

Non-Markovian dynamics of open quantum systems and its application

DISSERTATION

zur Erlangung des Grades eines Doktors
der Naturwissenschaften

vorgelegt von

Mei Yu

eingereicht bei der Naturwissenschaftlich-Technischen Fakultät
der Universität Siegen,
Siegen 2025

Betreuer und erster Gutachter

Jun. Prof. Dr. rer. nat. Stefan Nimmrichter
Universität Siegen

Zweiter Gutachter

Prof. Dr. rer. nat. Walter Strunz
Technische Universität Dresden

Abstract

In this thesis, we investigate non-Markovian dynamics across various physical scenarios, categorized into bosonic and finite spin baths, and apply these findings to the metrological task of quantum thermometry and the fundamental problem of quantum memory detection.

To begin, we explore non-Markovian dynamics of few-level giant atoms coupled to surface acoustic waves (SAWs), focusing on two-level and Λ -type three-level systems. With single-phonon excitation at zero temperature, we derive analytical solutions showing strong memory effects due to phonon-mediated self-feedback. Extending to finite temperatures, we study numerically thermal effects on non-Markovian behavior in two-level atoms. Comparing zero-temperature results with analytical solutions, we identify the most suitable numerical approach for simulating the dynamics at finite temperature and show that non-Markovianity can persist at finite temperatures.

Next, we apply the solutions for non-Markovian dynamics in two- and three-level giant atom systems to quantum memory detection. We introduce a criterion for the quantumness of memory approach based on the classical memory concept, reformulating it as a convex optimization problem. Additionally, we propose a metric to quantify the difference between the quantum memory required for a process and its classical memory counterpart. This framework can be extended to high-dimensional systems beyond qubits or two-level atom systems. By using the proposed method, we demonstrate that classical memory fails to describe spontaneous emission in these systems at zero temperature. Finally, we outline an experimental approach for detecting quantum memory in giant atoms.

Moving forward, we shift the focus on non-Markovian pure dephasing of a single or few central spins embedded in a finite spin bath, introducing a spin-lattice model to efficiently simulate the reduced system dynamics. We begin by investigating a single spin's behavior in uncorrelated and correlated spin baths, examining non-Markovian dephasing effects. The model is also applied to two case studies: entangled spins in a 2D lattice interacting with an evolving environment, and two nuclear spins in an organic molecule interacting with a thermal spin bath at finite temperatures for NMR applications.

Lastly, we employed the spin-lattice model to investigate non-Markovian phase thermometry, a non-invasive method in which a quantum spin probe interacts with a system, like a 2D Ising spin lattice, to estimate its temperature by observing the dephasing dynamics. As the system under consideration undergoes a phase transition, we evaluated the thermometric performance in the vicinity of the phase transition, utilizing the quantum Fisher information (QFI) to quantify the precision.

Zusammenfassung

In dieser Dissertation untersuchen wir nicht-Markovsche Dynamiken in verschiedenen physikalischen Szenarien, die in bosonische und endliche Spin-Bäder kategorisiert sind, und wenden diese Erkenntnisse auf die metrologische Aufgabe der Quantenthermometrie und das grundlegende Problem der Quantenspeicherdetektion an.

Zunächst erforschen wir die nicht-Markovsche Dynamik von Few-Level-Riesenatomen, die an akustische Oberflächenwellen (SAWs) gekoppelt sind, wobei der Schwerpunkt auf Zwei-Level- und Λ -Typ-Drei-Level-Systemen liegt. Mit Single-Phonon-Anregung bei Temperatur Null leiten wir analytische Lösungen ab, die starke Gedächtniseffekte aufgrund von phonon-vermitteltem Selbst-Feedback zeigen. Bei Ausdehnung auf endliche Temperaturen untersuchen wir numerisch die thermischen Effekte auf das nicht-Markovsche Verhalten in Zwei-Level-Atomen. Durch den Vergleich der Ergebnisse bei Temperatur Null mit analytischen Lösungen identifizieren wir den am besten geeigneten numerischen Ansatz zur Simulation der Dynamik bei endlicher Temperatur und zeigen, dass die Nicht-Markovianität bei endlichen Temperaturen bestehen bleiben kann.

Als nächstes wenden wir die Lösungen für die nicht-Markovsche Dynamik in Zwei- und Drei-Level-Riesenatomsystemen auf die Quantenspeicherdetektion an. Wir führen ein Kriterium für die Quantenhaftigkeit des Gedächtnisansatzes ein, das auf dem klassischen Gedächtniskonzept basiert und es als konvexes Optimierungsproblem neu formuliert. Zusätzlich schlagen wir eine Metrik vor, um den Unterschied zwischen dem für einen Prozess erforderlichen Quantengedächtnis und seinem klassischen Gegenstück zu quantifizieren. Dieser Rahmen kann auf hochdimensionale Systeme jenseits von Qubits oder Zwei-Level-Atom-Systemen erweitert werden. Mit der vorgeschlagenen Methode zeigen wir, dass das klassische Gedächtnis die spontane Emission in diesen Systemen bei Temperatur Null nicht beschreiben kann. Schließlich skizzieren wir einen experimentellen Ansatz zur Detektion von Quantengedächtnis in Riesenatomen.

Im weiteren Verlauf verlagern wir den Fokus auf die nicht-Markovsche reine Dephasierung eines einzelnen oder weniger zentraler Spins, die in ein endliches Spin-Bad eingebettet sind, und führen ein Spin-Gitter-Modell ein, um die reduzierte

Systemdynamik effizient zu simulieren. Wir beginnen mit der Untersuchung des Verhaltens eines einzelnen Spins in unkorrelierten und korrelierten Spin-Bädern und untersuchen nicht-Markovsche Dephasierungseffekte. Das Modell wird auch auf zwei Fallstudien angewendet: verschränkte Spins in einem 2D-Gitter, die mit einer sich entwickelnden Umgebung interagieren, und zwei Kernspins in einem organischen Molekül, die mit einem thermischen Spin-Bad bei endlichen Temperaturen für NMR-Anwendungen interagieren.

Schließlich verwendeten wir das Spin-Gitter-Modell, um die nicht-Markovsche Phasenthermometrie zu untersuchen, eine nicht-invasive Methode, bei der eine Quantenspinsonde mit einem System, wie einem 2D-Ising-Spin-Gitter, interagiert, um seine Temperatur durch Beobachtung der Dephasierungsdynamik abzuschätzen. Da das betrachtete System einen Phasenübergang durchläuft, bewerteten wir die thermometrische Leistung in der Nähe des Phasenübergangs unter Verwendung der Quanten-Fisher-Information (QFI), um die Präzision zu quantifizieren.

