frac{\partial \Delta^2(t)}{\partial \dot{\alpha}_k^I} = 2 \operatorname{Im} \left\langle \sum_{k'} O_k^*(x, \alpha) O_{k'}(x, \alpha) \dot{\alpha}_{k'} + \frac{i}{\hbar} O_k^*(x; \alpha) \mathcal{E}(x; \alpha) \right\rangle = 0 \quad (2.23)$$

the resulting conditions are

$$i\hbar \sum_{k'} \langle O_k^* O_{k'} \rangle \dot{\alpha}_{k'} = \langle O_k^* E_{\text{loc}} \rangle \quad \forall k \quad (2.24)$$

At this stage the equations still depend on the overall phase of the wavefunction. However, states differing only by a global complex factor represent the same physical state and should therefore be regarded as physically equivalent. To make this invariance explicit, let us introduce an additional variational parameter  $\phi$ , playing the role of a global complex phase,

$$|\Psi(\phi, \boldsymbol{\alpha})\rangle = e^{\phi} |\psi(\boldsymbol{\alpha})\rangle \quad (2.25)$$

where  $\psi$  denotes the original parametrized state and the remaining parameters are collectively denoted by  $\boldsymbol{\alpha}$ . The corresponding logarithmic derivative is simply

$$O_\phi(x) = \frac{\partial}{\partial \phi} \log \Psi(x) = 1 \quad (2.26)$$

Including  $\phi$  among the variational parameters, the stationarity conditions (2.24) become

$$i\hbar \sum_{k'} \langle O_k^* O_{k'} \rangle \dot{\alpha}_{k'} + i\hbar \langle O_k^* \rangle \dot{\phi} = \langle O_k^* E_{\text{loc}} \rangle \quad \forall k \quad (2.27)$$

$$i\hbar \sum_{k'} \langle O_{k'} \rangle \dot{\alpha}_{k'} + i\hbar \dot{\phi} = \langle E_{\text{loc}} \rangle \quad (2.28)$$

The second equation (2.28) can be solved explicitly for the phase velocity, then substituting it into (2.27) yields

$$i\hbar \sum_{k'} (\langle O_k^* O_{k'} \rangle - \langle O_k^* \rangle \langle O_{k'} \rangle) \dot{\alpha}_{k'} = \langle O_k^* E_{\text{loc}} \rangle - \langle O_k^* \rangle \langle E_{\text{loc}} \rangle \quad (2.29)$$

Defining the *Geometric Quantum Tensor* (GQT) as

$$S_{kk'} = \langle O_k^* O_{k'} \rangle - \langle O_k^* \rangle \langle O_{k'} \rangle \quad (2.30)$$

and the *Force Vector* as

$$F_k = \langle O_k^* E_{\text{loc}} \rangle - \langle O_k^* \rangle \langle E_{\text{loc}} \rangle \quad (2.31)$$

the equations of motion assume the compact form

$$i\hbar \sum_{k'} S_{kk'} \dot{\alpha}_{k'} = F_k \quad (2.32)$$

The matrix  $S$  is the covariance matrix of the logarithmic derivatives of the wavefunction and therefore is Hermitian and positive semidefinite. Geometrically, it corresponds to the quantum geometric tensor restricted to the variational manifold, while the vector  $F$  plays the role of a generalized force driving the variational dynamics. Finding the time-discretized updates  $\Delta\alpha \sim \dot{\alpha}dt$  amounts to inverting Eq (2.32). This is eased by the exact property that  $S$  is positive semidefinite, provided that care is taken regarding null or very small eigenvalues. We will discuss this issue in the context of the open systems variant in Section 4.4.1.

Equivalently, the same equations can be obtained by minimizing the infinitesimal Fubini–Study distance between the exact and variationally evolved states, making explicit that tVMC amounts to projecting the exact Schrödinger dynamics onto the tangent space of the variational manifold.

## Chapter 3

# Open time-dependent Variational Monte Carlo

The numerical simulation of open many-body quantum systems remains a challenging task due to the combined effects of environmental interactions and the exponential growth of the Hilbert space with system size. The open time-dependent Variational Monte Carlo (otVMC) method addresses these difficulties by combining the quantum trajectory formalism introduced in Chapter 1 with the Time-Dependent Variational Monte Carlo (tVMC) framework presented in Chapter 2.

The starting point of the method is the unraveling of the Lindblad master equation into an ensemble of stochastic pure-state evolutions. Rather than directly evolving the density matrix, one generates  $M$  independent realizations of an appropriate stochastic Schrödinger equation (SSE). Physical observables are then recovered by averaging over the ensemble of trajectories, reproducing the Markovian dynamics described by the Lindblad equation. Calling  $d$  the dimension of the associated Hilbert space, direct integration of the density matrix scales at worse as  $\mathcal{O}(d^4)$  in computational cost and requires  $\mathcal{O}(d^2)$  memory, the simulation of  $M$  pure-state trajectories scales as  $\mathcal{O}(Md^2)$ , or effectively as  $\mathcal{O}(d^2)$  when the trajectories are evolved in parallel and the parallelization overhead and scalar post-processing are negligible, requiring only  $\mathcal{O}(d)$  memory. In practice, accurate results are often obtained using a number of trajectories much smaller than the Hilbert-space dimension, namely  $M \ll d^2$ .

Despite this improvement, each trajectory is still represented by a wave function in the full Hilbert space that scales exponentially with the system size. This is precisely where the tVMC framework becomes essential. By introducing a suitable variational ansatz, the quantum state is constrained to evolve within a low-dimensional

variational manifold parametrized by a set of time-dependent parameters. The full Schrödinger dynamics is therefore replaced by the evolution of these variational parameters, whose equations of motion are obtained through a time-dependent variational principle, as discussed in the previous chapter. If the chosen parameterization efficiently captures the relevant physics of the system, the computational complexity can be reduced from an exponential dependence on system size to a polynomial one, often scaling quadratically or even linearly with the number of degrees of freedom. The price to pay for this reduction is that the resulting dynamics become approximate and depend on the expressive power of the selected variational ansatz.

In the following sections, the equations governing the evolution of the variational parameters for stochastic quantum trajectories are derived. Although the original motivation of the method is the simulation of Lindblad dynamics through ensemble averages, the same framework naturally extends to the description of conditioned dynamics associated with individual measurement records, allowing one to efficiently study continuously monitored open quantum systems and their conditional dynamics.

### 3.1 Equations of motion for otVMC

The derivation of the equations of motion for the variational parameters closely follows the procedure presented for the tVMC framework. The starting point is the diffusive stochastic Schrödinger equation introduced in Section 1.5. For convenience, we adopt its equivalent Stratonovich representation (see Eq. (1.48)), namely

$$d|\psi^{(c)}\rangle = \left\{ -\frac{i}{\hbar} \hat{H}_{\text{eff}}^{\text{Strat}} dt + \sum_n \left( \hat{c}_n - \frac{1}{2} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) \circ dW_n \right\} |\psi^{(c)}\rangle \quad (3.1)$$

where the effective Hamiltonian is

$$\hat{H}_{\text{eff}}^{\text{Strat}} = \hat{H} - \frac{i\hbar}{2} \sum_n \left( \hat{c}_n^\dagger \hat{c}_n - 2 \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \hat{c}_n + \hat{c}_n^2 + \langle \hat{c}_n + \hat{c}_n^\dagger \rangle^2 - \frac{1}{2} \langle \hat{c}_n^2 + 2 \hat{c}_n^\dagger \hat{c}_n + \hat{c}_n^{\dagger 2} \rangle \right) \quad (3.2)$$

The quantum state is parametrized by a set of complex variational parameters,  $\boldsymbol{\theta}(t) = \{\phi(t), \boldsymbol{\alpha}(t)\}$  where  $\phi$  is a global phase parameter and  $\boldsymbol{\alpha} = \{\alpha_1, \dots, \alpha_p\}$  denotes the set of variational parameters defining the ansatz,

$$\Psi(\boldsymbol{\theta}(t), \mathbf{x}) = e^{\phi(t)} \psi(\boldsymbol{\alpha}(t), \mathbf{x}) \quad (3.3)$$

Introducing a generic coordinate representation,  $\Psi(\mathbf{x}, \boldsymbol{\theta}) = \langle \mathbf{x} | \Psi(\boldsymbol{\theta}) \rangle$ , the stochastic Schrödinger equation can be written as

$$d\Psi(\mathbf{x}, \boldsymbol{\theta}) = \Psi(\mathbf{x}, \boldsymbol{\theta}) \left[ -\frac{i}{\hbar} \mathcal{E}_{\text{eff}}(\mathbf{x}, \boldsymbol{\alpha}) dt + \sum_{n=1}^N \left( \mathcal{B}^n(\mathbf{x}, \boldsymbol{\alpha}) - \frac{1}{2} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) \circ dW_n \right] \quad (3.4)$$

having conveniently introduced the *local effective energy* and the *local noise* terms,

$$\mathcal{E}_{\text{eff}}(\mathbf{x}, \boldsymbol{\alpha}) = \frac{\langle \mathbf{x} | \hat{H}_{\text{eff}}^{\text{Strat}} | \Psi(\boldsymbol{\theta}) \rangle}{\langle \mathbf{x} | \Psi(\boldsymbol{\theta}) \rangle} \quad (3.5)$$

$$\mathcal{B}^n(\mathbf{x}, \boldsymbol{\alpha}) = \frac{\langle \mathbf{x} | \hat{c}_n | \Psi(\boldsymbol{\theta}) \rangle}{\langle \mathbf{x} | \Psi(\boldsymbol{\theta}) \rangle} \quad (3.6)$$

On the variational manifold, the state variation induced by the time dependence of the parameters follows from the chain rule (valid thanks to the Stratonovich interpretation),

$$\begin{aligned} d\Psi_{\text{chain}}(\mathbf{x}, \boldsymbol{\theta}) &= \frac{\partial \Psi(\mathbf{x}, \boldsymbol{\theta})}{\partial \phi} d\phi + \sum_{k=1}^p \frac{\partial \Psi(\mathbf{x}, \boldsymbol{\theta})}{\partial \alpha_k} d\alpha_k \\ &= e^\phi \psi(\mathbf{x}, \boldsymbol{\alpha}) d\phi + \sum_{k=1}^p e^\phi \frac{\partial \psi(\mathbf{x}, \boldsymbol{\alpha})}{\partial \alpha_k} d\alpha_k \\ &= \Psi(\mathbf{x}, \boldsymbol{\theta}) \left( d\phi + \sum_{k=1}^p d\alpha_k \mathcal{O}_k(\mathbf{x}, \boldsymbol{\alpha}) \right) \end{aligned} \quad (3.7)$$

where  $p$  denotes the number of variational parameters  $\boldsymbol{\alpha}$  and

$$\mathcal{O}_k(\mathbf{x}, \boldsymbol{\alpha}) \equiv \frac{\partial \ln \psi(\mathbf{x}, \boldsymbol{\alpha})}{\partial \alpha_k} = \frac{1}{\psi(\mathbf{x}, \boldsymbol{\alpha})} \frac{\partial \psi(\mathbf{x}, \boldsymbol{\alpha})}{\partial \alpha_k} \quad (3.8)$$

are the *local operators* associated with the ansatz.

As in the closed-system case, the optimal evolution is determined by minimizing the Hilbert-space distance between the exact stochastic evolution and its variational projection,

$$\begin{aligned} \Delta^2(t) &= \sum_{\mathbf{x}} \left| d\Psi_{\text{chain}}(\mathbf{x}, \boldsymbol{\theta}) - d\Psi(\mathbf{x}, \boldsymbol{\theta}) \right|^2 = \sum_{\mathbf{x}} \left| \Psi(\mathbf{x}, \boldsymbol{\theta}) \left[ d\phi + \sum_{k=1}^p d\alpha_k \mathcal{O}_k(\mathbf{x}, \boldsymbol{\alpha}) \right. \right. \\ &\quad \left. \left. + \frac{i}{\hbar} \mathcal{E}_{\text{eff}}(\mathbf{x}, \boldsymbol{\alpha}) dt - \sum_{n=1}^N \left( \mathcal{B}^n(\mathbf{x}, \boldsymbol{\alpha}) - \frac{1}{2} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) \circ dW_n \right] \right|^2 \\ &= \sum_{\mathbf{x}} |\Psi(\mathbf{x}, \boldsymbol{\theta})|^2 |\mathcal{Z}(\mathbf{x}, t)|^2 \end{aligned} \quad (3.9)$$

where

$$\mathcal{Z}(\mathbf{x}, t) = d\phi + \sum_{k=1}^p d\alpha_k \mathcal{O}_k(\mathbf{x}, \boldsymbol{\alpha}) + \frac{i}{\hbar} \mathcal{E}_{\text{eff}}(\mathbf{x}, \boldsymbol{\alpha}) dt - \sum_{n=1}^N \left( \mathcal{B}^n(\mathbf{x}, \boldsymbol{\alpha}) - \frac{1}{2} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) \circ dW_n$$

The equations of motion are obtained by imposing that the first-order variations of  $\Delta^2(t)$  with respect to the parameter velocities vanish. This condition identifies the tangent vector on the variational manifold that best approximates the exact stochastic evolution in the least-squares sense.

At this stage, all terms appearing in the minimization functional can be expressed as expectation values with respect to the probability distribution induced by the variational state

$$\langle O(\mathbf{x}, t) \rangle = \sum_{\mathbf{x}} O(\mathbf{x}, t) |\psi(\mathbf{x}, \boldsymbol{\theta})|^2 \quad (3.10)$$

The stationarity conditions with respect to  $\dot{\phi}$  and  $\dot{\alpha}_k$  therefore yield

$$\begin{aligned} \frac{\partial \Delta^2(t)}{\partial d\phi^*} &= d\phi + \sum_{k=1}^p \langle O_k(\mathbf{x}, \boldsymbol{\alpha}) \rangle d\alpha_k + \frac{i}{\hbar} \langle \mathcal{E}_{\text{eff}}(\mathbf{x}, \boldsymbol{\alpha}) \rangle dt \\ &\quad - \sum_{n=1}^N \left( \langle \mathcal{B}^n(\mathbf{x}, \boldsymbol{\alpha}) \rangle - \frac{1}{2} \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) \circ dW_n = 0 \end{aligned} \quad (3.11)$$

$$\begin{aligned} \frac{\partial \Delta^2(t)}{\partial (d\alpha_j)^*} &= \langle \mathcal{O}_j^*(\mathbf{x}, \boldsymbol{\alpha}) \rangle d\phi + \sum_{k=1}^p \langle \mathcal{O}_j^*(\mathbf{x}, \boldsymbol{\alpha}) \mathcal{O}_k(\mathbf{x}, \boldsymbol{\alpha}) \rangle d\alpha_k \\ &\quad + \frac{i}{\hbar} \langle \mathcal{O}_j^*(\mathbf{x}, \boldsymbol{\alpha}) \mathcal{E}_{\text{eff}}(\mathbf{x}, \boldsymbol{\alpha}) \rangle dt \\ &\quad - \sum_{n=1}^N \left( \langle \mathcal{O}_j^*(\mathbf{x}, \boldsymbol{\alpha}) \mathcal{B}^n(\mathbf{x}, \boldsymbol{\alpha}) \rangle - \frac{1}{2} \langle \mathcal{O}_j^*(\mathbf{x}, \boldsymbol{\alpha}) \rangle \langle \hat{c}_n + \hat{c}_n^\dagger \rangle \right) \circ dW_n = 0 \end{aligned} \quad (3.12)$$

By substituting the global phase variation, obtained from the first equation, into the second one, one finally obtains

$$\sum_{k=1}^p S_{jk}(\boldsymbol{\alpha}) d\alpha_k + \frac{i}{\hbar} \mathcal{D}_j(\boldsymbol{\alpha}) dt - \sum_{n=1}^N \mathcal{N}_j^n(\boldsymbol{\alpha}) \circ dW_n = 0 \quad (3.13)$$

where we have introduced

$$\mathcal{S}_{jk}(\boldsymbol{\alpha}) \equiv \langle \mathcal{O}_j^* \mathcal{O}_k \rangle - \langle \mathcal{O}_j^* \rangle \langle \mathcal{O}_k \rangle \quad (3.14)$$

$$\mathcal{D}_j(\boldsymbol{\alpha}) \equiv \langle \mathcal{O}_j^* \mathcal{E}_{\text{eff}} \rangle - \langle \mathcal{O}_j^* \rangle \langle \mathcal{E}_{\text{eff}} \rangle \quad (3.15)$$

$$\mathcal{N}_j^n(\boldsymbol{\alpha}) \equiv \langle \mathcal{O}_j^* \mathcal{B}^n \rangle - \langle \mathcal{O}_j^* \rangle \langle \mathcal{B}^n \rangle \quad (3.16)$$

The matrix  $\mathcal{S}_{jk}$  is the quantum geometric tensor already encountered in the closed-system tVMC formalism. It encodes the geometry of the variational manifold and determines how parameter variations translate into changes of the quantum state.