Acknowledgements

First and foremost, I would like to express my deepest gratitude to my supervisor, Prof. Stefan Nimmrichter, for introducing me to the fascinating fields of open quantum systems and quantum thermodynamics. His open-mindedness, consistent support, and patient supervision have been invaluable throughout my PhD journey. His timely feedback and insightful suggestions have consistently guided me through both academic and personal challenges, for which I am profoundly thankful.

I am also sincerely grateful to Prof. Walter T. Strunz from TU Dresden for his guidance during my visit to his group in September and October 2024. Our frequent discussions significantly advanced my understanding and helped me overcome key challenges in my research. I am equally thankful to Dr. Alexander Eisfeld and Dr. Valentin Link from the same group for their inspiring discussions and the valuable insights I gained during my time there.

Special thanks go to Dr. Chau Nguyen from our group for the many discussions and valuable guidance he provided for my research, as well as to Prof. Otfried Ghne for his early mentorship during the initial stages of my PhD journey, which laid a strong foundation for my work.

I would also like to thank my colleagues Dr. Matthias Kleinmann, Dr. Ahana Ghoshal, Ties Ohst, Leonardo S. V. Santos, Julia Boeyens, and Michael Gaida for their collaboration and the engaging academic discussions that enriched my work. Special thanks go to Julia Boeyens and Michael Gaida, my office mates, for creating a positive and supportive working atmosphere. I am also deeply grateful to our group's secretary, Daniela Lehmann, for her kindness, patience, and invaluable assistance, which made many processes during my PhD much smoother.

Finally, I owe an immeasurable debt of gratitude to my family and my love for their endless love and unwavering support. Their belief in me has been my source of strength and motivation, enabling me to persevere through the challenges of this demanding PhD journey. Without their encouragement, I could not have reached this milestone.

List of Abbreviations

Abbreviation	Definition
BCF	bath correlation function
SD	spectral density
CPTP	completely positive and trace-preserving
HEOM	hierarchy equation of motion
ESPRIT	estimation of signal parameters via rotational invariance techniques
ADO	auxiliary density operator
SDP	semidefinite program
SAW	surface acoustic wave
PPT	positive partial transpose
FI	Fisher information
QFI	quantum Fisher information
POVM	positive operator-valued measure
SLD	symmetric logarithmic derivative
MFT	mean-field theory
HTE	high temperature expansion

Contents

Acknowledgements	vi
List of Abbreviations	vii
1 Introduction	1
2 Open quantum system theory	4
2.1 Open systems and non-unitary dynamics	4
2.2 Quantum dynamical maps	6
2.2.1 Kraus representation	6
2.2.2 Choi-Jamiołkowski isomorphism	7
2.2.3 CP divisibility	7
2.3 Markovian versus non-Markovian dynamics	8
2.4 Non-Markovian master equations	9
2.4.1 Nakajima-Zwanzig master equation	9
2.4.2 Time-convolutionless master equation	11
2.4.3 Quantum Redfield master equation	12
2.4.4 Quantum optical master equation	14
2.5 Numerical methods	15
2.6 Conclusion	17
3 Non-Markovian artificial giant atom dynamics	19
3.1 Motivation	19
3.2 The physical setup	20
3.3 Dynamics at zero temperature	22
3.3.1 Exact solution: probability amplitude method	22
3.3.2 Comparison with standard methods	26
3.4 Dynamics at finite temperature	32
3.5 Spontaneous emission in three-level giant atoms	34
3.6 Conclusion	37

4	Quantum memory detection using giant atom dynamics	39
4.1	Motivation	39
4.2	Characterisation of quantum memory	41
4.2.1	Quantization of deviation from classical memory	41
4.2.2	Witnesses of quantum memory	42
4.2.3	Choi representation and SDP relaxation	43
4.3	Quantum memory in giant atom dynamics	43
4.3.1	Two-level giant atom dynamics	44
4.3.2	Three-level giant atom dynamics	46
4.4	Conclusion	49
5	Non-Markovian dynamics in finite spin baths	51
5.1	Motivation	51
5.2	The spin-lattice model	52
5.3	Non-Markovian pure dephasing of single spin	56
5.4	Entanglement dynamics of two spins	61
5.4.1	2D lattice structure bath–Rydberg atoms	61
5.4.2	Organic molecule as a finite correlated spin bath	69
5.5	Conclusion	74
6	Non-Markovian phase thermometry	76
6.1	Motivation	76
6.2	Phase thermometry	77
6.3	Thermometric performance in physical models	81
6.3.1	Curie-Weiss model	82
6.3.2	2D Ising model at zero field	85
6.4	Conclusion	91
7	Conclusion	93
	List of Publications	95
	Bibliography	96
A	Appendix to Chapter 4	118
A.1	Quantum memory detection	118
A.1.1	Basic concepts	118
A.1.2	The classical future and its properties	118
A.1.3	SDP relaxations of the classical future	124

A.1.4	Witnesses of quantum memory	127
A.2	Quantum memory detection in giant atom dynamics	129
A.2.1	Two-level giant atom dynamics	129
A.2.2	Three-level giant atom dynamics	131
B	Appendix to Chapter 5 and 6	133
B.1	Magnetization in Curie-Weiss model	133
B.2	QFI derivation for Curie-Weiss model	133
B.3	Derivation in high temperature expansion	135

Introduction

” *The true sign of intelligence is not knowledge but imagination.*

— Albert Einstein

The study of open quantum systems, where a quantum system interacts with its surrounding environment, is central to understanding the complex dynamics that govern quantum behavior in real-world scenarios. In idealized conditions, quantum systems are often assumed to evolve in isolation, governed by the Schrödinger equation. However, in practice, quantum systems are rarely, if ever, perfectly isolated. Environmental interactions induce dissipation and decoherence, which disrupt quantum coherence—the essential feature that distinguishes quantum systems from classical ones [187, 237]. These effects impose substantial challenges for implementing and controlling quantum technologies [20, 164], including quantum computing [128, 197], quantum communication [68, 82], and quantum sensing [56, 64].

Therefore, understanding the dynamics of open quantum systems is crucial for advancing both our fundamental knowledge of quantum behavior and the practical application of quantum technologies. By studying how quantum systems interact with their environments, we can better manage dissipation and decoherence, ultimately improving the reliability and efficiency of quantum technologies [14, 29, 216].

Traditionally, the dynamics of open quantum systems have been modeled within the Markovian approximation, where the environment is assumed to have no memory [20, 222]. In this framework, once information is lost to the environment, it does not return to the system. While this approach has been widely used due to its mathematical simplicity and applicability to many systems, it fails to capture important features of real-world interactions, where memory effects and temporal correlations between the system and its environment play a crucial role. These memory effects lead to non-Markovian dynamics, where the system’s evolution is influenced not only by the current state of the system but also by its past history [22, 180].

The investigation of non-Markovian dynamics has gained significant interest in recent years, driven by the increasing accessibility of proof-of-principle experiments, primarily operating at radio or microwave resonance frequencies. Relevant platforms include superconducting circuits, where Josephson loops function as artificial atoms interacting with microwave or acoustic waveguide radiation [94, 121], quantum transport systems [219], spin lattice models [165, 167], optomechanical systems [85, 132, 135, 192], and photonic simulators [12, 41, 137].

In addition, non-Markovian dynamics have attracted widespread attention in various areas, including the implementation of quantum heat engines within quantum thermodynamics [73, 163], the investigation of energy excitation transfer in quantum biological systems [38], and the study of photosynthetic complexes [37], where memory effects are fundamental to understanding system behavior. Moreover, non-Markovianity is increasingly regarded as a valuable resource in quantum information processing, offering distinct advantages in maintaining quantum coherence [10, 200], enhancing quantum control [6, 60, 135], and improving error correction [175, 215].

Theoretical methods for addressing non-Markovian dynamics encompass perturbation expansions beyond the weak-coupling regime [21, 35, 127], trajectory-based approaches [62, 116, 201], collision-model techniques [44, 45, 126], and a variety of numerical methods [133, 199, 205, 206]. Each of these methods has its own strengths and limitations, making them suitable for different scenarios.

This thesis aims to explore non-Markovian dynamics across various physical systems by combining existing techniques. These systems include artificial giant atoms coupled to surface acoustic waves [4, 94], NV centers interacting with nearby charge spins [1, 57, 89, 112, 113, 181], and Rydberg atoms interacting with neighboring atoms [8, 13, 24, 86]. Moreover, we examine how these dynamic models can be applied to enhance temperature estimation accuracy in quantum thermodynamics [55, 152] and quantum memory detection [7, 81, 154, 162, 208]. To lay the groundwork for this, Chapter 2 introduces key concepts and mathematical tools necessary for understanding the results presented in subsequent chapters.

In Chapter 3, we investigate the dynamics of few-level giant atoms, focusing on two-level and Λ -type three-level systems. We derive the exact solution for the non-Markovian dynamics of two-level giant atoms at zero temperature, using it as a benchmark to evaluate standard methods for open quantum system dynamics. By comparing these methods with the exact solution, we assess their effectiveness in capturing non-Markovian effects arising from time-delayed self-interaction. Based on this comparison, we identify the most accurate method and apply it to study the

finite-temperature dynamics of giant atoms. Additionally, we extend our analysis to three-level giant atoms, particularly in relation to spontaneous emission.

In Chapter 4, we build on the previous chapter and explore the use of non-Markovian dynamics in two- and three-level giant atoms for quantum memory detection. Notably, we propose a new approach based on the classical memory definition and reformulate it as a convex optimization problem. Furthermore, we introduce a metric to quantify the discrepancy between the quantum memory required for a process and its classical memory counterpart. Finally, we demonstrate the detection of quantum memory within the non-Markovian dynamics of giant atoms.

Chapter 5 introduces a spin-lattice model that enables the study of non-Markovian pure dephasing in central spins embedded in finite spin baths. In this model, an adjacency matrix is used to encode all the accumulated phases from historical interactions, allowing for efficient simulation of the reduced system dynamics. We examine two exemplary scenarios: a two-dimensional, partially filled lattice with hopping and nearest-neighbor interactions and a practical rigid molecular structure with fixed positions and long-range interactions that depend on the distance.

Finally, in Chapter 6, we use the spin-lattice model from the previous chapter to study non-Markovian phase thermometry. This is a non-invasive method where a quantum spin probe interacts with either a small part of the system or the entire system, such as a two-dimensional Ising spin lattice, to measure the temperature by observing its dephasing dynamics. The model from the previous chapter provides a clear framework to describe and analyze this dephasing behavior. Additionally, we consider the effect of a phase transition in the system, which can help improve the accuracy of temperature estimation, measured by the Quantum Fisher Information (QFI).

In summary, this thesis seeks to advance both the foundational and applied aspects of non-Markovian dynamics of open quantum systems.

Open quantum system theory

In this chapter, we present the fundamental concepts and formalisms in the theory of open quantum systems that form the basis for the considerations in the subsequent chapters. We start by outlining the general framework of open quantum systems, accompanied by a brief discussion of key concepts such as the evolution of the reduced density matrix, dynamical maps, and the distinctions between Markovian and non-Markovian dynamics. Building on these foundations, we introduce the perturbative master equation as a tool for describing non-Markovian dynamics. Finally, we present the numerical methods essential for investigating non-Markovian systems that allow for the simulation of complex dynamics in cases where analytical solutions are unattainable.

2.1 Open systems and non-unitary dynamics

In quantum mechanics, the state of a system is represented by a wave function $|\psi\rangle$, which encodes all the essential information about the system. The time evolution of the wave function is determined by the Schrödinger equation

$$\frac{d|\psi(t)\rangle}{dt} = -\frac{i}{\hbar}\hat{H}|\psi(t)\rangle, \quad (2.1)$$

where $\hat{H}$ is the Hamiltonian of the system, which may depend on time due to external driving fields. When the system is in a statistical mixture of states, or its exact state is unknown, it is described by a density operator

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad (2.2)$$

where p_i represents the probability that the system is in the state $|\psi_i\rangle$. The evolution of the density operator is governed by the Liouville-von Neumann equation

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[\hat{H}, \rho(t)]. \quad (2.3)$$

Systems described by Eq. (2.3) exhibit unitary dynamics. However, in practice, most quantum systems interact with their environment, making them open quantum systems. This interaction causes the system's evolution to become non-unitary. The

study of open quantum systems is fundamental for understanding how quantum systems behave in realistic settings, where processes like decoherence and dissipation play a crucial role.

To model an open quantum system S , it is often viewed as a part of a larger composite system that includes both S and its environment B . The environment is typically chosen to be much larger than the system, such as a reservoir with infinitely many degrees of freedom. Although covering the full system dynamics may not be feasible due to the vast size of the environment, it is often possible to extract the essential system dynamics under certain assumptions, especially in the weak coupling regime. The total system, comprising the open system and its environment, remains closed and its unitary dynamics is governed by the microscopic Hamiltonian with a general form

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_I, \quad (2.4)$$

where $\hat{H}_S$ and $\hat{H}_B$ are the Hamiltonians of the system and the environment, respectively, and $\hat{H}_I$ is the interaction Hamiltonian that couples the system and the environment. The time evolution of the global system is still unitary and described by the Liouville-von Neumann equation

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[\hat{H}, \rho(t)]. \quad (2.5)$$

The formal solution to it is given by $\rho(t) = \hat{U}(t)\rho(0)\hat{U}^\dagger(t)$, where the unitary time-evolution operator $\hat{U}(t) = \exp(-i\hat{H}t/\hbar)$, which evolves the composite system from its initial state to the state at a given time moment t . Here, we assume the total Hamiltonian to be time-independent.