The vector  $\mathcal{D}_j$  plays the role of a generalized drift term. In analogy with closed-system tVMC, it can be interpreted as the gradient of the effective energy; however, due to the non-Hermitian nature of the effective Hamiltonian, it now also contains the dissipative contributions arising from the coupling to the environment.

Finally, the quantities  $\mathcal{N}_j^n$  constitute the noise-coupling vectors and are a distinctive feature of open-system dynamics. They describe how the independent Wiener processes associated with the environmental channels are projected onto the variational manifold. Consequently, each realization of the stochastic evolution experiences a different local decoherence process, giving rise to diffusive dynamics and, in general, to trajectory-dependent symmetry breaking.

Equivalently, the previous equation can be written in compact vector form as

$$\mathcal{S}(\boldsymbol{\alpha}) d\boldsymbol{\alpha} = \mathcal{F}(\boldsymbol{\theta}) \quad (3.17)$$

where we have introduced the stochastic generalized force variation

$$\mathcal{F}_j(\boldsymbol{\theta}) \equiv -\frac{i}{\hbar} \mathcal{D}_j(\boldsymbol{\theta}) dt + \sum_{n=1}^N \mathcal{N}_j^n(\boldsymbol{\theta}) \circ dW_n \quad (3.18)$$

By inverting the matrix  $\mathcal{S}$ , one finally obtains the stochastic differential equations governing the evolution of the variational parameters,

$$d\boldsymbol{\alpha} = \mathcal{S}^{-1}(\boldsymbol{\alpha}) \mathcal{F}(\boldsymbol{\theta}) \quad (3.19)$$

or, explicitly,

$$d\boldsymbol{\alpha} = -\frac{i}{\hbar} \mathcal{S}^{-1}(\boldsymbol{\alpha}) \mathcal{D}(\boldsymbol{\theta}) dt + \sum_{n=1}^N \mathcal{S}^{-1}(\boldsymbol{\alpha}) \mathcal{N}^n(\boldsymbol{\theta}) \circ dW_n \quad (3.20)$$

It is worth noting that the quantities defined in Eqs. (3.14)–(3.16) are covariance-like objects and are therefore invariant under constant shifts of the corresponding local estimators. Consequently, scalar contributions to the effective Hamiltonian, including the Itô correction terms, do not influence the evolution of the variational parameters.

Finally, it should be noted that the derivation does not require the variational states to be normalized. Repeating the minimization procedure for unnormalized states leads to exactly the same equations of motion for the parameters  $\alpha$ . The only modification concerns the equation for the global phase parameter  $\phi$ . Since  $\phi$  merely accounts for an overall normalization and phase factor, it does not affect physical observables nor the resulting dynamics of the system.

## 3.2 Algorithmic Structure

Having derived the equations of motion and all the quantities required for their numerical evaluation, a general overview of the implemented otVMC algorithm can now be given. Although the unconditional and conditional formulations share the same variational framework, they differ in the way observables are averaged and in the role played by stochastic trajectories. For clarity, the computational workflow for the two cases is discussed separately.

### 3.2.1 Unconditional Dynamics

Once the physical model and the variational ansatz have been specified, the otVMC simulation proceeds by generating an ensemble of  $M$  independent stochastic trajectories. All trajectories are initialized in the same quantum state and subsequently evolved independently according to the stochastic equations of motion derived in the previous section.

For a given trajectory and at a given time  $t$ , a set of system configurations  $\sigma$  is sampled using the Metropolis-Hastings algorithm. The sampled configurations are employed to obtain Monte Carlo estimates of all quantities entering the equations of motion, namely the covariance matrix  $\mathcal{S}$ , the generalized drift  $\mathcal{D}$ , the noise vectors  $\mathcal{N}_n$ , and any observable of interest.

The Wiener increments  $\Delta W_n(t)$  associated with the environmental channels are then generated and the stochastic differential equations for the variational parameters

are integrated over a time step  $\delta t$ , yielding the updated parameters  $\boldsymbol{\theta}(t + \delta t)$ . The procedure is repeated until the final simulation time is reached.

After all trajectories have been propagated, expectation values of physical observables are obtained by averaging over the entire ensemble of trajectories. A schematic summary of the procedure is given in Algorithm 1.

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**Algorithm 1** Unconditional otVMC

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- 1: **Input:** physical model, variational ansatz, initial condition,  $\delta t$ : time step,  $N_{\text{traj}}$ : number of trajectories
  - 2: **for**  $\text{traj} = 1, \dots, N_{\text{traj}}$  **do**
  - 3:   Set initial condition  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}(t_0)$
  - 4:   **for**  $t = t_0, \delta t, \dots, t_{\text{final}}$  **do**
  - 5:     Generate Wiener increments  $\Delta W_n(t)$
  - 6:     Sample configurations  $\sigma \sim |\psi(\sigma, \boldsymbol{\theta})|^2$  using the Metropolis algorithm
  - 7:     Estimate  $\mathcal{S}$ ,  $\mathcal{D}$ ,  $\mathcal{N}_n$ , and observables
  - 8:     Compute  $d\phi$  and  $d\boldsymbol{\alpha}$
  - 9:     Update  $\boldsymbol{\theta}(t + \delta t)$  using a SDE integrator
  - 10:   **end for**
  - 11: **end for**
  - 12: Average observables over the  $N_{\text{traj}}$  trajectories
  - 13: **Output:** Trajectory-averaged expectation values of the observables
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### 3.2.2 Conditional Dynamics

The conditional formulation aims at simulating experimental realizations of a continuously monitored open quantum system. In this context, an experiment is specified by the choice of the observables being continuously measured and by the corresponding measurement records.

The interaction between the system and the environment can be decomposed into different channels, each representing one kind of coupling to the surroundings. Depending on whether their outputs are measured or not, these channels can be divided into monitored and unmonitored channels.

Monitored channels are continuously observed and therefore produce a time-resolved stochastic measurement record. In the diffusive formulation adopted in this work, the stochastic parts of such records are represented by the Wiener increments associated with the corresponding channels. By contrast, unmonitored channels still contribute

to the system dynamics through decoherence and dissipation, but their outputs are inaccessible and no measurement record is available.

Mathematically, a conditioned trajectory is completely determined by the initial state together with the realizations of all Wiener increments. A crucial distinction, however, must be made between the increments associated with monitored and unmonitored channels. The former represent the actual measurement outcomes and therefore uniquely define a given experimental realization. Consequently, they are generated once and kept fixed throughout the simulation of that experiment. The latter instead account for environmental fluctuations that are not observed and must therefore be independently sampled for each stochastic trajectory.

From a computational perspective, the simulation naturally acquires a hierarchical structure. For a given experimental realization, all trajectories share the same Wiener increments associated with the monitored channels, while independent increments are generated for the unmonitored channels. Conditional expectation values are then obtained by averaging over this ensemble of trajectories. Statistical properties over different experimental realizations can subsequently be estimated by repeating the procedure for independent realizations of the monitored-channel increments. In the present implementation, observables are stored for every trajectory and every experimental realization. The averages over trajectories and experiments, together with the corresponding statistical estimators, are evaluated in a separate post-processing stage. In the postprocessing stage, the observables are first averaged over the internal trajectories associated with the same experimental realization. This gives the conditional expectation values corresponding to a fixed measurement record. By subsequently averaging these conditional expectation values over the different experimental realizations, one recovers the unconditional expectation values. However, for nonlinear quantities such as variances and covariances, the order of operations is important. In this case, the nonlinear combination of observables should be performed after the average over internal trajectories, but before the average over experimental realizations. This distinction is particularly relevant in the monitored case, since each experimental realization corresponds to a different measurement record, and combining already unconditional averages is in general not equivalent to averaging the corresponding conditional nonlinear quantities. This approach provides greater flexibility in the analysis and allows different statistical quantities to be computed from the same raw dataset. The overall workflow is summarized in Algorithm 2.

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**Algorithm 2** Conditional otVMC

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- 1: **Input:** physical model, variational ansatz, initial condition,  $\delta t$ : time step,  $N_{\text{traj}}$ : number of trajectories,  $N_{\text{exp}}$ : number of experiments
- 2: **for**  $\text{exp} = 1, \dots, N_{\text{exp}}$  **do**
- 3:     Generate Wiener increments  $\Delta W_m(t)$  for each monitored channel
- 4:     **for**  $\text{traj} = 1, \dots, N_{\text{traj}}$  **do**
- 5:         Set initial condition  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}(t_0)$
- 6:         **for**  $t = t_0, \delta t, \dots, t_{\text{final}}$  **do**
- 7:             Generate Wiener increments  $\Delta W_n(t)$  for unmonitored channels
- 8:             Sample configurations  $\sigma \sim |\psi(\sigma, \boldsymbol{\theta})|^2$  using the Metropolis algorithm
- 9:             Estimate  $\mathcal{S}$ ,  $\mathcal{D}$ ,  $\mathcal{N}_n$ , and observables
- 10:            Compute  $d\phi$  and  $d\boldsymbol{\alpha}$
- 11:            Update  $\boldsymbol{\theta}(t + \delta t)$  using a SDE integrator
- 12:         **end for**
- 13:         Store trajectory observables
- 14:     **end for**
- 15: **end for**
- 16: **Output:** Time series of observables for each trajectory and experimental realization.

**Postprocessing**

Compute conditional expectation values, averaging over the internal trajectories for each experiment. Optionally, subsequently performing statistical analysis of experiments

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# Chapter 4

## Numerical Implementation

The numerical implementation employed in this work is based on an existing C++ realization of the open time-dependent Variational Monte Carlo (otVMC) algorithm [1, 3, 36], stored on a private gitlab repository. The code is designed to simulate both closed and open quantum systems within a unified framework and follows an object-oriented architecture based on abstract interfaces and modular components. Such a design facilitates the implementation of different physical models, variational wave functions, and integration schemes while maintaining a clear separation between physical and numerical aspects of the algorithm.

Linear algebra operations are performed using the Armadillo library, whereas the Monte Carlo sampling is parallelized through MPI, allowing independent Markov chains to be distributed across multiple processes and substantially reducing the computational cost of each variational time step.

Although the otVMC framework can, in principle, be extended to more general quantum systems, the present implementation is specifically designed for systems composed of discrete two-level degrees of freedom, such as spin-1/2 particles or effective two-level atoms. The computational basis is therefore represented by configurations

$$\sigma = (\sigma_1, \dots, \sigma_N) \quad \text{with } \sigma_i = \pm 1$$

where each component denotes the local state of one constituent.

The implementation is organized around three core classes:

- **WaveFunction**: responsible for the definition of the variational ansatz and the computation of all wave-function-dependent quantities.

- **SpinHamiltonian**: encodes the physical model and provides the local estimators required by the variational algorithm.
- **SamplerOpen**: orchestrates the Monte Carlo sampling and the stochastic time evolution of the variational parameters.

The work carried out in the present Thesis introduces several extensions to the original implementation. In particular, the code has been generalized to two-dimensional spin geometries and to physically relevant monitored Ising systems, additional variational ansätze have been implemented for benchmarking purposes, and the random number generation framework has been redesigned to improve computational performance. The main implementation choices and their motivations are discussed in the following sections. Furthermore, a scaling analysis of the code, including its parallel performance, has been carried out. The results are reported in Appendix A.

## 4.1 WaveFunction Class

The `WaveFunction` class provides the interface between the variational ansatz and the Monte Carlo engine. Its purpose is to represent the parameterized quantum state

$$\psi(\sigma; \boldsymbol{\theta}) \tag{4.1}$$

where  $\sigma$  denotes a spin configuration and  $\boldsymbol{\theta}$  collectively represents the variational parameters. In addition to storing and updating the variational parameters, the class evaluates all wavefunction-dependent quantities required by the otVMC algorithm.

In particular, its main tasks include:

- evaluating the wavefunction amplitude and the local operators,

$$O_k(\sigma) = \frac{\partial}{\partial \theta_k} \log \psi(\sigma; \boldsymbol{\theta}) \tag{4.2}$$

which enter the definition of the quantum geometric tensor and the generalized force vector;

- computing the probability ratios required by the Metropolis-Hastings sampling procedure.

As discussed in Section 2.1.2, the auxiliary distribution in the Metropolis-Hastings algorithm is chosen to be symmetric. Under this assumption, the acceptance probability (2.5) depends solely on the ratio between the probabilities associated with the proposed and current configurations,

$$\frac{P(\sigma_{\text{new}})}{P(\sigma_{\text{old}})} = \frac{|\psi(\sigma_{\text{new}}; \boldsymbol{\theta})|^2}{|\psi(\sigma_{\text{old}}; \boldsymbol{\theta})|^2} \quad (4.3)$$

The evaluation of this quantity depends on the specific variational ansatz and is implemented analytically whenever possible in order to minimize the computational cost of each Monte Carlo update. The different parameterizations of the wave function considered in this work are discussed in the following sections.

### 4.1.1 Exact Hilbert-Space Parameterization

During the preliminary stages of the development and validation of the otVMC implementation, it is particularly useful to have an exact representation of the Hilbert space. Such a representation allows one to isolate numerical and implementation issues without introducing the additional uncertainty associated with an approximate variational wavefunction. For this reason, an exact parameterization based on the full expansion of the quantum state in the computational basis has been implemented.

For a system of  $N$  spin-1/2 degrees of freedom, the Hilbert space has dimension  $\dim \mathcal{H} = 2^N$ , and the variational state is written as

$$|\psi(\phi, \boldsymbol{\alpha})\rangle = e^{\phi} \sum_{n=0}^{2^N-1} \alpha_n |n\rangle \quad (4.4)$$

where  $\{|n\rangle\}$  denotes the computational basis and

$$\boldsymbol{\alpha} = (\alpha_0, \alpha_1, \dots, \alpha_{2^N-1})$$

contains one complex variational parameter for each basis state. The explicit introduction of the parameter  $\phi$  separates the global amplitude and phase of the wavefunction from the relative amplitudes encoded in the coefficients  $\alpha_n$ , consistently with the parameterization adopted throughout this work.

Consequently, the ansatz contains  $2^N + 1$  complex variational parameters and its computational cost grows exponentially with the system size, making it impractical for large systems. Its use is therefore restricted to small-scale simulations and

benchmarking tests. Although this representation spans the entire Hilbert space and is therefore exact, it remains fully embedded within the otVMC framework and evolves according to the same variational equations of motion employed by the approximate ansätze.

Since the computational basis depends only on the number of spins and not on their spatial arrangement, the implementation is completely independent of the underlying geometry and can therefore be employed for both one- and two-dimensional systems, as well as more general interaction graphs.

As a simple example, for a system of two spins one has

$$|\psi(\phi, \boldsymbol{\alpha})\rangle = e^{\phi} (\alpha_0 |\downarrow\downarrow\rangle + \alpha_1 |\uparrow\downarrow\rangle + \alpha_2 |\downarrow\uparrow\rangle + \alpha_3 |\uparrow\uparrow\rangle) \quad (4.5)$$

To compute quantities required by the Monte Carlo algorithm, such as acceptance probabilities and local operators, it is necessary to evaluate the wavefunction amplitude corresponding to a given spin configuration,

$$\psi(\sigma; \phi, \boldsymbol{\alpha}) = \langle \sigma | \psi(\phi, \boldsymbol{\alpha}) \rangle \quad (4.6)$$

For instance, for the configuration  $\sigma = (-1, +1)$ , corresponding to the basis state  $|\downarrow\uparrow\rangle$ , one simply obtains

$$\psi((-1, +1); \phi, \boldsymbol{\alpha}) = \langle \downarrow\uparrow | \psi(\phi, \boldsymbol{\alpha}) \rangle = e^{\phi} \alpha_2 \quad (4.7)$$

More generally, since every spin configuration corresponds to exactly one element of the computational basis, the projection operation merely selects the coefficient associated with that basis state. The implementation therefore requires a one-to-one correspondence between a configuration

$$\sigma = (\sigma_1, \sigma_2, \dots, \sigma_N) \quad \sigma_i = \pm 1 \quad (4.8)$$

and an index of the basis expansion.

This mapping is obtained by interpreting the spin configuration as a binary number. Each spin is first mapped according to  $b_i = \frac{1-\sigma_i}{2}$  so that  $\sigma_i = +1$  is associated with  $b_i = 0$  and  $\sigma_i = -1$  with  $b_i = 1$ . The resulting binary sequence is then interpreted as

the integer label of the corresponding basis state. For example,

$$\sigma = (+1, -1, +1, -1) \longrightarrow b = (0, 1, 0, 1) \longrightarrow 0101_2 = 5$$

and therefore  $\psi(\sigma; \phi, \boldsymbol{\alpha}) = e^\phi \alpha_5$ .

As a consequence, the acceptance probability required by the Metropolis algorithm can be computed directly from the amplitudes associated with the current and proposed configurations,

$$\frac{P(\sigma_{\text{new}})}{P(\sigma_{\text{old}})} = \frac{|\alpha_{i_{\text{new}}}|^2}{|\alpha_{i_{\text{old}}}|^2} \quad (4.9)$$

where  $i_{\text{old}}$  and  $i_{\text{new}}$  denote the basis indices corresponding to the two configurations.

Similarly, the logarithmic derivatives assume a particularly simple form. Since one obtains, for the configuration associated with index  $i$

$$O_\phi(\sigma) = \partial_\phi \log \psi(\sigma) = 1 \quad (4.10)$$

$$O_{\alpha_k}(\sigma) = \partial_{\alpha_k} \log \psi(\sigma) = \frac{\delta_{ik}}{\alpha_i} \quad (4.11)$$

where  $\delta_{ik}$  denotes the Kronecker delta. Therefore, the vector of logarithmic derivatives is extremely sparse: for each sampled configuration only one component associated with the parameters  $\alpha_k$  is non-vanishing, while all remaining entries are identically zero.

### 4.1.2 Spin-Jastrow Ansatz

One of the simplest yet physically motivated classes of variational wavefunctions is represented by the spin-Jastrow ansätze. Their main strength lies in the ability to capture many-body correlations through pairwise interaction terms while avoiding the exponential growth in the number of variational parameters characteristic of exact Hilbert-space parameterizations.

A general spin-Jastrow wavefunction can be written as

$$\psi(\sigma; \mathbf{a}, \boldsymbol{\eta}) = \exp \left( \sum_{i=1}^N a_i \sigma_i + \sum_{i < j} \eta_{ij} \sigma_i \sigma_j \right) \quad (4.12)$$

where the parameters  $a_i$  are usually referred to as *independent biases*, while the coefficients  $\eta_{ij}$  describe pairwise correlations between spins.

Different Jastrow ansätze are obtained by imposing different structures on the correlation parameters  $\eta_{ij}$ . At one extreme, one may assign an independent parameter to every pair of spins, leading to the so-called *Long-Range Inhomogeneous Jastrow with Independent Bias*. In this case, the total number of variational parameters is

$$N_{\text{par}} = N + \frac{N(N-1)}{2} \quad (4.13)$$

which scales quadratically with the system size. At the opposite extreme, one may impose translational invariance and let the coefficients depend only on the distance between spins, considerably reducing the number of parameters at the expense of a more constrained variational manifold.

In this work, a compromise between these two limiting cases has been adopted through the implementation of the *Long-Range Partially Homogeneous Jastrow with Independent Bias* (LRPHJasIB). A cutoff distance  $l_{\text{inh}}$  is introduced such that all pairs of spins satisfying  $d(i, j) \leq l_{\text{inh}}$  are assigned independent variational parameters, whereas all pairs with  $d(i, j) > l_{\text{inh}}$  share a parameter that depends only on their mutual distance,

$$\eta_{ij} = \eta(d(i, j)) \quad (4.14)$$

For a fixed value of  $l_{\text{inh}}$  and regular lattice geometries, the number of variational parameters grows linearly with the system size. This construction therefore retains long-range correlations while avoiding the strong symmetry constraints imposed by fully homogeneous Jastrow states, maintaining sufficient flexibility to describe dynamical and out-of-equilibrium phenomena.

The expressions for the local operators  $O_k$  assume particularly simple expressions. For the independent biases one obtains

$$O_{a_i}(\sigma) = \frac{\partial}{\partial a_i} \log \psi(\sigma) = \sigma_i \quad (4.15)$$

Similarly, for a generic correlation parameter  $\eta_\mu$ ,

$$O_{\eta_\mu}(\sigma) = \frac{\partial}{\partial \eta_\mu} \log \psi(\sigma) = \sum_{(i,j) \in \mathcal{C}_\mu} \sigma_i \sigma_j \quad (4.16)$$

where  $\mathcal{C}_\mu$  denotes the set of spin pairs associated with the parameter  $\eta_\mu$ . This expres-

sion naturally encompasses both limiting cases. For an inhomogeneous parameter

$$\mathcal{C}_\mu = \{(i, j)\} \quad \rightarrow \quad O_{\eta_\mu} = \sigma_i \sigma_j$$

whereas for a homogeneous parameter associated with a given distance  $r$ , one has

$$\mathcal{C}_\mu = \{(i, j) : d(i, j) = r\} \quad \rightarrow \quad O_{\eta_\mu} = \sum_{d(i, j)=r} \sigma_i \sigma_j$$

To efficiently evaluate these quantities, the correspondence between spin pairs and variational parameters is precomputed during the initialization stage. More precisely, a lookup matrix is constructed whose entry  $(i, j)$  stores the index of the variational parameter associated with the pair of spins  $(i, j)$ . Once this mapping has been generated, the local operators can be evaluated by iterating only once over all spin pairs and accumulating the contribution  $\sigma_i \sigma_j$  into the appropriate component of the local operators vector.

Finally, the exponential structure of the Jastrow ansatz considerably simplifies the computation of the acceptance probability in the Metropolis algorithm. Defining

$$\Delta = \log \psi(\sigma_{\text{new}}) - \log \psi(\sigma_{\text{old}}) \quad (4.17)$$

the probability ratio can be written as

$$\frac{P(\sigma_{\text{new}})}{P(\sigma_{\text{old}})} = \exp[2 \operatorname{Re}(\Delta)]. \quad (4.18)$$

In the present implementation, candidate configurations are generated through single-spin-flip updates. Consequently, the configurations  $\sigma_{\text{old}}$  and  $\sigma_{\text{new}}$  differ only on one site, say  $k$ , and the logarithmic difference can be computed without reevaluating the complete wavefunction. The contribution of the independent biases reduces to the single term

$$\Delta_a = a_k (\sigma_k^{\text{new}} - \sigma_k^{\text{old}}) \quad (4.19)$$

while for the pairwise correlations only the interaction terms involving the flipped spin contribute,

$$\Delta_\eta = \sum_{j \neq k} \eta_{kj} (\sigma_k^{\text{new}} \sigma_j - \sigma_k^{\text{old}} \sigma_j) \quad (4.20)$$

From an implementation standpoint, this update requires accessing only the row of the lookup matrix corresponding to the flipped spin. Therefore, the computational

cost of evaluating the acceptance probability scales linearly with the number of spins rather than quadratically, providing a significant improvement in the efficiency of the Monte Carlo sampling.

## 4.2 SpinHamiltonian class

The `SpinHamiltonian` class encapsulates the definition of the physical model under investigation and provides all model-dependent quantities entering the stochastic variational dynamics. Its primary role is to evaluate the contributions arising from the coherent Hamiltonian evolution, dissipative processes, and continuous measurements, while remaining independent of the specific variational ansatz employed.

More specifically, the class provides routines for computing:

- local energies associated with the Hamiltonian dynamics;
- local estimators of dissipative and measurement operators;
- drift and noise terms entering the stochastic equations of motion;
- expectation values of generic observables.

As discussed in the previous chapters, all expectation values can be reformulated as statistical averages over spin configurations sampled accordingly. For a generic operator  $\hat{O}$ , the expected value can be written as

$$\langle \hat{O} \rangle = \frac{1}{\langle \psi(\boldsymbol{\theta}) | \psi(\boldsymbol{\theta}) \rangle} \sum_{\sigma} |\psi(\sigma, \boldsymbol{\theta})|^2 O_{\text{loc}}(\sigma, \boldsymbol{\theta}) \quad (4.21)$$

where

$$O_{\text{loc}}(\sigma, \boldsymbol{\theta}) = \sum_{\sigma'} \frac{\langle \sigma | \hat{O} | \sigma' \rangle \psi(\sigma', \boldsymbol{\theta})}{\psi(\sigma, \boldsymbol{\theta})} \quad (4.22)$$

is the corresponding local estimator. Hence

$$\langle \hat{O} \rangle = \frac{1}{\langle \psi(\boldsymbol{\theta}) | \psi(\boldsymbol{\theta}) \rangle} \sum_{\sigma} |\psi(\sigma, \boldsymbol{\theta})|^2 \sum_{\sigma'} \langle \sigma | \hat{O} | \sigma' \rangle \frac{\psi(\sigma', \boldsymbol{\theta})}{\psi(\sigma, \boldsymbol{\theta})} \quad (4.23)$$

This framework applies equally to observables and to the quantities entering the otVMC equations, such as the local effective energy (3.5) and local noise (3.6). Although Eq. (4.23) formally involves a sum over all configurations  $\sigma'$ , only those

for which  $\langle \sigma | \hat{O} | \sigma' \rangle \neq 0$  contribute. These matrix elements define the *connections* of  $\sigma$ . Since physically relevant operators are generally sparse, the number of such connections grows only polynomially with system size.

The central task of the `SpinHamiltonian` class is the generation of the connections associated with the various operators entering the dynamics. Given a configuration  $\sigma$ , the class constructs the set of configurations  $\sigma'$  for which the matrix elements  $\langle \sigma | \hat{O} | \sigma' \rangle$  are non-vanishing, together with their corresponding coefficients. Different operators may induce different connectivity patterns. In particular, an operator can be diagonal in the computational basis, for which only the connection  $\sigma' = \sigma$  contributes, or it can generate off-diagonal connections, such as configurations differing by a single-spin flip or, more generally, by multiple spin updates. The same framework is employed to evaluate all quantities appearing in the simulation, including the Hamiltonian and measurement terms entering the stochastic dynamics, the effective open-system contributions, and the physical observables of interest.

### 4.3 Implementation of the Ising model

The implementation of the long-range interacting Ising model introduced in Sec. 1.6 is based on a separation between the geometrical structure of the system and the Monte Carlo and stochastic-evolution routines. The latter do not require direct access to the spatial coordinates of the spins, but only to the interaction coefficients between pairs of sites. For this reason, the geometry is processed once during initialization and encoded in an interaction lookup matrix.

A spin configuration is represented in the computational basis as a one-dimensional vector

$$\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \dots, \sigma_N) \quad \sigma_i = \pm 1 \quad (4.24)$$

This representation is independent of the specific geometry: the sampling procedure, the variational wave function, and the stochastic evolution act directly on the spin vector. All geometrical information is instead contained in the matrix

$$I_{ij} = \begin{cases} r_{ij}^{-\beta} & i \neq j \\ 0 & i = j \end{cases} \quad (4.25)$$

where  $r_{ij}$  is the distance between sites  $i$  and  $j$ . The diagonal entries are set to zero in order to exclude self-interactions. Once the matrix has been constructed, no

further distance calculations are required during the simulation. The long-range Ising contribution can therefore be evaluated by repeatedly accessing the precomputed coefficients.

In the simulations presented in this thesis, the general structure described above is specialized to regular two-dimensional lattices with periodic boundary conditions. For a lattice of size  $L_x \times L_y$ , sites are mapped to the configuration vector using a row-major convention. A site with coordinates  $(x, y)$  is assigned the linear index

$$i = x + L_x y \quad x = 0, \dots, L_x - 1 \quad y = 0, \dots, L_y - 1 \quad (4.26)$$

With this convention, consecutive entries of the spin vector correspond to consecutive sites along the same row, while different rows are stored sequentially. This indexing provides a simple way to construct the coordinate list needed during initialization.

The distance between two sites is computed using the minimum-image convention. Along the two spatial directions one defines

$$\Delta x_{ij} = \min(|x_i - x_j|, L_x - |x_i - x_j|) \quad (4.27)$$

and

$$\Delta y_{ij} = \min(|y_i - y_j|, L_y - |y_i - y_j|) \quad (4.28)$$

The distance entering the interaction matrix is then

$$r_{ij} = \sqrt{\Delta x_{ij}^2 + \Delta y_{ij}^2} \quad (4.29)$$

This prescription implements periodic boundary conditions by selecting the shortest distance between two sites on the periodic lattice, thus reducing boundary effects in the finite system.

This organization also simplifies the construction of connected configurations. Long-range interaction terms are diagonal in the computational basis and therefore do not generate new configurations. The same holds for collective operators diagonal in this basis. Non-diagonal single-site operators, instead, generate configurations differing by local spin flips. As a result, even though the interaction is long-ranged, the number of explicitly generated connected configurations grows at most linearly with the number of spins.

Overall, the implementation consists of a general geometry-independent layer, which acts on vectorized spin configurations and on the precomputed interaction matrix, and

a geometry-dependent initialization layer, which constructs  $I_{ij}$ . Although only regular square lattices are considered in this thesis, different geometries, boundary conditions, or interaction graphs could be included by modifying only this initialization step.

## 4.4 **SamplerOpen** class

At the core of the otVMC algorithm lies the **SamplerOpen** class, which acts as the main driver of the variational dynamics. Its primary purpose is to evolve the variational parameters  $\boldsymbol{\theta}(t)$  according to the stochastic equations of motion derived in the previous chapter.

At each time step, the class performs a sequence of operations that closely mirrors the theoretical structure of the algorithm. First, a Markov chain of spin configurations is generated using the Metropolis-Hastings sampling procedure described previously. Configurations are distributed according to the variational probability distribution  $P(\sigma) = \frac{|\psi(\sigma; \boldsymbol{\theta})|^2}{\mathcal{N}}$  where the normalization constant does not need to be computed explicitly.

The sampled configurations are then used to estimate all Monte Carlo quantities entering the equations of motion. These include the local estimators associated with the effective Hamiltonian and the jump operators, the local operators, the generalized forces, the quantum geometric tensor (QGT), and the stochastic noise vector generated by the monitored channels.

Finally, a realization of the Wiener increments is generated and the resulting stochastic differential equation for the variational parameters is integrated over a finite time step, producing the update  $\boldsymbol{\theta}(t) \mapsto \boldsymbol{\theta}(t + \Delta t)$ .

Each trajectory corresponds to an independent realization of this stochastic evolution. Repeating the procedure over many trajectories and experimental realizations allows one to reconstruct ensemble-averaged observables and characterize the statistical properties of the monitored quantum dynamics.