To derive the reduced dynamics of the open system S , we trace out the environmental degrees of freedom from the total density matrix $\rho(t)$, resulting in the reduced density matrix

$$\rho_S(t) = \text{tr}_B\{\rho(t)\} = \text{tr}_B\{\hat{U}(t)\rho(0)\hat{U}^\dagger(t)\}. \quad (2.6)$$

By inserting the unitary operator into the right-hand side of the equation and expanding it, one could find that the resulting solution is not closed, making it unhelpful for obtaining a final description. Here we mainly analyze the concepts and the approaches to describe the system dynamics that will be discussed in later sections in detail.

2.2 Quantum dynamical maps

In open quantum systems, the quantum dynamical map is a fundamental concept for describing the system's evolution under environmental interactions. To introduce this concept, we first consider an initially uncorrelated system-environment state, given by $\rho(0) = \rho_S(0) \otimes \rho_B(0)$. The time evolution of the reduced density matrix, as obtained from (2.6), is expressed as

$$\rho_S(t) = \text{tr}_B\{\hat{U}(t)\rho_S(0) \otimes \rho_B(0)\hat{U}^\dagger(t)\}. \quad (2.7)$$

This naturally leads to the definition of a linear map acting on the system's state space $S(\mathcal{H}_S)$

$$\mathcal{E}(t) : S(\mathcal{H}_S) \rightarrow S(\mathcal{H}_S), \quad (2.8)$$

which governs the transformation of the initial system state $\rho_S(0)$ into the corresponding state $\rho_S(t)$ at time t

$$\rho_S(0) \mapsto \rho_S(t) = \mathcal{E}(t) [\rho_S(0)]. \quad (2.9)$$

2.2.1 Kraus representation

For a fixed initial environmental state $\rho_B(0)$, the dynamical map can be expressed in terms of its Kraus decomposition [124]

$$\mathcal{E}(t) [\rho_S(t)] = \sum_{\alpha} \hat{K}_{\alpha}(t) \rho_S(t_0) \hat{K}_{\alpha}^{\dagger}(t), \quad (2.10)$$

where the index $\alpha = \{i, j\}$ and the Kraus operators

$$\hat{K}_{\{i,j\}}(t) = \sqrt{q_i} \langle \psi_i | \hat{U}(t) | \psi_j \rangle \quad (2.11)$$

satisfy the completeness relation

$$\sum_i \hat{K}_i^{\dagger}(t) \hat{K}_i(t) = \mathbb{1}. \quad (2.12)$$

Here, we have used the spectral decomposition of the initial environmental state, $\rho_B(0) = \sum_i q_i |\psi_i\rangle \langle \psi_i|$. The Kraus operators encapsulate the effects of the environment on the open system, incorporating phenomena such as decoherence and dissipation.

From the decomposition, it is straightforward to verify that the linear dynamical map (2.10) is Hermitian, trace-preserving, and positive, meaning it maps positive

operators to positive operators. Consequently, $\mathcal{E}(t)$ ensures that physical states are mapped to physical states. Another key property of the dynamical map $\mathcal{E}(t)$ is that it is not only positive but also completely positive (CPTP) [164]. This property guarantees that the map remains positive not only for the system it directly acts upon but also for any larger system that includes the original system as a subsystem.

2.2.2 Choi-Jamiołkowski isomorphism

An alternative approach to characterizing quantum dynamical maps is provided by the Choi-Jamiołkowski (CJ) isomorphism [115, 144], which establishes a fundamental correspondence between CPTP maps and density operators of a composite system SA . Here, A is an auxiliary system of the same dimension d as S , and the corresponding density operator is known as the Choi state. To construct the Choi state, the map is applied to one part of a maximally entangled state $|\Psi^+\rangle$ in the extended Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_A$, where the auxiliary space $\mathcal{H}_A$ has the same dimension as $\mathcal{H}_S$ [164, 179]. The maximally entangled state is given by

$$|\Psi^+\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^d |i\rangle_S \otimes |i\rangle_A, \quad (2.13)$$

where $\{|i\rangle\}$ forms an orthonormal basis for both $\mathcal{H}_S$ and $\mathcal{H}_A$, with $d = \dim(\mathcal{H}_S)$. The Choi state $E(t)$ associated with the dynamical map $\mathcal{E}$ is then defined as

$$E(t) = (\mathbb{1} \otimes \mathcal{E}) (|\Psi^+\rangle \langle \Psi^+|) = \frac{1}{d} \sum_{i,j=1}^d |i\rangle_A \langle j| \otimes \mathcal{E}_S(|i\rangle_S \langle j|). \quad (2.14)$$

A map $\mathcal{E}$ is said to be completely positive if the extended map $(\mathbb{1} \otimes \mathcal{E})$ preserves positivity. This ensures that the map remains physically valid even when applied to a subsystem of a larger entangled system, making complete positivity a stricter condition than mere positivity. Thus, complete positivity is a stronger condition than mere positivity, guaranteeing that not only all physical states of S evolve into valid physical states, but also that any physical state of the extended system SA is mapped to a legitimate physical state.

2.2.3 CP divisibility

By allowing t to vary over the time interval $[0, T]$, where T can be either finite or infinite, we obtain a family of dynamical maps parameterized by t

$$\mathcal{E} = \{\mathcal{E}(t) \mid 0 \leq t \leq T, \mathcal{E}(0) = \mathbb{1}\}, \quad (2.15)$$

where $\mathbb{I}$ denotes the identity map. This family fully characterizes the time evolution of all initial states of the open system within the given time interval, providing a comprehensive description of its dynamics.

Given inverse map $\mathcal{E}^{-1}$ exists for all time t in the considered time interval, one could always decompose the map at time t into intermediate steps as follows

$$\mathcal{E}(t) = \mathcal{E}(t, s) \circ \mathcal{E}(s, 0), \quad \forall s \in [0, t]. \quad (2.16)$$

This property is referred to as divisibility [179, 180]. If the intermediate map $\mathcal{E}(t, s)$ is positive for all intermediate times s , the family of dynamical maps is said to be P-divisible, indicating that the evolution preserves positivity. However, if the map $\mathcal{E}(t, s)$ is completely positive for all $0 \leq s \leq t$, the dynamics is classified as CP-divisible [23, 179].