### 4.4.1 Quantum geometric tensor regularization

The equations of motion of the otVMC method require the inversion of the quantum geometric tensor. Recalling the compact form of the equations of motion (3.17)

$$\sum_j \mathcal{S}_{ij} d\alpha_j = \mathcal{F}_i \quad (4.30)$$

The matrix  $\mathcal{S}$  is Hermitian and positive semidefinite. In practical calculations, however, it is estimated through Monte Carlo sampling and therefore inevitably contains statistical noise. As a consequence, some of its eigenvalues may become extremely small or even numerically indistinguishable from zero, rendering the inversion ill-conditioned. Direct inversion in these situations leads to large and unphysical parameter updates, since fluctuations in poorly determined directions of the variational manifold become strongly amplified.

To stabilize the numerical evolution, the implementation adopts a Moore–Penrose pseudoinverse [37]. Since  $\mathcal{S}$  is Hermitian and positive semidefinite, it admits the eigenvalue decomposition

$$\mathcal{S}_{kl} = \sum_j V_{kj} s_j (V^\dagger)_{jl} \quad (4.31)$$

where  $s_j \geq 0$  are the eigenvalues and  $V$  is the unitary matrix whose columns are the corresponding eigenvectors.

The regularized pseudoinverse is then defined as

$$(S^+)_{kl} = \sum_j V_{kj} \tilde{s}_j (V^\dagger)_{jl} \quad (4.32)$$

with

$$\tilde{s}_j = \begin{cases} \frac{1}{s_j} & s_j > \lambda_{\text{th}} \\ 0 & \text{otherwise} \end{cases} \quad (4.33)$$

where  $\lambda_{\text{th}}$  is a numerical cutoff parameter.

This procedure selectively removes the directions of the variational manifold that are insufficiently resolved by the Monte Carlo sampling while preserving the physically meaningful components of the dynamics. Consequently, the pseudoinverse regularization provides a robust method for stabilizing the integration of the otVMC equations without introducing appreciable biases in the evolution.

### 4.4.2 Numerical integration of the stochastic equations

The stochastic equations governing the evolution of the variational parameters are written in the Stratonovich form,

$$d\theta_k = f_k(\boldsymbol{\theta}, t) dt + \sum_j g_k^j(\boldsymbol{\theta}, t) \circ dW_j \quad (4.34)$$

where  $f_k$  and  $g_k^{(n)}$  denote the deterministic and stochastic contributions, respectively, and  $dW_n$  are independent Wiener increments.

Since the stochastic coefficients depend explicitly on the variational parameters, a simple Euler discretization generally provides insufficient accuracy and may lead to numerical instabilities. Moreover, a single Euler step would only converge to the Ito interpretation. For this reasons, the implementation employs a predictor-corrector scheme, which represents a straightforward extension of the Euler-Maruyama method to Stratonovich stochastic differential equations [38, 39].

Given the parameter vector at time  $t_n$ , an intermediate predictor value is first computed through an explicit Euler step,

$$\tilde{\theta}_k^{(n+1)} = \theta_k^{(n)} + f_k(\boldsymbol{\theta}^{(n)})\Delta t + \sum_j g_k^j(\boldsymbol{\theta}^{(n)})\Delta W_j^{(n)} \quad (4.35)$$

The final update is then obtained by evaluating the drift and diffusion terms at the midpoint between the predictor and the previous value,

$$\theta_k^{(n+1)} = \theta_k^{(n)} + f_k\left(\frac{\tilde{\theta}_k^{(n+1)} + \theta_k^{(n)}}{2}\right)\Delta t + \sum_j g_k^j\left(\frac{\tilde{\theta}_k^{(n+1)} + \theta_k^{(n)}}{2}\right)\Delta W_j^{(n)} \quad (4.36)$$

The same Wiener increments are employed in both stages of the algorithm. This predictor-corrector procedure preserves the essential properties of Stratonovich calculus while providing significantly improved stability compared with a purely explicit integration scheme, making it particularly suitable for long-time simulations of monitored many-body quantum systems.

The method is of strong convergence order 1/2 in case there are multiple generic noise channels [39].

## 4.5 Random Number Generation

Monte Carlo methods rely heavily on the generation of high-quality pseudo-random numbers, making the choice of the underlying generator an important aspect of the overall implementation. In the original version of the code, random numbers were produced using a linear congruential generator (LCG). Generators of this class construct a sequence of pseudo-random integers through the recursive relation

$$x_{n+1} = (ax_n + c) \bmod m \quad (4.37)$$

where  $a$ ,  $c$ , and  $m$  are fixed constants. Although linear congruential generators are computationally inexpensive and simple to implement, they can exhibit non-negligible correlations between different streams, making them less suitable for large-scale parallel Monte Carlo simulations.

For these reasons, the original generator has been replaced by the **Philox** generator [40] provided by the Intel Math Kernel Library (MKL) [41]. Philox belongs to the class of *counter-based* pseudo-random number generators. In contrast to recursive generators, a counter-based generator does not obtain the next random number from the previous one. Instead, random numbers are generated by applying a deterministic transformation

$$x_n = F(\text{counter}, \text{key}) \quad (4.38)$$

where the output depends only on the current value of an integer counter and on a user-defined key.

This construction offers several advantages. Since the generated sequence is entirely determined by the pair (counter, key), any element of the sequence can be accessed directly without evaluating all preceding values. More importantly, independent pseudo-random streams can be generated simply by assigning different keys. This property is particularly advantageous in parallel environments, where each MPI process can be associated with a distinct key and can therefore generate statistically independent random sequences without requiring communication or synchronization with other processes.

A further optimization introduced in the present implementation concerns the generation of random numbers in batches. Rather than requesting a new pseudo-random number every time one is needed by the Monte Carlo routines, random variates are generated in blocks and stored in memory buffers. The simulation then consumes the numbers sequentially from the current buffer. Once the buffer is

exhausted, a new batch is generated and the process is repeated.

This strategy reduces the overhead associated with repeated calls to the random number generator and allows the highly optimized vectorized routines provided by the Intel MKL library to be exploited more effectively. Although conceptually simple, this modification results in a measurable improvement in the overall efficiency of the Monte Carlo sampling procedure.

# Chapter 5

## Results

The purpose of this chapter is to assess the numerical capabilities and reliability of the otVMC implementation. Since the method is intended to simulate the dynamics of open quantum many-body systems beyond the range accessible to exact approaches, a systematic validation is required before applying it to regimes where no direct benchmark is available.

The chapter is organized as follows. Section 5.1 introduces the general simulation setup, the observables considered, and the main numerical parameters. Sections 5.2 and 5.3 present the comparison between otVMC and QuTiP for conditional dynamics in a few-spin system, using the exact ansatz. Section 5.4 investigates the effect of changing the number of local dissipative channels, again in a few-spin regime where the exact ansatz (Section 4.1.1) can be used and QuTiP simulations remain feasible. Section 5.5 then discusses the unconditional dynamics of a system with  $N = 49$  spins, using the LRPJasIB ansatz (Section 4.1.2) and comparing the variational evolution with an exact solution. Section 5.6 considers a simplified monitored dynamics for  $N = 49$  spins, in which only the collective monitored channel is present, allowing for a comparison with an approximate analytical prediction. Section 5.7 shows the dynamics for  $N = 64$  spins in the presence of Hamiltonian evolution with a transverse field and monitoring, but without local dissipation. Finally, Section 5.8 is devoted to nonlinear observables, in particular variances and covariances, whose estimation requires additional care in the conditional setting.

The numerical simulations presented in this chapter were carried out using high-performance computing resources made available through the CINECA award Is-crC\_otVMC2D, granted under the ISCRA initiative. Additional computational resources were provided by INRiM through the Legion and Battery workstations,

whose support was essential for performing the calculations discussed in the following sections.

## 5.1 General simulation setup

The simulations are performed for the long-range dissipative transverse-field Ising model introduced in Section 1.6. The variational wave functions employed in the numerical analysis are presented in Chapter 4. Two different representations of the quantum state are used, depending on the system size considered.

For the few-spin benchmarks, the exact ansatz is adopted. This means that the variational manifold coincides with the full Hilbert space of the system. In this way, the comparison with QuTiP directly tests the implementation of the otVMC stochastic evolution, the sampling procedure, and the treatment of monitored and unmonitored channels, without introducing an additional approximation due to the structure of the variational wave function.

For the many-body simulations with  $N = 49$  spins, the LRPJasIB ansatz is used. This ansatz provides a compact variational representation suitable for larger two-dimensional systems. In all simulations performed with the LRPJasIB ansatz, the inhomogeneous cutoff distance is set to one,  $l_{\text{inh}} = 1$ . Moreover, the cutoff parameter used in the pseudoinverse regularization is fixed to  $10^{-7}$  for all simulations.

Unless stated otherwise, the system consists of a two-dimensional lattice of  $N = L \times L$  spins with periodic boundary conditions. The Hamiltonian and dissipative parameters are chosen in order to probe different physical regimes, ranging from unconditional Lindblad evolution to conditional dynamics dominated by continuous monitoring. In all simulations, the long-range interaction exponent is fixed at  $\beta = 2$ . This value, which is equal to the system dimension, has been argued to represent a particularly challenging regime, lying at the boundary between simple mean-field dynamics and the more entangled short-range dynamics [22]. Unless explicitly specified, the initial state is a coherent spin state (CSS) polarized along the  $x$  direction. This state, obtained by setting  $\theta = \frac{\pi}{2}$  and  $\varphi = 0$  in equation (1.62), corresponds to the maximally delocalized and uniform state in the chosen computational basis. When explicitly indicated in the label of the vertical axis, the variance of  $M_z$  is normalized to its CSS value,  $\text{Var}(M_{z,\text{CSS}}) = \frac{1}{N}$ .

For the benchmark simulations, the agreement between otVMC and the reference

solution is assessed both qualitatively and quantitatively. On the qualitative side, the time evolution of the relevant observables is compared in order to verify whether the method correctly reproduces the physical trends of the dynamics. On the quantitative side, the corresponding deviations and relative errors with respect to the reference results are analysed. Since otVMC is a stochastic method, particular attention is devoted to the estimation of statistical uncertainty. Error bars are therefore included not only for the observables themselves, but also, when relevant, for the relative errors used to compare different simulations.

## 5.2 Benchmark against exact stochastic simulations

As a validation of the implementation, the monitored dynamics obtained with otVMC was compared with exact stochastic simulations performed with QuTiP. The benchmark was carried out for a small system of  $N = 6$  spins, for which the exact Hilbert-space evolution is still numerically accessible. In all simulations discussed in this section the time step was fixed to  $dt = 0.01$  and the interaction strength to  $J = 1$ . The variational ansatz was taken to be exact, so that possible discrepancies are not related to a limited expressivity of the wave function, but rather to the stochastic sampling, the integration scheme, and the implementation of the monitored dynamics.

Two different dynamical regimes were considered. First, the case with Hamiltonian evolution and continuous monitoring only was studied by setting the local dissipative rate to  $\kappa = 0$  and the monitoring rate to  $\Gamma = 0.5$ . In this case, a single internal trajectory was used,  $N_{\text{traj}} = 1$ , since no additional averaging over unmonitored jumps is required. The results are shown in Fig. 5.1. The agreement between otVMC and QuTiP is overall satisfactory for both values of the transverse field,  $h = \pm 0.5$ . In particular, the variance of the magnetization,  $\text{Var}(M_z)$ , is accurately reproduced over the whole time interval. The average magnetization  $\langle M_z \rangle$  remains close to zero, as expected for this parameter regime, and the otVMC results are compatible with the exact evolution within the statistical fluctuations. This confirms that the monitored part of the evolution is correctly implemented and that the stochastic measurement noise is consistently treated.

The full dynamics, including Hamiltonian evolution, monitoring with  $\Gamma = 0.5$ , and local dissipation with  $\kappa = 0.1$ , was then analyzed. In this case the simulation

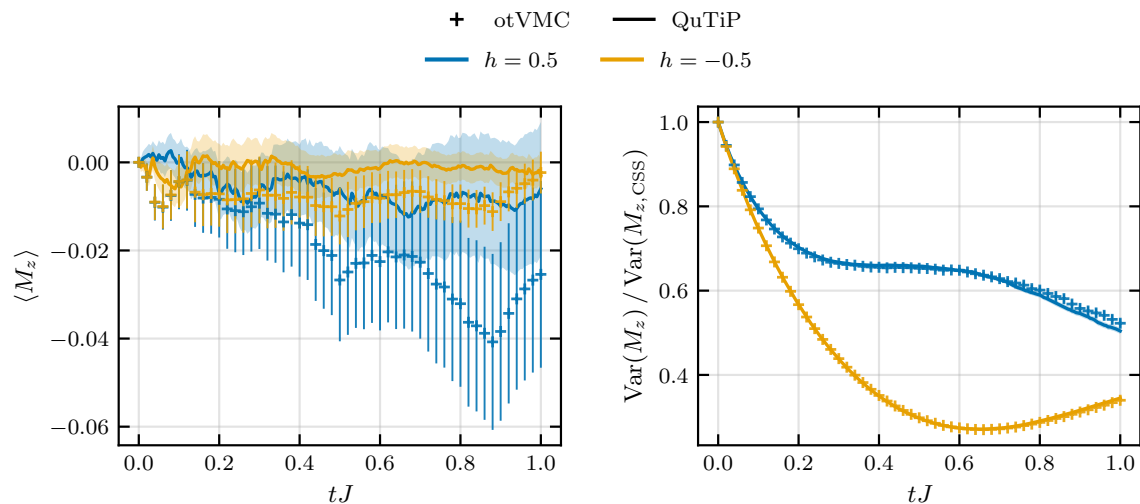


Figure 5.1: Comparison between otVMC and exact QuTiP simulations for  $N = 6$  spins,  $dt = 0.01$  and  $J = 1$ , in the presence of Hamiltonian evolution, continuous monitoring only with rate  $\Gamma = 0.5$ , and no dissipation ( $\kappa = 0$ ).

was performed with  $N_{\text{exp}} = 1000$  monitored experiments and  $N_{\text{traj}} = 2$  internal trajectories for each experiment. The results are reported in Fig. 5.2. A clear dependence on the sign of the transverse field is observed. For  $h = -0.5$ , otVMC remains in good agreement with QuTiP for both  $\langle M_z \rangle$  and  $\text{Var}(M_z)$ , reproducing not only the qualitative behavior but also the quantitative evolution of the exact curves. By contrast, for  $h = 0.5$  the agreement deteriorates in both observables.

Since the ansatz used in this benchmark is exact, the observed disagreement cannot be attributed to variational limitations. Instead, it indicates that the combined action of the transverse Hamiltonian term, dissipation, and monitoring introduces a numerical difficulty that is not present when the local dissipative channel is removed. This result motivates the analysis presented in the following sections, where the transverse field is progressively simplified or removed in order to isolate the origin of the discrepancy. In particular, by suppressing the transverse-field contribution one can test whether the problematic behavior is associated with the off-diagonal Hamiltonian dynamics or with the treatment of the dissipative and monitored terms themselves.

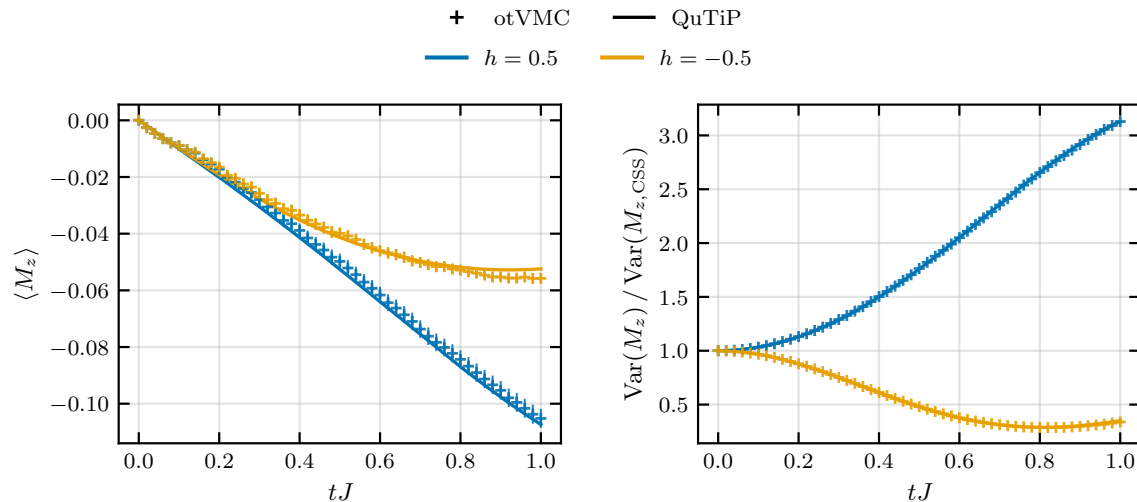


Figure 5.2: Comparison between otVMC and exact QuTiP simulations for  $N = 6$  spins,  $dt = 0.01$ ,  $J = 1$  and local dissipation rate  $\kappa = 0.1$ .

### 5.3 Comparison with QuTiP of conditional dynamics for few spins

The first benchmark concerns the conditional dynamics of few-spin system in the presence of both the monitored collective channel and local dissipative processes and in the absence of transverse field. In this regime, no simple analytical solution is available. The validation is therefore performed by comparing the otVMC dynamics with reference simulations obtained with QuTiP. The QuTiP code used to generate the reference results is reported in Appendix B.

The simulations in this section are performed using the exact ansatz. Since the system size is small, the variational state can represent the full wave function without any restriction due to an approximate parametrization. As a consequence, possible discrepancies between otVMC and QuTiP are not associated with the expressivity of the ansatz, but rather with the numerical implementation of the conditional dynamics, the stochastic integration, and the Monte Carlo sampling.

A crucial aspect of this comparison is that the dynamics is conditional on a specific measurement record. Therefore, the benchmark does not correspond to unconditional evolution and is not based only on ensemble-averaged quantities. Instead, a single experimental realization is considered, and the same measurement record is imposed in both simulations. In practice, the QuTiP trajectory is generated using the option `run_from_experiment`, so that the same Wiener increments are used for the monitored channel in the QuTiP and otVMC evolutions. This way, the two

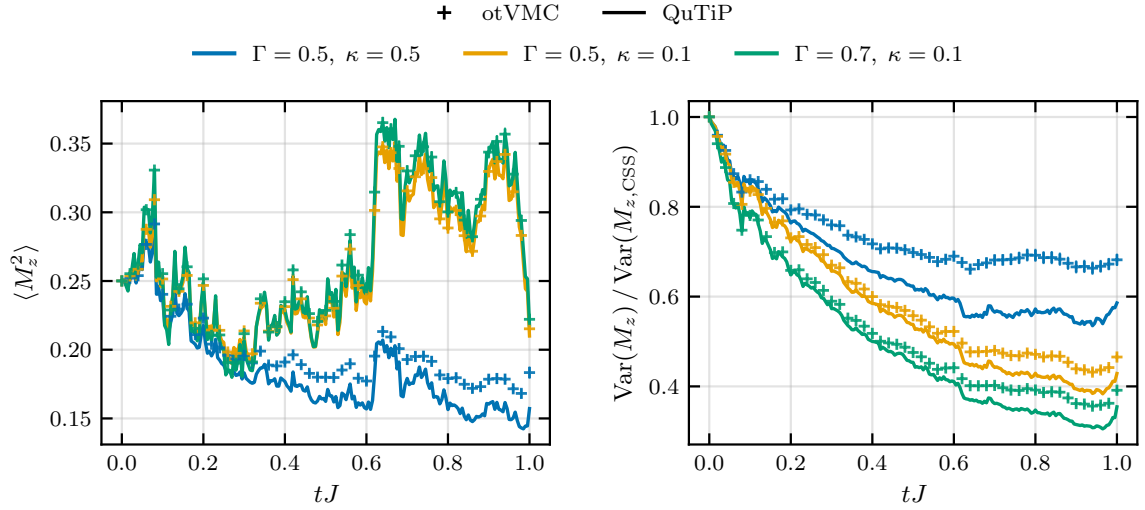


Figure 5.3: Comparison between otVMC and QuTiP for a conditional trajectory of a  $2 \times 2$  spin system with a fixed measurement record. The otVMC simulation is performed using the exact ansatz.

trajectories are conditioned on the same stochastic signal, and the comparison directly tests the implementation of the conditional update.

The simulations are performed for a system of  $N = 4$  spins arranged on a  $2 \times 2$  lattice. The Hamiltonian parameters are fixed to  $J = 1$  (which is then the reference energy) and  $\hbar = 0$ , while the time step is set to  $\Delta t = 0.005$ . Since a single measurement record is considered, the number of experiments is  $N_{\text{exp}} = 1$ . For the otVMC simulation,  $N_{\text{traj}} = 400$  internal trajectories are used to represent the conditional state associated with this record.

Figure 5.3 shows the comparison between otVMC and QuTiP for different values of the measurement strength  $\Gamma$  and of the local dissipation rate  $\kappa$ . The agreement improves when the monitored dynamics becomes dominant with respect to the local dissipative processes. This leads to a more accurate reconstruction of the QuTiP trajectory for linear observables, such as expectation values of fixed operators. The situation is more delicate for nonlinear observables, such as variances. Although an improvement is also observed when the relative weight of the local dissipation is reduced, visible deviations remain present. A more systematic analysis of this issue, and in particular of the role played by the local dissipation, is presented in the next section.

This benchmark confirms that the conditional dynamics at the trajectory level is correctly reproduced in regimes where the monitored collective channel is sufficiently dominant. At the same time, it highlights the increasing numerical difficulty

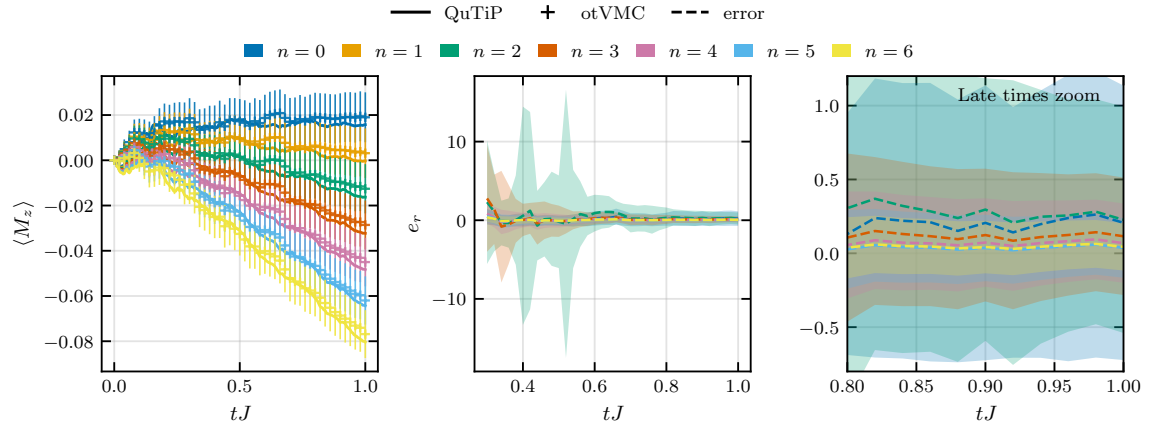


Figure 5.4: Dependence on the number of local dissipators for the linear observable  $\langle M_z \rangle$ . The otVMC simulations are performed using the exact ansatz.

associated with nonlinear observables and competing local dissipative processes.

## 5.4 Dependence on the number of local dissipators

After validating the conditional dynamics for a fixed set of dissipative channels, the dependence on the number of local dissipators is investigated. The analysis is performed for a system of  $N = 6$  spins arranged on a  $2 \times 3$  lattice, where QuTiP simulations remain feasible and can be used as a reference. Also in this section, the exact ansatz is used in the otVMC simulations, so that the effect of the local dissipative channels can be analysed without introducing an additional approximation due to the variational representation.

The parameters are fixed to  $J = 1$ ,  $h = 0$ ,  $\Gamma = 0.5$ ,  $\kappa = 0.1$ , and  $\Delta t = 0.01$ . The number of active local dissipative channels is then varied from  $n = 0$  to  $n = 6$ , while all other parameters are kept unchanged.

The comparison is performed both qualitatively, by directly comparing the time evolution of the observables, and quantitatively, by considering the relative error with respect to the QuTiP result. The relative error is defined using QuTiP as reference value,

$$e_r(t) = \frac{O_{\text{otVMC}}(t) - O_{\text{QuTiP}}(t)}{|O_{\text{QuTiP}}(t)|} \quad (5.1)$$

where  $O(t)$  denotes the observable under consideration. The uncertainty associated with  $e_r(t)$  is obtained by error propagation, taking into account both the statistical

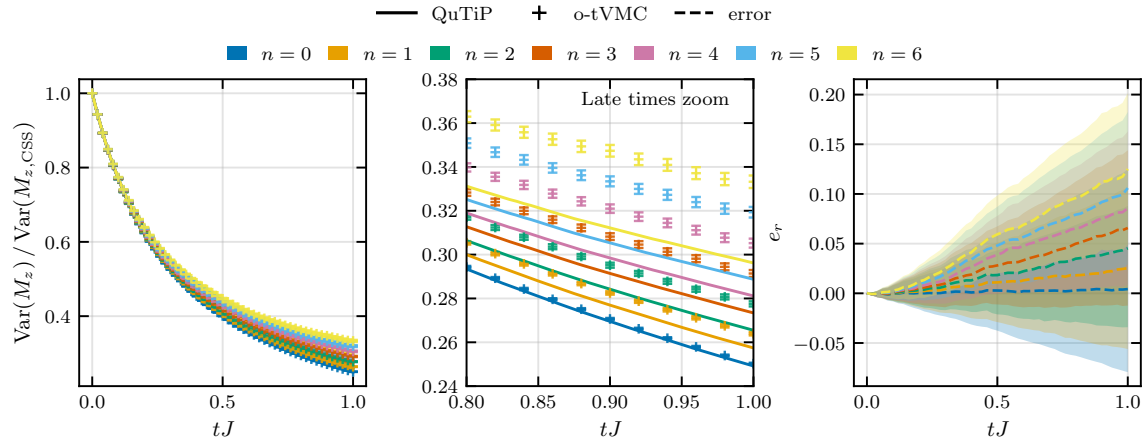


Figure 5.5: Dependence on the number of local dissipators for the nonlinear observable  $\text{Var}(M_z)$ . The otVMC simulations are performed using the exact ansatz.

uncertainty of the otVMC estimate and that of the QuTiP reference.

Figure 5.4 shows the results for the linear observable  $\langle M_z \rangle$ . In this case, the otVMC dynamics remains in good agreement with the QuTiP reference for all the considered values of  $n$ . The qualitative behaviour is correctly reproduced as the number of local dissipators is increased, and the relative error remains statistically compatible with zero within the corresponding uncertainty. This indicates that, for linear observables, the effect of the additional local dissipative channels is accurately captured by the variational dynamics.

The situation is substantially different for nonlinear observables. Figure 5.5 shows the same analysis for  $\text{Var}(M_z)$ . Although the overall decreasing trend of the variance is reproduced, the quantitative agreement deteriorates as the number of local dissipators is increased. This is particularly visible at late times, where the otVMC estimates progressively deviate from the QuTiP curves for larger values of  $n$ .

This behaviour is confirmed by the relative error. For a small number of local dissipators, the error remains compatible with zero within the statistical uncertainty. Conversely, when more local dissipative channels are included, the relative error becomes systematically different from zero, even after accounting for the propagated error bars. This suggests that, in this regime, the two simulations are no longer statistically compatible for the nonlinear observable.

These results show that the treatment of multiple local dissipators is reliable for linear observables, for which otVMC and QuTiP remain statistically consistent across the full range of  $n$ . Nonlinear observables, on the other hand, show significant

inaccuracies that become relevant when the number of local dissipators increases.

There are a few possible explanations for the discrepancy:

- Inaccuracy of the employed stochastic solver. We have tested different stochastic solvers both with QuTiP and otVMC [38, 39], also reducing the timestep, finding however that their results do not significantly vary.
- Inaccuracy of the ansatz. This is excluded since we are using the exact ansatz for few spins.
- Erroneous stochastic equations in the mixed SME case. There is more evidence pointing in this direction, since both the purely unconditional and the purely monitored cases show good agreement with exact results. It appears that the discrepancy arises when we consider both a monitored operator and local unmonitored ones. There might be a wrong assumption in how to correctly manage the conditional averages, since we are still employing the SSE equations which assume pure state stochastic evolution.

## 5.5 Unconditional dynamics for large systems

The next benchmark concerns the unconditional dynamics of a system with  $N = 49$  spins. This regime provides a direct test of the variational implementation in a many-body setting, since the otVMC results can be compared with the exact solution derived for long-range Ising dynamics with local decoherence [42]. No measurement record is involved, and the evolution corresponds to the ensemble-averaged Lindblad dynamics.

In contrast to the few-spin benchmarks discussed in the previous sections, the simulations in this section are performed using the `LRPHJasIB` ansatz. This choice is required in order to treat a system size beyond the range where an exact representation of the wave function is practical. Therefore, this benchmark tests not only the numerical integration and sampling procedure, but also the accuracy of the variational approximation in a many-body regime.

The simulations are performed with  $J = 1$ ,  $\kappa = 0.1$ ,  $h = 0$ . The two otVMC simulation (1) and (2) are obtained with time-step  $\Delta t = 0.01$  and  $\Delta t = 0.005$ . For the comparison shown in Fig. 5.6,  $N_{\text{traj}} = 1000$  trajectories are used.

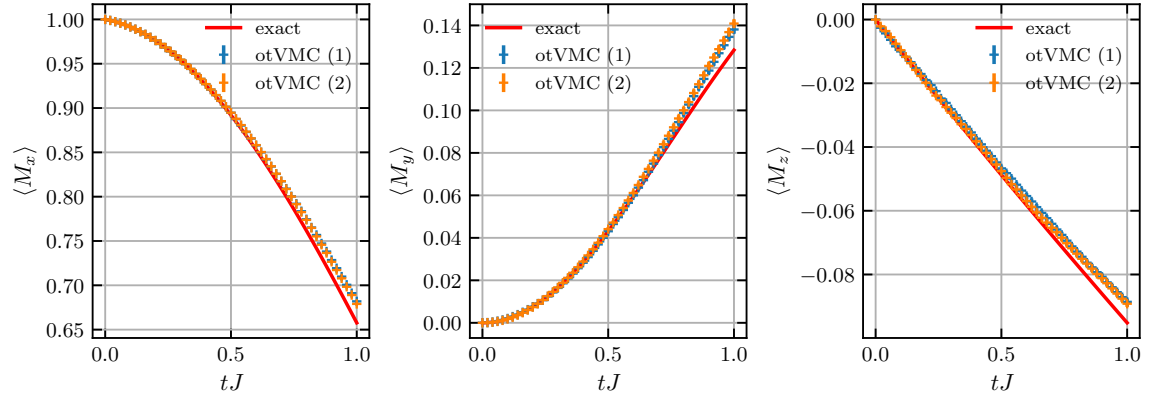


Figure 5.6: Unconditional dynamics for  $N = 49$  spins. otVMC simulations use the **LRPHJasIB** ansatz, with time steps  $dt = 0.01$  for otVMC (1) and  $dt = 0.005$  for otVMC (2).

For this choice of parameters, the exact solution for the magnetization components can be written as

$$\langle M_x(t) \rangle_{\text{ex}} = e^{-\kappa t/2} \text{Re} \left[ \prod_{j \neq i} \phi(J_{ij}, t, \kappa) \right] \quad (5.2)$$

$$\langle M_y(t) \rangle_{\text{ex}} = -e^{-\kappa t/2} \text{Im} \left[ \prod_{j \neq i} \phi(J_{ij}, t, \kappa) \right] \quad (5.3)$$

$$\langle M_z(t) \rangle_{\text{ex}} = e^{-\kappa t} - 1 \quad (5.4)$$

with

$$\begin{aligned} \phi(J_{ij}, t, \kappa) &= e^{-\frac{\kappa t}{2}} \left( \cos(ts) + \frac{\kappa}{2s} \sin(ts) \right) \\ s &= \frac{i}{2} \kappa + 2 \frac{J_{ij}}{N} \end{aligned}$$

Here,  $\phi(J_{ij}, t, \kappa)$  is the two-spin contribution entering the exact solution and  $J_{ij}$  denotes the long-range coupling between sites  $i$  and  $j$ . Due to translational invariance, the product can be evaluated by fixing an arbitrary reference site  $i$ .