2.3 Markovian versus non-Markovian dynamics

A quantum process is classified as Markovian if its evolution is CP-divisible, meaning that the intermediate dynamical map $\mathcal{E}(t, s)$ remains completely positive for all $0 \leq s \leq t$. This condition ensures a memoryless process, where information transferred to the environment does not return to the system [180]. From a differential perspective, Markovian evolution is governed by a time-local master equation of the Lindblad form [134, 148]

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}(t)\rho_S(t), \quad (2.17)$$

where the generator $\mathcal{L}(t)$ has the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) form

$$\mathcal{L}(t) = -\frac{i}{\hbar} [\hat{H}_S, \rho_S(t)] + \sum_k \gamma_k(t) \left(\hat{L}_k \rho_S(t) \hat{L}_k^\dagger - \frac{1}{2} \{ \hat{L}_k \hat{L}_k^\dagger, \rho_S(t) \} \right), \quad (2.18)$$

with non-negative decay rates $\gamma_k(t)$ for all times. This form of dynamics typically arises in weakly interacting systems coupled to large, unstructured environments at or near thermal equilibrium, where individual interactions average out, resulting in a net one-way dissipation of information [20, 23, 180].

Non-Markovian dynamics, in contrast, exhibit memory effects due to the breakdown of CP-divisibility in the dynamical map [22, 180]. If the intermediate map $\mathcal{E}(t, s)$ is positive (P-divisible) but not completely positive, the evolution is no longer CP-divisible, indicating the presence of reversibility or feedback in the system's dynamics. This breakdown results in information backflow from the environment, meaning that previous interactions influence the future evolution of the system [22,

180]. Consequently, the dynamical map can no longer be described as a simple, memoryless process. Instead, the system's evolution is typically governed by a time-dependent master equation, where the decay rates may temporarily become negative [20, 23].

A thorough understanding of non-Markovian dynamics has significant potential for advancing quantum technologies [102, 140, 141]. Systems that exhibit non-Markovian behavior can maintain coherence for extended periods [139, 153], facilitate error correction [175, 215], and support entanglement preservation [204, 209, 232] etc. In the following, we explore different approaches and techniques for describing the non-Markovian dynamics of open quantum systems.

2.4 Non-Markovian master equations

A fundamental method for describing such dynamics involves deriving the master equation governing the evolution of the system's reduced density matrix, $\rho_S(t)$. This section presents some of the most relevant master equations used to model open quantum system dynamics.

2.4.1 Nakajima-Zwanzig master equation

To rigorously describe the dynamics of open quantum systems, where the system interacts with an external environment, it is crucial to employ techniques that describe the reduced system dynamics independently. One of the most effective methods is the Nakajima-Zwanzig projection operator technique, which provides a systematic framework for deriving the exact master equation that governs the evolution of the reduced density matrix [159, 238].

The projection operator technique begins by defining a projection operator $\mathcal{P}$ as follows

$$\mathcal{P}\rho(t) = \rho_S(t) \otimes \rho_B(0), \quad (2.19)$$

which projects the state onto the relevant subspace, with its complementary projector $\mathcal{Q} = 1 - \mathcal{P}$ projecting onto the irrelevant part.

Starting from the global system Hamiltonian (2.4), we analyze the system dynamics in the interaction picture with respect to the free Hamiltonians. In this picture, the global state and interaction Hamiltonian take the following forms

$$\tilde{\rho}(t) = e^{i(\hat{H}_S + \hat{H}_B)t/\hbar} \rho(t) e^{-i(\hat{H}_S + \hat{H}_B)t/\hbar}, \quad (2.20)$$

$$\tilde{H}_I(t) = e^{i(\hat{H}_S + \hat{H}_B)t/\hbar} \hat{H}_I e^{-i(\hat{H}_S + \hat{H}_B)t/\hbar}. \quad (2.21)$$

and the von-Neumann equation for the whole system is given by

$$\frac{d}{dt}\tilde{\rho}(t) = -\frac{i}{\hbar} [\tilde{H}_I(t), \tilde{\rho}(t)] = \mathcal{L}(t)\tilde{\rho}(t). \quad (2.22)$$

This formulation simplifies the analysis by isolating the effects of the interaction from the free evolution of the system and environment.

Applying the defined projector and its complement $\mathcal{P} + \mathcal{Q} = \mathbb{I}$ on both sides of Eq. (2.22), we can obtain the equation of motion for $\mathcal{P}\tilde{\rho}(t)$ and $\mathcal{Q}\tilde{\rho}(t)$ as follows

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \mathcal{P}\mathcal{L}(t)\mathcal{P}\tilde{\rho}(t) + \mathcal{P}\mathcal{L}(t)\mathcal{Q}\tilde{\rho}(t), \quad (2.23)$$

$$\frac{d}{dt}\mathcal{Q}\tilde{\rho}(t) = \mathcal{Q}\mathcal{L}(t)\mathcal{P}\tilde{\rho}(t) + \mathcal{Q}\mathcal{L}(t)\mathcal{Q}\tilde{\rho}(t). \quad (2.24)$$

In order to obtain the above two equations, we also used the identity $\mathcal{P} + \mathcal{Q} = \mathbb{I}$ and insert it between Liouville operator and the density matrix. To get a closed equation for the relevant part of the density matrix, we firstly solve Eq. (2.24) formally and substitute into Eq. (2.23). The formal solution of Eq. (2.24) reads

$$\mathcal{Q}\tilde{\rho}(t) = \mathcal{G}(t, 0)\mathcal{Q}\tilde{\rho}(0) + \int_0^t ds \mathcal{G}(t, s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\tilde{\rho}(s), \quad (2.25)$$

where the propagator $\mathcal{G}(t, s)$ is defined as

$$\mathcal{G}(t, s) = \mathcal{T}_{\leftarrow} \exp \left(\int_s^t ds' \mathcal{Q}\mathcal{L}(s') \right). \quad (2.26)$$

The symbol $\mathcal{T}_{\leftarrow}$ indicates the chronological time ordering. Substituting the expression for $\mathcal{Q}\tilde{\rho}(t)$ into the equation of motion of the relevant part of the state Eq. (2.23) yields the generalized master equation for $\mathcal{P}\tilde{\rho}(t)$

$$\begin{aligned} \frac{d}{dt}\mathcal{P}\tilde{\rho}(t) &= \mathcal{P}\mathcal{L}(t)\mathcal{P}\tilde{\rho}(t) + \mathcal{P}\mathcal{L}(t)\mathcal{G}(t, 0)\mathcal{Q}\tilde{\rho}(0) \\ &+ \int_0^t ds \mathcal{P}\mathcal{L}(t)\mathcal{G}(t, s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\tilde{\rho}(s). \end{aligned} \quad (2.27)$$

For an uncorrelated initial state $\rho(0) = \rho_S(0) \otimes \rho_B(0)$, we have $\mathcal{Q}\tilde{\rho}(0) = (1 - \mathcal{P})\tilde{\rho}(0) = 0$. Therefore, the equation simplifies to

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \mathcal{P}\mathcal{L}(t)\mathcal{P}\tilde{\rho}(t) + \int_0^t ds \mathcal{K}_{\text{NZ}}(t, s)\mathcal{P}\tilde{\rho}(s), \quad (2.28)$$

with the memory kernel

$$\mathcal{K}_{\text{NZ}}(t, s) = \mathcal{P}\mathcal{L}(t)\mathcal{G}(t, s)\mathcal{Q}\mathcal{L}(s). \quad (2.29)$$

The generalized master equation derived here is called Nakajima-Zwanzig projection formalism and is exact, although calculating $\mathcal{K}_{\text{NZ}}(t, s)$ is often complicated or impossible exactly. Nevertheless, this framework is the basis for systematic approximations. For instance, a second-order perturbative expansion in the coupling strength leads to the master equation under the Born approximation [20]. Despite the simplifications from perturbative methods, the resulting equation remains an integro-differential form that can be challenging to solve. This can be alleviated by employing the time-convolutionless projection operator technique, which will be discussed next.

2.4.2 Time-convolutionless master equation

The basic idea of time-convolutionless (TCL) projection operator technique is to remove the memory kernel from the Eq. (2.28) by introducing the backward propagator of the composite system which is defined as [35, 191]

$$\tilde{\mathcal{G}}(t, s) = \mathcal{T}_{\rightarrow} \exp \left(- \int_s^t ds' \mathcal{L}(s') \right), \quad (2.30)$$

and $\mathcal{T}_{\rightarrow}$ indicates the antichronological time ordering. The following involves using the backward propagator to replace the state $\tilde{\rho}(s)$ on the right-hand side of the formal solution for $\mathcal{Q}\tilde{\rho}(t)$ in Eq. (2.25)

$$\mathcal{Q}\tilde{\rho}(t) = \mathcal{G}(t, 0)\mathcal{Q}\tilde{\rho}(0) + \int_0^t ds \mathcal{G}(t, s) \mathcal{Q}\mathcal{L}(s) \mathcal{P}\tilde{\mathcal{G}}(t, s) (\mathcal{P} + \mathcal{Q}) \tilde{\rho}(t). \quad (2.31)$$

Since the integration in Eq. (2.28) arises from solving the irrelevant part $\mathcal{Q}\tilde{\rho}(t)$, introducing the backward propagator at this stage provides a systematic approach to eliminating the memory kernel. Then we can regroup Eq. (2.31) and obtain

$$\mathcal{Q}\tilde{\rho}(t) = \frac{\int_0^t ds \mathcal{G}(t, s) \mathcal{Q}\mathcal{L}(s) \mathcal{P}\tilde{\mathcal{G}}(t, s)}{1 - \int_{t_0}^t ds \mathcal{G}(t, s) \mathcal{Q}\mathcal{L}(s) \mathcal{P}\tilde{\mathcal{G}}(t, s)} \mathcal{P}\tilde{\rho}(t) = \frac{\Sigma(t)}{1 - \Sigma(t)} \mathcal{P}\tilde{\rho}(t), \quad (2.32)$$

with $\Sigma(t) = \int_{t_0}^t ds \mathcal{G}(t, s) \mathcal{Q}\mathcal{L}(s) \mathcal{P}\tilde{\mathcal{G}}(t, s)$. As we can see, the solution explicitly depends on time t which can be substituted into Eq. (2.23) to obtain the exact TCL master equation

$$\frac{d}{dt} \mathcal{P}\tilde{\rho}(t) = \mathcal{P}\mathcal{L}(t) \mathcal{P}\tilde{\rho}(t) + \mathcal{P}\mathcal{L}(t) \frac{\Sigma(t)}{1 - \Sigma(t)} \mathcal{P}\tilde{\rho}(t) = \mathcal{K}_{\text{TCL}}(t) \mathcal{P}\tilde{\rho}(t). \quad (2.33)$$

The equation is local in time now. The generator $\mathcal{K}_{\text{TCL}}(t)$ is defined as

$$\mathcal{K}_{\text{TCL}}(t) = \mathcal{P}\mathcal{L}(t) [1 - \Sigma(t)]^{-1} = \sum_{n=0}^{\infty} \mathcal{P}\mathcal{L}(t) \Sigma^n(t), \quad (2.34)$$

which exists if and only if $1 - \Sigma(t)$ is invertible. This form is the starting point for a perturbative expansion of $\mathcal{K}_{\text{TCL}}(t)$ in powers of the coupling strength [21].

2.4.3 Quantum Redfield master equation

The Redfield master equation is widely used to describe open quantum systems in the weak coupling regime, particularly with bosonic baths modeled by harmonic oscillators [20, 177, 222]. To derive the Redfield master equation for the reduced state, we start with the Nakajima-Zwanzig projection formalism (2.28). Additionally, we apply the assumption $[\hat{H}_B, \rho_B(0)] = 0$, which leads to the result that

$$\mathcal{P}\mathcal{L}(t)\mathcal{P}\tilde{\rho}(t) = 0. \quad (2.35)$$

With these considerations and in the lowest order of the coupling strength, we obtain the following expression (in the interaction picture).

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\frac{1}{\hbar^2} \int_0^t d\text{str}_B \{ [\tilde{H}_I(t), [\tilde{H}_I(s), \tilde{\rho}_S(s) \otimes \rho_B(0)]] \}, \quad (2.36)$$

which is known as the master equation in Born approximation. The initial product state $\rho(0) = \rho_S(0) \otimes \rho_B(0)$ has been assumed.