Figure 5.6 shows the comparison between the exact solution and the otVMC evolutions for the three magnetization components. Good agreement is observed at short times for all observables. At longer times, the discrepancy with respect to the exact reference solution increases, indicating a progressive loss of accuracy during the time evolution. However, the two otVMC simulations, performed with different time steps, are almost indistinguishable. This suggests that the observed deviation is not primarily due to the finite time-step discretization, but is more likely associated

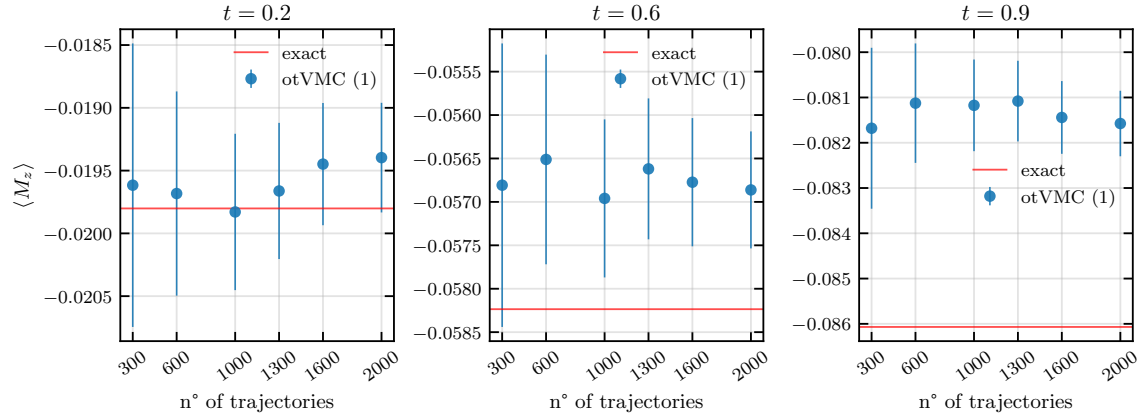


Figure 5.7: Dependence of  $\langle M_z \rangle$  on the number of trajectories for  $N = 49$  spins at three representative times. The otVMC simulations are performed using the LRPJasIB ansatz.

with the limited expressivity of the variational ansatz and with the accumulation of statistical errors.

The dependence on the number of trajectories is analysed in Fig. 5.7, where  $\langle M_z \rangle$  is shown at three representative times. The convergence is reached rather quickly: the results obtained with different numbers of trajectories are mostly compatible within their statistical uncertainty. As expected, increasing  $N_{\text{traj}}$  reduces the size of the error bars. Up to intermediate times, the otVMC estimates remain compatible with the exact value, while at longer times a systematic deviation from the exact solution becomes visible.

This benchmark shows that the unconditional dynamics is accurately reproduced at short and intermediate times by the LRPJasIB ansatz, while long-time simulations require additional care due to the accumulation of statistical and variational errors.

## 5.6 Measurement-only conditional dynamics

As a final many-body benchmark, a conditional dynamics is considered in which only the monitored collective channel is retained. In previous sections, it was observed that such a setting is recovered quite accurately in the case of few spins. The Hamiltonian evolution and the local dissipative processes are switched off by setting  $J = 0$ ,  $h = 0$ , and  $\kappa = 0$ . In this limit, the dynamics is entirely induced by the continuous measurement process, and therefore provides a direct test of the stochastic part of the otVMC equations in a large system.

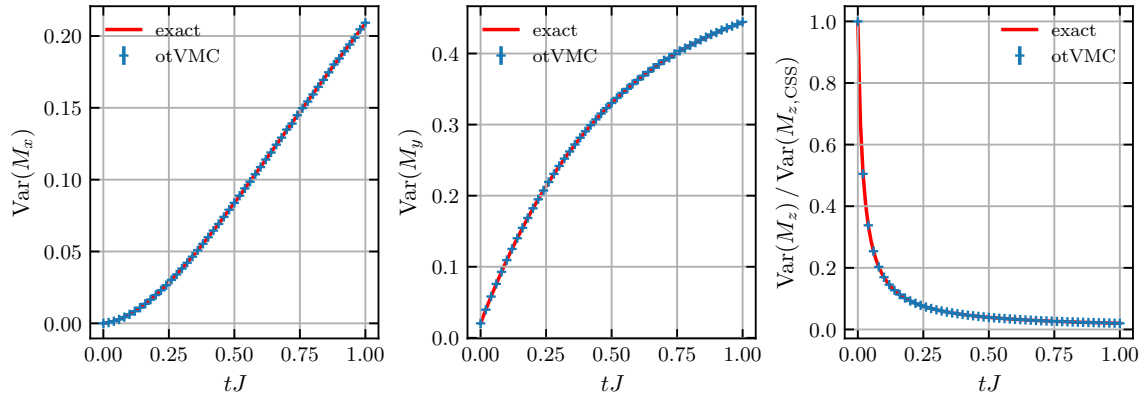


Figure 5.8: Measurement-only conditional dynamics for  $N = 49$  spins. The otVMC simulation is performed using the `LRPHJasIB` ansatz.

The simulation is performed for  $N = 49$  spins using the `LRPHJasIB` ansatz. This makes it possible to test the measurement-induced dynamics in a many-body regime where the exact ansatz is no longer practical. The measurement strength is set to  $\Gamma = 1.0$  and the time step is  $\Delta t = 0.01$ . The final averages are obtained over  $N_{\text{exp}} = 400$  independent experiments. The choice of this decomposition of the computational cost between internal trajectories and independent experiments is discussed in Section 5.8.

In this regime, the numerical results can be compared with an approximate analytical description [21] valid in the large-system limit. Introducing  $\tau = \Gamma t$  and  $S = N/2$ , the predicted variances are given by

$$\begin{aligned}\text{Var}(M_x) &= \frac{S(1 - e^{-\tau})^2 + \frac{1}{2}(1 - e^{-2\tau})}{N} \\ \text{Var}(M_y) &= \frac{S(1 - e^{-2\tau}) + \frac{1}{2}(1 + e^{-2\tau})}{N} \\ \text{Var}(M_z) &= \frac{1}{N(1 + 2S\tau)}\end{aligned}$$

Figure 5.8 shows the comparison between the otVMC results and the analytical approximation for the variances of the three magnetization components. The agreement is very good over the whole time interval considered. The growth of  $\text{Var}(M_x)$  and  $\text{Var}(M_y)$  is reproduced accurately, as well as the rapid decrease of  $\text{Var}(M_z)$  induced by the continuous monitoring of the collective channel.

This benchmark validates the implementation of the measurement-induced stochastic evolution in a regime where no deterministic Hamiltonian dynamics or additional dissipative channel competes with the monitored process. Moreover, the agreement

obtained for  $N = 49$  indicates that the LRPHJasIB ansatz is able to reproduce the collective measurement dynamics with good accuracy in the time interval considered. It therefore provides a clean many-body reference case before considering the full conditional dynamics, where measurement backaction, Hamiltonian evolution, and local dissipation are simultaneously present.

## 5.7 Monitored dynamics for $N = 64$ spins

As a final application, the monitored dynamics of a larger two-dimensional system is considered. The simulation is performed for  $N = 64$  spins, with interaction strength  $J = 1$ , transverse field  $h = \pm 0.5$ , monitoring strength  $\Gamma = 0.5$ , and no local dissipation,  $\kappa = 0$ . The variational state is parametrized by the LRPHJasIB ansatz. The final averages are obtained over  $N_{\text{exp}} = 700$  independent experiments and a single internal trajectory,  $N_{\text{traj}} = 1$ , since no additional averaging over unmonitored jumps is required. In contrast to the benchmarks discussed in the previous sections, no exact reference solution is available for this system size and set of parameters. The purpose of this calculation is therefore not to provide a quantitative validation, but rather to show that the implemented otVMC code can be applied to genuinely larger monitored many-body systems and produces physically consistent dynamics.

Figure 5.9 shows the time evolution of the magnetization  $\langle M_z \rangle$  and of the variance  $\text{Var}(M_z)$ , normalized to the coherent-spin-state value  $\text{Var}(M_{z,\text{CSS}}) = 1/N$ . The average magnetization remains compatible with zero within the statistical uncertainty over the whole time interval. At the same time, the variance rapidly decreases from its initial CSS value and reaches values much smaller than one. This behaviour is consistent with the effect of the continuous measurement of the collective operator  $\hat{J}_z$ . The residual oscillations observed in the variance indicate that the monitored dynamics is not purely dissipative, but is affected by the coherent Hamiltonian evolution.

The observed behaviour can be understood qualitatively from the competition between continuous monitoring and coherent Hamiltonian dynamics. In the absence of the transverse field, both the Ising interaction and the monitored operator  $\hat{J}_z$  are diagonal in the computational basis and commute. In that case, the monitoring tends to reduce the fluctuations of  $\langle M_z \rangle$  without producing a systematic drift of its mean value. This is consistent with the fact that  $\langle M_z \rangle$  remains compatible with zero, while  $\text{Var}(M_z)$  is strongly suppressed.

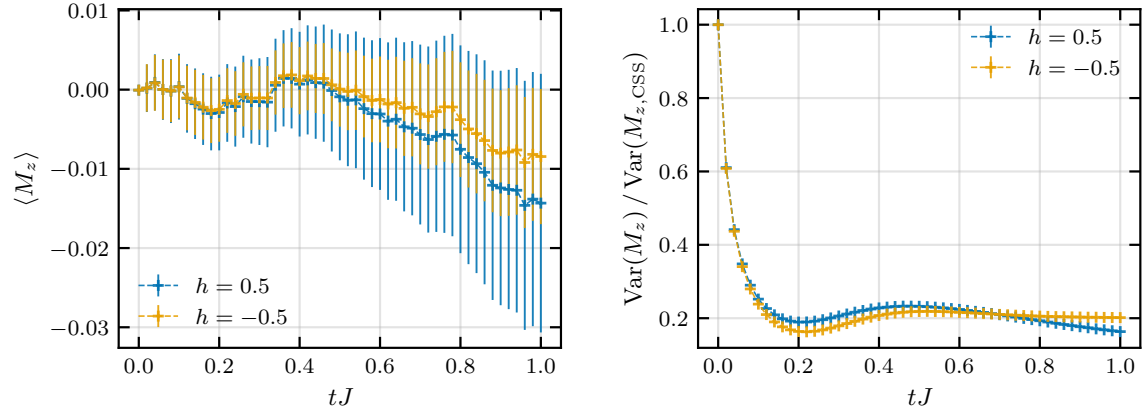


Figure 5.9: Conditional dynamics without local dissipators for  $N = 64$  spins. The otVMC simulation is performed using the LRPHJasIB ansatz.

The presence of the transverse field modifies this simple picture, since it does not commute with  $\hat{J}_z$  and the spin-spin interaction. The field couples the  $y$  and  $z$  spin components. Starting from a state with  $\langle M_y \rangle = 0$ , the initial change of  $\langle M_z \rangle$  is expected to be weak, whereas the effect on the fluctuations can be more visible. The oscillations observed in  $\text{Var}(M_z)$  can therefore be interpreted as the result of coherent rotations induced by the transverse field, superimposed on the measurement-induced reduction of the fluctuations. Depending on the relative effect of the transverse field and of the Ising interaction, these rotations may partially enhance or counteract the squeezing generated by the monitoring.

It should be stressed that, for this system size, no independent reference solution is available. Moreover, only the LRPHJasIB ansatz is considered in this simulation. Therefore, although the dynamics appears physically consistent, a systematic study with different variational parametrizations would be required to assess the possible role of ansatz-dependent effects.

## 5.8 Statistical analysis of variance and covariance estimators

The last numerical analysis concerns the estimation of nonlinear observables in the conditional dynamics. In contrast to linear observables, quantities such as variances and covariances are not obtained by a direct average over all sampled trajectories. This distinction is specific to the monitored case, where each experiment corresponds to a different measurement record and therefore to a different conditional state.

As a consequence, the averaging over internal trajectories and the averaging over independent experiments play different statistical roles.

At fixed computational budget, increasing the number of internal trajectories improves the estimate of each single conditional expectation. However, it also reduces the number of independent experiments that can be performed. Since nonlinear observables depend on the fluctuations of conditional expectation values over different measurement records, this trade-off is nontrivial. In order to quantify it, an analytical expression for the variance of the estimators was derived. The derivation is reported below and gives the dependence of the estimator variance on the number of internal trajectories  $N$  and on the number of experiments  $M$ .

The quantity of interest is the covariance function

$$\text{Cov}(\hat{A}, \hat{B}) = \mathbb{E}_{\text{exp}} \left[ \mathbb{E}_{\text{traj}} [\langle \hat{A}\hat{B} \rangle_{\text{MC}}] - \mathbb{E}_{\text{traj}} [\langle \hat{A} \rangle_{\text{MC}}] \mathbb{E}_{\text{traj}} [\langle \hat{B} \rangle_{\text{MC}}] \right] \quad (5.5)$$

For convenience, at a fixed time step, we introduce the notation

$$X_i^k := \langle \hat{A} \rangle_i^k, \quad Y_i^k := \langle \hat{B} \rangle_i^k, \quad Z_i^k := \langle \hat{A}\hat{B} \rangle_i^k$$

where the index  $k$  labels the  $M$  independent experiments, each consisting of  $N$  internal trajectories indexed by  $i$ .

It is useful to regard these random variables as depending on two distinct sources of randomness, namely

$$X[\xi, \eta]$$

where  $\xi$  denotes the stochastic monitoring process shared among all trajectories belonging to the same experiment, while  $\eta$  represents the trajectory-dependent noise. In this framework, Eq. (5.5) can be rewritten as

$$\text{Cov}(\hat{A}, \hat{B}) = \mathbb{E}_{\xi} [C(\xi)] \quad (5.6)$$

$$C(\xi) = \mathbb{E}_{\text{traj}} [\langle \hat{A}\hat{B} \rangle_{\text{MC}} | \xi] - \mathbb{E}_{\text{traj}} [\langle \hat{A} \rangle_{\text{MC}} | \xi] \mathbb{E}_{\text{traj}} [\langle \hat{B} \rangle_{\text{MC}} | \xi] \quad (5.7)$$

As discussed in the Thesis [3], particular care must be taken in constructing an estimator for Eq. (5.7), due to the nonlinearity introduced by the product of expectation values. Indeed, a naive estimator generally leads to a biased result. This issue can

be avoided by employing a U-statistic estimator [43, 44], namely

$$\hat{C}_k = \frac{1}{N} \sum_i Z_i^k - \frac{1}{N(N-1)} \sum_{i \neq j} X_i^k Y_j^k \quad (5.8)$$

which satisfies

$$\mathbb{E}[\hat{C}_k \mid \xi] = C(\xi).$$

The corresponding unbiased estimator for Eq. (5.5) is therefore

$$\hat{C} = \frac{1}{M} \sum_{k=1}^M \hat{C}_k \quad (5.9)$$

Assuming that the estimators  $\hat{C}_k$  are independent and identically distributed, the variance of Eq. (5.9) is

$$\text{Var}(\hat{C}) = \text{Var}\left(\frac{1}{M} \sum_{k=1}^M \hat{C}_k\right) = \frac{1}{M} \text{Var}(\hat{C}_k) \quad (5.10)$$

The remaining task is therefore the computation of  $\text{Var}(\hat{C}_k)$ . To this end, we first apply the law of total variance:

$$\text{Var}(\hat{C}_k) = \text{Var}_\xi\left(\mathbb{E}[\hat{C}_k \mid \xi]\right) + \mathbb{E}_\xi\left[\text{Var}(\hat{C}_k \mid \xi)\right] \quad (5.11)$$

Since the estimator is unbiased, the first contribution reduces to  $\text{Var}_\xi(C(\xi))$ .

To evaluate the second term, namely the variance conditioned on the monitoring realization  $\xi$ , we simplify the notation by omitting both the superscript  $k$  and the explicit conditioning on  $\xi$ . We decompose the random variables as

$$X_i := \mu_X + \delta X_i \quad Y_i := \mu_Y + \delta Y_i \quad Z_i := \mu_Z + \delta Z_i$$

where

$$\mu_X = \mathbb{E}[X] \quad \mu_Y = \mathbb{E}[Y] \quad \mu_Z = \mathbb{E}[Z]$$

With these definitions, the first term in Eq. (5.8) becomes

$$\bar{Z} = \frac{1}{N} \sum_i Z_i = \mu_Z + \frac{1}{N} \sum_i \delta Z_i \quad (5.12)$$

Similarly, the second contribution can be rewritten as

$$\begin{aligned}
 U &= \frac{1}{N(N-1)} \sum_{i \neq j} (\mu_X + \delta X_i)(\mu_Y + \delta Y_j) \\
 &= \frac{1}{N(N-1)} \sum_{i \neq j} (\mu_X \mu_Y + \mu_X \delta Y_j + \mu_Y \delta X_i + \delta X_i \delta Y_j) \\
 &= \mu_X \mu_Y + \frac{1}{N} \sum_i (\mu_X \delta Y_i + \mu_Y \delta X_i) + \frac{1}{N(N-1)} \sum_{i \neq j} \delta X_i \delta Y_j \quad (5.13)
 \end{aligned}$$

Substituting these expressions into Eq. (5.8), one obtains

$$\begin{aligned}
 \hat{C}_k &= (\mu_Z - \mu_X \mu_Y) + \frac{1}{N} \sum_i (\delta Z_i - \mu_Y \delta X_i - \mu_X \delta Y_i) \\
 &\quad - \frac{1}{N(N-1)} \sum_{i \neq j} \delta X_i \delta Y_j \\
 &= (\mu_Z - \mu_X \mu_Y) + \frac{1}{N} \sum_i \Psi_i - R \quad (5.14)
 \end{aligned}$$

where we introduced the quantities

$$\Psi_i = \delta Z_i - \mu_Y \delta X_i - \mu_X \delta Y_i$$

and

$$R = \frac{1}{N(N-1)} \sum_{i \neq j} \delta X_i \delta Y_j$$

The conditional variance therefore reads

$$\text{Var}(\hat{C}_k) = \text{Var}\left(\frac{1}{N} \sum_i \Psi_i\right) + \text{Var}(R) - 2 \text{Cov}\left(\frac{1}{N} \sum_i \Psi_i, R\right) \quad (5.15)$$

By construction,  $\mathbb{E}[\delta X_i] = \mathbb{E}[\delta Y_i] = 0$ , and, for  $i \neq j$ , the variables  $\delta X_i$  and  $\delta Y_j$  are independent. Assuming that the variables are i.i.d. conditioned on the monitoring process, the individual terms can be evaluated explicitly.

The first contribution is

$$\text{Var}\left(\frac{1}{N} \sum_i \Psi_i\right) = \frac{1}{N} \text{Var}(\Psi) \quad (5.16)$$

For the second term, because the trajectories are independent and the fluctuations are centered, all contributions vanish with the exception of paired indices (e.g.  $i = \ell$ ,

$j = k$ ). The surviving contractions generate two distinct contributions, proportional respectively to  $\text{Var}(X) \text{Var}(Y)$  and  $\text{Cov}(X, Y)^2$ . One therefore obtains

$$\begin{aligned}
 \text{Var}(R) &= \mathbb{E}[R^2] - \mathbb{E}[R]^2 = \mathbb{E}[R^2] \\
 &= \mathbb{E} \left[ \frac{1}{N^2(N-1)^2} \sum_{i \neq j} \sum_{\ell \neq k} \delta X_i \delta Y_j \delta X_\ell \delta Y_k \right] \\
 &= \frac{\text{Var}(X) \text{Var}(Y) + \text{Cov}(X, Y)^2}{N(N-1)}
 \end{aligned} \tag{5.17}$$

Finally, the covariance term vanishes; indeed, every contribution to the expectation value contains at least one independent centered fluctuation appearing linearly. As a consequence, all terms factorize into products containing a zero expectation value, leading to:

$$\begin{aligned}
 \text{Cov} \left( \frac{1}{N} \sum_i \Psi_i, R \right) &= \mathbb{E} \left[ \frac{1}{N} \sum_i \Psi_i R \right] - \mathbb{E} \left[ \frac{1}{N} \sum_i \Psi_i \right] \mathbb{E}[R] \\
 &= \mathbb{E} \left[ \frac{1}{N} \sum_i \Psi_i R \right] \\
 &= \mathbb{E} \left[ \frac{1}{N} \sum_i \Psi_i \frac{1}{N(N-1)} \sum_{\ell \neq k} \delta X_\ell \delta Y_k \right] \\
 &= 0
 \end{aligned} \tag{5.18}$$

Substituting Eqs. (5.16)–(5.18) into Eq. (5.15), the conditional variance becomes

$$\begin{aligned}
 \text{Var}(\hat{C}_k | \xi) &= \frac{1}{N} \text{Var}(\delta Z - \mu_Y \delta X - \mu_X \delta Y | \xi) \\
 &\quad + \frac{\text{Var}(X | \xi) \text{Var}(Y | \xi) + \text{Cov}(X, Y | \xi)^2}{N(N-1)}
 \end{aligned} \tag{5.19}$$

Using Eq. (5.11), one finally obtains

$$\begin{aligned}
 \text{Var}(\hat{C}_k) &= \text{Var}_\xi(C(\xi)) \\
 &\quad + \frac{1}{N} \mathbb{E}_\xi [\sigma_\Psi^2(\xi)] \\
 &\quad + \frac{1}{N(N-1)} \mathbb{E}_\xi [\text{Var}(X | \xi) \text{Var}(Y | \xi) + \text{Cov}(X, Y | \xi)^2]
 \end{aligned} \tag{5.20}$$

Substituting this result into Eq. (5.10), the variance of the estimator for the covariance

function is

$$\begin{aligned} \text{Var}(\hat{C}) = & \frac{1}{M} \text{Var}_\xi (C(\xi)) + \frac{1}{MN} \mathbb{E}_\xi [\sigma_\Psi^2(\xi)] \\ & + \frac{1}{MN(N-1)} \mathbb{E}_\xi [\text{Var}(X | \xi) \text{Var}(Y | \xi) + \text{Cov}(X, Y | \xi)^2] \end{aligned} \quad (5.21)$$

The final expression for the variance separates into three contributions. The first term describes fluctuations between different monitoring realizations and therefore scales inversely with the number of experiments  $M$ . The second term corresponds to the leading statistical uncertainty associated with the finite sampling of trajectories for a fixed monitoring realization, exhibiting the standard scaling proportional to  $1/N$ . Finally, the third term represents a subleading correction originating from the U-statistic structure required to obtain an unbiased estimator of the covariance.

Finally, defining the total computational budget  $T = NM = \text{constant}$ , the variance can be rewritten as

$$\begin{aligned} \text{Var}(\hat{C}) = & \frac{N}{T} \text{Var}_\xi (C(\xi)) + \frac{1}{T} \mathbb{E}_\xi [\sigma_\Psi^2(\xi)] \\ & + \frac{1}{T(N-1)} \mathbb{E}_\xi [\text{Var}(X | \xi) \text{Var}(Y | \xi) + \text{Cov}(X, Y | \xi)^2] \end{aligned} \quad (5.22)$$

The prediction was tested numerically by performing simulations at fixed total cost

$$T = NM = 2100$$

For each value of  $N$ , the number of experiments was chosen as  $M = T/N$ . The analysis was repeated 120 times in order to estimate the variance of the final estimators. The simulations were initialized from random initial conditions and evolved only for a small number of time steps.

Figure 5.10 shows the quantity  $T \text{Var}[\hat{C}]$  as a function of  $N$  for the covariance  $\text{Cov}(M_x, M_y)$  and for the variance  $\text{Var}(M_z)$ . The numerical data are compared with the fit obtained from the analytical expression derived above. The agreement confirms that the formula captures the relevant dependence of the estimator variance on the way in which the fixed computational budget is split between trajectories and experiments.

The fitted curves show that the estimator variance increases when  $N$  is increased. Therefore, within the explored parameter regime, the optimal strategy is to use the smallest number of internal trajectories compatible with the unbiased estimator. Since

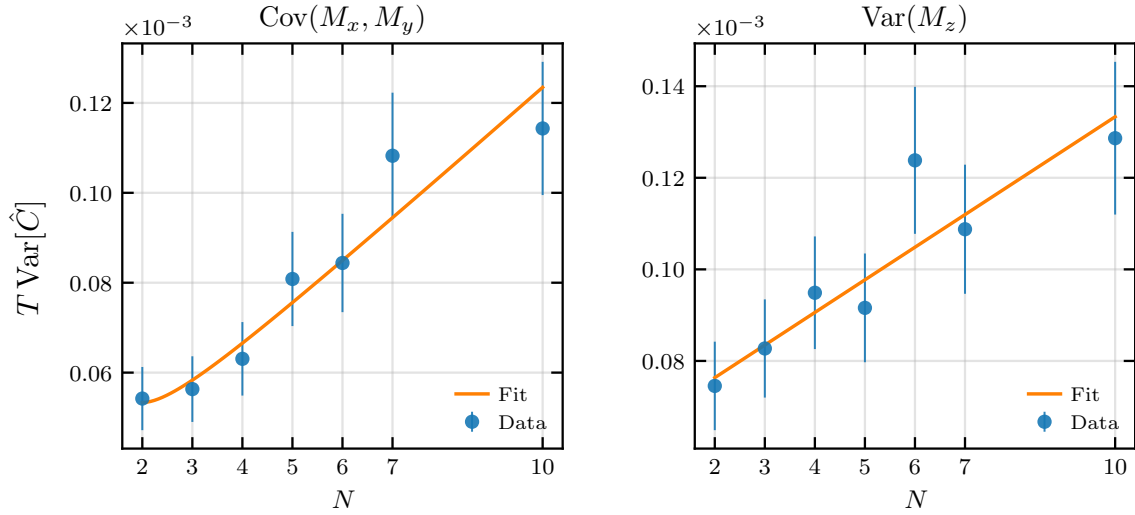


Figure 5.10: Variance of the estimators for nonlinear observables at fixed computational cost  $T = N_{\text{traj}}N_{\text{exp}} = 2100$ . The analysis is performed for  $\text{Cov}(M_x, M_y)$  and  $\text{Var}(M_z)$  using 120 independent repetitions.

the estimation of a variance or covariance requires at least two internal trajectories, this corresponds to  $N = 2$ .

This result suggests that the dominant contribution to the statistical uncertainty is the one associated with fluctuations between independent experiments. In the analytical expression, this corresponds to the term proportional to the number of internal trajectories once the total cost is kept fixed.

This analysis provides a practical criterion for the simulations of conditional dynamics. When nonlinear observables such as variances and covariances are the quantities of interest, the computational effort should preferentially be invested in increasing the number of independent experiments rather than increasing the number of internal trajectories per experiment. This the reason why we have typically considered  $N_{\text{traj}} = 2$  when studying monitored dynamics.

# Chapter 6

## Conclusions

The objective of this thesis was to extend the method proposed in Ref. [3] for the simulation of monitored open quantum dynamics with otVMC to two-dimensional many-body systems, and to apply it to the paradigmatic case of a long-range dissipative transverse-field Ising model.

A two-dimensional implementation of the long-range dissipative transverse-field Ising model was developed and integrated within the otVMC framework. Particular attention was devoted to separating the geometrical structure of the lattice from the stochastic and variational evolution, so that the code could be made efficient and easily generalized to different two-dimensional geometries.

The numerical results show that, in the presence of Hamiltonian dynamics and continuous monitoring, the implemented code correctly reproduces the expected conditional dynamics. In this regime, the otVMC approach was found to be stable and accurate, and it allowed simulations to be extended to system sizes significantly larger than those accessible by direct exact integration of the stochastic master equation. These results confirm the potential of the method for the study of monitored many-body dynamics in the class of two-dimensional systems considered.

At the same time, the analysis highlighted some limitations when local dissipative processes are included. In this regime, the accuracy observed in the purely monitored Hamiltonian case is not always preserved. This indicates that the extension of the method to dynamics combining continuous monitoring and local dissipation requires further investigation.

Several benchmarks were performed to analyse the scaling behaviour of the code and to assess its computational efficiency for increasing system sizes. In this context,

particular effort was devoted to optimizing the routines associated with random-number generation, which represent a crucial component of both the Monte Carlo sampling and the stochastic evolution. These optimizations improved the practical performance of the implementation and provided a clearer picture of the numerical cost of the different parts of the algorithm.

Several directions for future work naturally follow from these results. First, a more detailed profiling of the code would be necessary in order to identify the dominant computational bottlenecks and improve the scaling for large two-dimensional systems. This includes a careful analysis of the parallelization strategies and of the interaction between the libraries used for linear algebra, random-number generation, and Monte Carlo sampling.

A further development would consist in testing more expressive variational ansätze for conditional dissipative dynamics. While the present implementation is able to capture the monitored Hamiltonian evolution with good accuracy, more flexible variational states may be required to describe regimes in which monitoring and dissipation act simultaneously.

In conclusion, this thesis provides a first extension of the otVMC approach for monitored open quantum systems to two-dimensional long-range spin models. The results demonstrate that the method can successfully describe monitored Hamiltonian dynamics and can reach relatively large system sizes. At the same time, the difficulties encountered in the presence of local dissipators identify clear targets for future investigations. Addressing these issues would make it possible to apply the method to a broader class of open quantum many-body systems and to investigate regimes in which interactions, dissipation, and measurement are all present.

# Appendix A

## Scaling

Figure A.1 reports the execution time of the simulation as a function of the number of spins for different numbers of MPI processes on two computational platforms: the Galileo100 cluster at CINECA and the INRiM workstation Legion. The left panel presents the data on a logarithmic scale to emphasize the scaling behaviour, the right panel shows the same data on a linear scale to highlight the absolute runtime differences. Figure A.2 displays the percentage differences between selected configurations, as indicated in the legend.

This analysis, although not central to the physical results of the thesis, is relevant in view of the primary research objective of performing simulations at progressively larger system sizes. Understanding how the computational cost grows with the number of spins and with the degree of parallelization is therefore essential both for assessing the practical feasibility of large-scale simulations and for identifying potential inefficiencies that may affect the use of high-performance computing resources.

A first important observation emerges from the log-log representation. For sys-

| Dataset          | Full range | $N \leq 64$ | $N \geq 81$ |
|------------------|------------|-------------|-------------|
| Legion, 10 ranks | 2.143      | 1.863       | 3.302       |
| Legion, 19 ranks | 2.425      | 1.848       | 3.339       |
| G100, 10 ranks   | 2.184      | 1.917       | 3.249       |
| G100, 32 ranks   | 2.419      | 1.847       | 3.570       |

Table A.1: Power-law exponents obtained by fitting the computational time as  $t \sim N^\alpha$ . The fits are performed over the full range of system sizes and separately in the small- and large-size regimes.