For the microscopic model, the bosonic environment is generally modeled as linear harmonic oscillators with bath Hamiltonian $\hat{H}_B = \sum_\lambda \hbar\omega_\lambda a_\lambda^\dagger a_\lambda$. The interaction between system and environment is also considered as linear coupling with the interaction Hamiltonian $\tilde{H}_I(t) = \hbar\tilde{L}(t) \otimes \tilde{B}(t)$ in the interaction picture, where the typical bath operator is defined as $\tilde{B}(t) = \sum_\lambda (g_\lambda^* a_\lambda^\dagger e^{i\omega_\lambda t} + g_\lambda a_\lambda e^{-i\omega_\lambda t})$ with the environmental modes indexed by λ . The coupling constants g_λ account for the individual coupling strength between the system and the discrete mode characterized by frequency ω_λ . Note that the coupling operator $\tilde{L}(t)$ is generally considered to be Hermitian. Under these conditions, the equation governing the evolution of the system's density operator becomes

$$\frac{d}{dt}\tilde{\rho}_S(t) = - \int_0^t dt' \{ C(t-t') [\tilde{L}(t), \tilde{L}(t') \tilde{\rho}_S(t')] + \text{h.c.} \}, \quad (2.37)$$

with the bath correlation function (BCF) $C(s) = \text{tr}_B \{ \tilde{B}(t) \tilde{B}(t+s) \tilde{\rho}_B(0) \}$. In the case of a thermal environment, the initial bath state is taken to be the Gibbs state, $\tilde{\rho}_B(0) \sim e^{-\beta \hat{H}_B}$ with the inverse bath temperature $\beta = \hbar/k_B T$. Then the BCF has

$$C(s) = \text{tr}_B \{ \tilde{B}(t) \tilde{B}(t+s) \tilde{\rho}_B(0) \} = \sum_\lambda |g_\lambda|^2 [2\bar{n}(\beta\omega_\lambda) \cos \omega_\lambda s + e^{-i\omega_\lambda s}], \quad (2.38)$$

where $\bar{n}(\beta\omega_\lambda) = 1/(e^{\beta\omega_\lambda} - 1)$ denotes the Bose-Einstein distribution.

In the case of a continuous environment, the discrete set of environmental modes transitions to an infinite collection, leading to a dense distribution of frequencies ω_λ . In this limit, the sum over λ is approximated by an integral $\sum_\lambda |g_\lambda|^2 \rightarrow \int_0^\infty d\omega J(\omega)$, which gives rise to the definition of the spectral density (SD). Here, the coupling strengths g_λ are represented as a continuous function

$$J(\omega) := \sum_\lambda |g_\lambda|^2 \delta(\omega - \omega_\lambda). \quad (2.39)$$

Consequently, for a continuous environment, the BCF takes the form

$$C(s) = \int_0^\infty d\omega J(\omega) [2\bar{n}(\beta\omega) \cos \omega s + e^{-i\omega s}]. \quad (2.40)$$

When the BCF decays faster than the timescale of the system's dynamics in the interaction picture, we can approximate $\rho(t') \approx \rho(t)$ inside the integral of Eq. (2.37). Replacing $t-t'$ by τ and transforming back to Schrödinger picture, yield the following evolution equation

$$\frac{d}{dt} \rho_S(t) = -\frac{i}{\hbar} [\hat{H}_S, \rho_S(t)] - \int_0^t d\tau \{C(\tau) [\hat{L}, \tilde{L}(-\tau) \rho_S(t)] + \text{h.c.}\}, \quad (2.41)$$

where $\tilde{L}(-\tau)$ still remains in the interaction picture. To eliminate the time-dependent coupling operator, it is useful to decompose the coupling operator $\hat{L}$ in the following manner:

$$\hat{L} = \sum_\omega \hat{L}_\omega, \quad (2.42)$$

where ω run over all the possible transition frequencies of the system and $\hat{L}_\omega$ is written in terms of eigenstate projectors of $\hat{H}_S|E\rangle = E|E\rangle$

$$\hat{L}_\omega = \sum_{E, E': E-E'=\omega} |E\rangle \langle E| \hat{L} |E'\rangle \langle E'|. \quad (2.43)$$

Consequently, for an operator $\hat{L}$ in the interaction picture we can write

$$\tilde{L}(t) = \sum_\omega e^{i\hat{H}_S t/\hbar} \hat{L}_\omega e^{-i\hat{H}_S t/\hbar} = \sum_\omega \hat{L}_\omega e^{-i\omega t}. \quad (2.44)$$

With this, Eq. (2.41) can be reexpressed as simpler form

$$\frac{d}{dt} \rho_S(t) = -\frac{i}{\hbar} [\hat{H}_S, \rho_S(t)] + \sum_\omega \chi(\omega, t) \{ [\hat{L}_\omega \rho_S(t), \hat{L}] + \text{h.c.} \}. \quad (2.45)$$

with the time-dependent coefficients $\chi(\omega, t) = \int_0^t d\tau C(\tau) e^{i\omega\tau}$. The derived Redfield master equation does not inherently conform to the GKSL form, which means that the positivity of the reduced density matrix is not assured in general. This can result in unphysical states over time, such as negative probabilities. Nonetheless, when the system-bath coupling is sufficiently weak and the BCF decays rapidly, the approximations underlying the Redfield equation can be justified, making its solutions valid within an acceptable margin of error. To ensure the reduced density matrix always remains positive, additional approximations, such as the rotating wave approximation or secular approximation, can be applied to bring the master equation into GKSL form, the so called quantum optical master equation, thereby preserving physicality at all times.

2.4.4 Quantum optical master equation

To derive the GKSL form, we take the Eq. (2.37) as starting point. Since the coupling operator is Hermitian $\hat{L}^\dagger = \hat{L}$, we rewrite the $\tilde{L}(t) = \tilde{L}^\dagger(t) = \sum_\omega \hat{L}_\omega^\dagger e^{i\omega t}$ and $\tilde{L}(t') = \sum_{\omega'} \hat{L}_{\omega'} e^{-i\omega' t'}$. As before, for a sufficiently fast decaying BCF, the $\tilde{\rho}_S(t')$ can be approximated by $\tilde{\rho}_S(t)$. We also again replace the $t - t'$ by τ and the equation has following form

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}_S(t) &= \sum_{\omega, \omega'} \left\{ \int_0^t d\tau C(\tau) e^{i\omega'\tau} e^{i(\omega - \omega')t} [\hat{L}_{\omega'} \tilde{\rho}_S(t), \hat{L}_\omega^\dagger] + \text{h.c.} \right\} \\ &\approx \sum_{\omega, \omega'} e^{i(\omega - \omega')t} \chi(\omega', t) [\hat{L}_{\omega'} \tilde{\rho}_S(t), \hat{L}_\omega^\dagger] + \text{h.c.} \end{aligned} \quad (2.46)$$

If the magnitude of $\chi(\omega', t)$ is comparable to the system-environment coupling strength, which is generally much smaller than the transition frequency $\omega - \omega'$, certain simplifications can be made. In quantum optics, for instance, the interaction strength between an atom and light is much weaker than the optical mode frequency. This causes the secular terms with $\omega \neq \omega'$ to oscillate rapidly and average out to zero. As a result, only the terms with $\omega = \omega'$ contribute meaningfully. This simplification leads to the quantum optical master equation. Additionally, we can replace the time-dependent coefficients $\chi(\omega, t)$ with their asymptotic values $\chi'(\omega)$ by considering the limit as $t \rightarrow \infty$, making them independent of time. Transforming back to the Schrödinger picture yields the GKSL form

$$\begin{aligned} \frac{d}{dt} \rho_S(t) &= -i[\hat{H}_S/\hbar + \chi'_I(\omega) \hat{L}_\omega^\dagger \hat{L}_\omega, \rho_S(t)] \\ &+ \sum_\omega \left\{ \chi'_R(\omega) [\hat{L}_\omega \rho_S(t), \hat{L}_\omega^\dagger] + \text{h.c.} \right\}. \end{aligned} \quad (2.47)$$

The terms $\chi'_I(\omega)$ and $\chi'_R(\omega)$ represent the imaginary and real parts, respectively. The operators $\hat{L}_\omega$ denote the Lindblad operators. The asymptotic coefficients are constant and positive, resulting in Markovian dynamics.