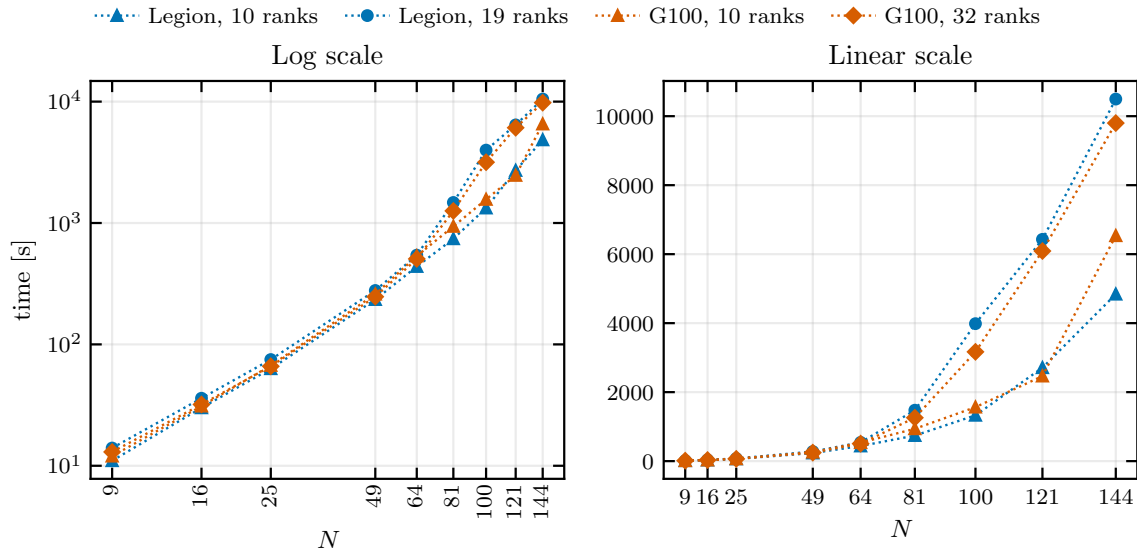


Figure A.1: Scaling.

tem sizes below approximately 100 spins, the execution time scales approximately quadratically with the number of spins. Above this threshold, however, the effective scaling exponent increases to a value slightly larger than three, as obtained from linear fits in the log-log plane whose results are shown in Table A.1. This crossover in computational complexity is consistently observed on both machines and for different numbers of MPI processes. In contrast, it is not observed in the single-process runs, where the scaling remains close to quadratic up to the largest simulated size (144 spins). This indicates that the change in scaling is not intrinsic to the core algorithm, but rather associated with the parallel execution. Profiling analysis performed with Intel VTune Profiler in the single-process case shows no qualitative change in the relative weight of the main computational kernels across the two regimes, further supporting the hypothesis that the effect originates from MPI-related operations. The precise mechanism responsible for this behavior could not be fully identified within the scope of this work.

A second relevant aspect is the systematic increase in runtime when the number of MPI processes is increased at a fixed system size. This effect is clearly visible in the linear-scale plot of Figure A.1 and quantified in the percentage differences shown in Figure A.2. In an ideal scenario with negligible communication cost, one would expect the execution time to remain approximately constant when distributing the workload over a larger number of processes. In practice, communication and synchronization introduce an overhead that becomes more significant as the amount of exchanged data increases with system size. However, the magnitude and the non-monotonic behavior of the observed overhead suggest that additional factors

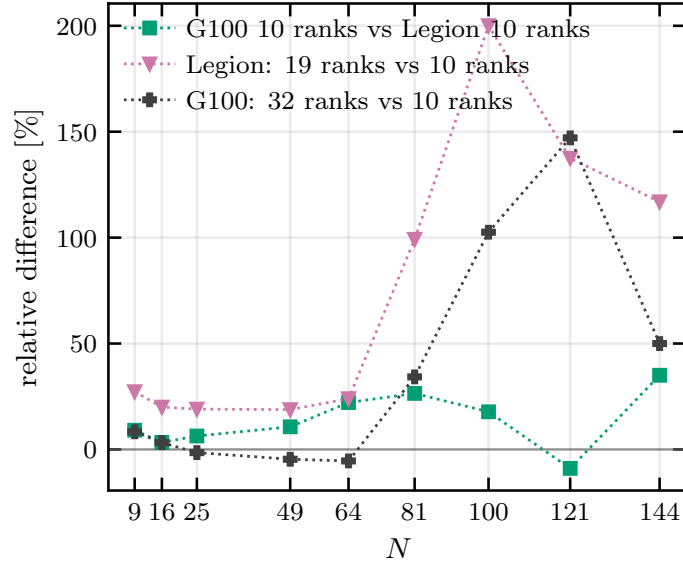


Figure A.2: Scaling difference.

may be involved.

To exclude possible inefficiencies related to unintended hybrid parallelism, several tests were performed. Since the code parallelization relies exclusively on MPI, care was taken to ensure that external numerical libraries did not spawn additional threads that could lead to oversubscription of computational resources. MPI is used by each trajectory to parallelize the VMC random walks. Currently, trajectories are instead performed sequentially. In particular, the libraries MKL and OpenMP (implicitly used by matrix operations in Armadillo) were forced to use a single thread per process by setting the environment variables `MKL_NUM_THREADS=1` and `OMP_NUM_THREADS=1`, and by enforcing the same behaviour at compilation time. These adjustments did not produce any appreciable change in the observed scaling.

It is worth noting that all simulations were performed with identical physical parameters and Monte Carlo settings. Consequently, increasing the number of processes also increases the total Monte Carlo statistics collected in a given wall-clock time, resulting in improved statistical accuracy. Achieving the same level of accuracy with fewer processes would require proportionally longer runtimes. From this perspective, parallel execution remains advantageous despite the communication overhead. Nevertheless, the observed growth of the runtime with both system size and number of processes has practical implications for the efficient use of large HPC clusters and indicates that further optimization of the MPI communication patterns could lead to a significant reduction in computational cost for large-scale simulations.

Overall, the results reported in Figures A.1 and A.2 highlight two aspects that are

particularly relevant for the extension of the simulations to larger systems: the emergence of an effectively cubic scaling regime in the parallel case and the non-negligible overhead associated with increasing the number of MPI processes. Both effects directly impact the feasibility and the computational cost of large-scale simulations, and therefore represent important considerations for future code development and optimisation.

# Appendix B

## QuTiP simulations

This appendix reports the QuTiP code used to produce the exact numerical benchmarks discussed in Chapter 5. QuTiP, the Quantum Toolbox in Python, is an open-source Python library for the simulation of closed and open quantum systems [45]. In this work it was used as an independent benchmark for small system sizes, where the full Hilbert-space representation is still accessible.

The conditional dynamics was simulated with the stochastic master-equation solver `smesolve`. As discussed in Section 1.4, monitored and unmonitored environmental channels play different roles. In QuTiP this distinction is implemented through the two lists `c_ops` and `sc_ops`: the former contains the unmonitored collapse operators. In contrast, the latter contains the monitored channels responsible for the stochastic measurement backaction.

The following code is not meant to reproduce all the auxiliary options used in the simulations, but only the main structure of the implementation.

The geometry, physical parameters and time grid are initialized as follows.

```
1 import numpy as np
2 import qutip as q
3
4 # Geometry
5 n_rows = 3
6 n_cols = 3
7 N = n_rows * n_cols
8
9 # Physical parameters
10 J = 1.0 # Ising interaction strength
```

```

11 h = 0.0 # transverse field
12 l = 0.0 # longitudinal field
13 beta = 2.0 # power-law exponent
14 k = 0.1 # local decay rate
15 Gamma = 0.5 # global dephasing rate
16
17 # Number of stochastic experiments
18 n_experiments = 2000
19
20 # Time grid
21 t_start = 0.0
22 t_end = 1.0
23 dt = 0.005
24 num_steps = int((t_end - t_start) / dt) + 1
25 t_span = np.linspace(t_start, t_end, num_steps)

```

The many-body spin operators are built by tensoring a single-site Pauli operator with the identity on all remaining sites.

```

1 def total_operator(N, index, operator):
2     return q.tensor([
3         operator if n == index else q.qeye(2)
4         for n in range(N)
5     ])
6
7 SigmaX_list = [total_operator(N, i, q.sigmax()) for i in
8     range(N)]
9 SigmaY_list = [total_operator(N, i, q.sigmay()) for i in
10    range(N)]
11 SigmaZ_list = [total_operator(N, i, q.sigmaz()) for i in
12    range(N)]

```

For the long-range Ising Hamiltonian introduced in Section 1.6, the distances are computed on the two-dimensional lattice with periodic boundary conditions, and the interaction is normalized with the same Kac factor used in the variational simulations.

```

1 def ind_to_pos(n, l_row):
2     row = n // l_row
3     col = n % l_row
4     return row, col
5

```

```

6 def distance_matrix(N, l_row, l_col):
7     dist_matrix = np.zeros((N, N))
8
9     for n_i in range(N):
10         for n_j in range(n_i):
11             i, j = ind_to_pos(n_i, l_row)
12             ii, jj = ind_to_pos(n_j, l_row)
13
14             d_row = abs(i - ii)
15             d_col = abs(j - jj)
16
17             d_row = min(d_row, l_col - d_row)
18             d_col = min(d_col, l_row - d_col)
19
20             d = np.sqrt(d_row**2 + d_col**2)
21
22             dist_matrix[n_i, n_j] = d
23             dist_matrix[n_j, n_i] = d
24
25     return dist_matrix
26
27 def kac_normalization(N, beta, Dist):
28     K = 0.0
29     for i in range(N):
30         for j in range(i):
31             K += 1.0 / Dist[i, j]**beta
32
33     return K / (N - 1)
34
35 Dist = distance_matrix(N, n_cols, n_rows)
36 K = kac_normalization(N, beta, Dist)
37
38 H = q.qzero([2] * N)
39 interaction_term = q.qzero([2] * N)
40
41 for i in range(N):
42     H = H - h * SigmaX_list[i] - l * SigmaZ_list[i]
43
44     for j in range(i):
45         d = Dist[i, j]
    
```

```

46         interaction_term += SigmaZ_list[i] * SigmaZ_list[j]
47         / d**beta
48 H = H - (J / K) * interaction_term

```

The local unmonitored channels and the collective monitored channel are defined according to the model described in Section 1.6.

```

1 c_unmon = [
2     total_operator(N, i, np.sqrt(k) * q.sigmam())
3     for i in range(N)
4 ]
5
6 Jz = sum(SigmaZ_list) / 2
7 c_mon = [np.sqrt(Gamma) * Jz]

```

The list `c_unmon` is passed to `c_ops`, while `c_mon` is passed to `sc_ops`. Removing the monitored channels from `sc_ops` gives the corresponding unmonitored evolution. Notice that when `sc_ops` is present, QuTiP correctly assumes that a corresponding dissipator should also be included in the solver.

The observables are collected in a single list. Besides the linear magnetizations, quadratic and mixed operators are included in order to compute the variances and covariances discussed in Sec. 5.8.

```

1 Mx = sum(SigmaX_list) / N
2 My = sum(SigmaY_list) / N
3 Mz = sum(SigmaZ_list) / N
4
5 Obs = [
6     H,
7     Mx,
8     My,
9     Mz,
10    Mx * Mx,
11    My * My,
12    Mz * Mz,
13    0.5 * (Mx * My + My * Mx),
14    0.5 * (Mx * Mz + Mz * Mx),
15    0.5 * (My * Mz + Mz * My),
16 ]

```

Each stochastic experiment is obtained by calling `smesolve` with a single trajectory. The expectation values are stored in an array labelled by experiment, observable and time step.

```

1 expectations = np.zeros((n_experiments, len(Obs),
2                           len(t_span)))
3
4 for r in range(n_experiments):
5     result = q.smesolve(
6         H,
7         Psi0,
8         t_span,
9         c_ops=c_unmon,
10        sc_ops=c_mon,
11        e_ops=Obs,
12        ntraj=1,
13    )
14
15    for j in range(len(Obs)):
16        expectations[r, j, :] = result.expect[j]
```

With this convention, `expectations[r,j,t]` contains the expectation value of the  $j$ -th observable at the selected time step for the experiment labelled by  $r$ .

Linear observables are averaged directly over the stochastic experiments. This is the same procedure used for the comparison with the variational results.

```

1 expectations_avg = np.mean(expectations, axis=0)
2
3 expectations_std = (
4     np.std(expectations, axis=0)
5     / np.sqrt(n_experiments - 1)
6 )
```

For nonlinear quantities, the operation is performed experiment by experiment before taking the average. This distinction, already discussed in Sec. 5.8, is essential for conditional dynamics.

```

1 idx = {
2     "Mx": 1,
3     "My": 2,
4     "Mz": 3,
```

```

5     "MxMx": 4,
6     "MyMy": 5,
7     "MzMz": 6,
8     "MxMy": 7,
9     "MxMz": 8,
10    "MyMz": 9,
11 }

```

The trajectory-resolved variances and covariances are then reconstructed from the stored expectation values.

```

1 covMxMx = (
2     expectations[:, idx["MxMx"], :]
3     - expectations[:, idx["Mx"], :] * expectations[:,
4         idx["Mx"], :]
5 )
6 covMyMy = (
7     expectations[:, idx["MyMy"], :]
8     - expectations[:, idx["My"], :] * expectations[:,
9         idx["My"], :]
10 )
11 covMzMz = (
12     expectations[:, idx["MzMz"], :]
13     - expectations[:, idx["Mz"], :] * expectations[:,
14         idx["Mz"], :]
15 )
16 covMxMy = (
17     expectations[:, idx["MxMy"], :]
18     - expectations[:, idx["Mx"], :] * expectations[:,
19         idx["My"], :]
20 )
21 covMxMz = (
22     expectations[:, idx["MxMz"], :]
23     - expectations[:, idx["Mx"], :] * expectations[:,
24         idx["Mz"], :]
25 )

```

```

25
26 covMyMz = (
27     expectations[:, idx["MyMz"], :]
28     - expectations[:, idx["My"], :] * expectations[:,
29         idx["Mz"], :]

```

Finally, the mean values and standard errors are computed over the stochastic ensemble.

```

1 covariance_avg = np.zeros((6, len(t_span)))
2
3 covariance_avg[0] = np.mean(covMxMx, axis=0)
4 covariance_avg[1] = np.mean(covMyMy, axis=0)
5 covariance_avg[2] = np.mean(covMzMz, axis=0)
6 covariance_avg[3] = np.mean(covMxMy, axis=0)
7 covariance_avg[4] = np.mean(covMxMz, axis=0)
8 covariance_avg[5] = np.mean(covMyMz, axis=0)
9
10 covariance_std = np.zeros((6, len(t_span)))
11
12 covariance_std[0] = np.std(covMxMx, axis=0) /
13     np.sqrt(n_experiments - 1)
14 covariance_std[1] = np.std(covMyMy, axis=0) /
15     np.sqrt(n_experiments - 1)
16 covariance_std[2] = np.std(covMzMz, axis=0) /
17     np.sqrt(n_experiments - 1)
18 covariance_std[3] = np.std(covMxMy, axis=0) /
19     np.sqrt(n_experiments - 1)
20 covariance_std[4] = np.std(covMxMz, axis=0) /
21     np.sqrt(n_experiments - 1)
22 covariance_std[5] = np.std(covMyMz, axis=0) /
23     np.sqrt(n_experiments - 1)

```

This post-processing is the one used for the QuTiP benchmarks shown in Chapter 5. Linear observables are averaged directly, while variances and covariances are first reconstructed for each stochastic experiment and only afterwards averaged over the ensemble.

For the simulations in which the monitored evolution was compared directly with

the corresponding variational trajectories, the same Wiener increments were imposed in both calculations. This was done by using the lower-level `SMESolver` interface and the method `run_from_experiment`. In this way, the stochastic noise entering the QuTiP evolution is not generated internally by the solver, but is instead read from the same file used in the variational simulation. This allows a comparison of the conditional dynamics, rather than only a comparison between ensemble averages.

```

1 solver = q.SMESolver(
2     H,
3     sc_ops=c_mon,
4     heterodyne=False,
5     c_ops=c_unmon,
6 )
7
8 dW = np.loadtxt(
9     "Wiener_monitored_exp0_dW_dt1.dat",
10    comments="#",
11    usecols=1,
12 )
13
14 for r in range(n_experiments):
15     result = solver.run_from_experiment(
16         state=Psi0,
17         tlist=t_span,
18         noise=dW.reshape(1, -1),
19         e_ops=Obs,
20         measurement=False,
21     )
22
23     for j in range(len(Obs)):
24         expectations[r, j, :] = result.expect[j]
```

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