2.5 Numerical methods

When the coupling strength between a system and its environment extends beyond the weak coupling regime or when the dynamics involve significant feedback mechanisms, traditional perturbative approaches become inadequate. Simulating non-Markovian open quantum dynamics is inherently challenging due to the pronounced memory effects, where the system's evolution depends on its interaction history with the environment.

To address these complexities, a range of advanced numerical methods have been developed. These include the Hierarchical Equations of Motion (HEOM) [205, 207], Time-Evolving Matrix Product Operator (TEMPO) algorithms [133, 199], and non-Markovian quantum state diffusion techniques [62, 63], among others. Each of these methods provides distinct strengths and applicability based on the system-environment characteristics. In this part, we mainly introduce the HEOM method.

Again, consider the microscopic model of an arbitrary system with single bosonic environment, the total system Hamiltonian reads

$$\hat{H} = \hat{H}_S(t) + \sum_{\lambda} \hbar \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} + \hbar \hat{L} \otimes \hat{B} \quad (2.48)$$

with the system operator $\hat{L}$ and the bath operator $\hat{B} = \sum_{\lambda} (g_{\lambda}^* a_{\lambda}^{\dagger} + g_{\lambda} a_{\lambda})$. They are linearly coupled to each other. The exact dynamics of the system in the interaction picture with respect to $\hat{H}_S(t) + \hat{H}_B$ can be derived in terms of the time-ordered influence functional as [129, 142, 205, 207]

$$\begin{aligned} \tilde{\rho}_S(t) = & \mathcal{T} \exp \left\{ - \int_0^t dt_2 \int_0^{t_2} dt_1 \tilde{L}(t_2)^{\times} [C_R(t_2 - t_1) \tilde{L}^{\times}(t_1)] \right. \\ & \left. + i C_I(t_2 - t_1) \tilde{L}^{\circ}(t_1) \right\} \tilde{\rho}_S(0). \end{aligned} \quad (2.49)$$

As one can see, the effect from the bath on the system is included the BCF $C(s)$, which is defined as Eq. (2.38) with the assumptions i.e., the initial product system-environment state and the environment is initially thermal equilibrium state. Note that the notation $O^{\times}(t)$ and $O^{\circ}(t)$ in the equation represent that they act to the

right part as superoperators and are defined as $O^\times(t)A = [O(t), A]$ and $O^\circ(t)A = \{O(t), A\}$ with the commutation and anti-commutation form, respectively.

The Eq. (2.49) is exact but still difficult to directly solve since it includes the time-ordered exponential function with integrals inside. In order to get the exact solution, one first decomposes the real and imaginary parts of BCF into the sum of exponential functions as

$$\begin{aligned} C_R(t) &= \sum_{k=1}^{N_R} c_k^R e^{-\gamma_k^R t}, \\ C_I(t) &= \sum_{k=1}^{N_I} c_k^I e^{-\gamma_k^I t}, \end{aligned} \quad (2.50)$$

where c_k^j and γ_k^j can be real or complex. Then one inserts them into Eq. (2.49) to have

$$\tilde{\rho}_S(t) = \exp \left\{ \int_0^t dt_2 \int_0^{t_2} dt_1 \Phi^\times(t_2) \sum_{j=R,I} \sum_{k=1}^{N_j} e^{-\gamma_k^j(t_2-t_1)} \Omega_k^j(t_1) \right\} \tilde{\rho}_S(0), \quad (2.51)$$

where we introduce the new superoperators defined as

$$\begin{aligned} \Phi(t) &= -i\tilde{L}(t)^\times, \\ \Omega_k^R &= -ic_k^R \tilde{L}^\times(t), \\ \Omega_k^I &= c_k^I \tilde{L}^\circ(t). \end{aligned} \quad (2.52)$$

The purpose of these new superoperators is to simplify expressions as much as possible and to avoid errors caused by imaginary and negative signs during derivations. Then one takes the first derivative of Eq. (2.51) and transforming back to Schrödinger picture, we obtain

$$\begin{aligned} \frac{d}{dt} \rho_S(t) &= -i\hat{H}_S(t)^\times \rho_S(t) + \hat{U}_t \dot{\tilde{\rho}}_S(t) \hat{U}_t^\dagger \\ &= -i\hat{H}_S(t)^\times \rho_S(t) + \Phi(t) \sum_{j=R,I} \sum_{k=1}^{N_j} \hat{U}_t \mathcal{T} \left\{ \int_0^t d\tau \Omega_k^j(\tau) e^{-\gamma_k^j(t-\tau)} \right. \\ &\quad \times \left. \exp \left[\int_0^t dt_2 \int_0^{t_2} dt_1 \Phi(t_2) \sum_{j=R,I} \sum_{k=1}^{N_j} \Omega_k^j(t_1) e^{-\gamma_k^j(t_2-t_1)} \right] \right\} \tilde{\rho}_S(0) \hat{U}_t^\dagger, \end{aligned} \quad (2.53)$$

where $\hat{U}_t = \exp(-i\hat{H}_S t/\hbar)$. Now we can consider the Eq. (2.53) as the starting point and introduce the auxiliary density operators (ADOs). For instance, we can

introduce the first order ADOs in the right-hand side of the equation, which leads to

$$\frac{d}{dt}\rho_S(t) = -i\hat{H}_S(t)^\times \rho_S(t) + \Phi(t) \sum_{j=R,I} \sum_{k=1}^{N_j} \rho_S^{1jk}(t). \quad (2.54)$$

Repeatedly taking the time derivative of introduced ADOs, one ultimately finds the following set of coupled differential equations

$$\begin{aligned} \frac{d}{dt}\rho_S^n(t) = & \left(-i\hat{H}_S^\times - \sum_{j=R,I} \sum_{k=1}^{N_j} n_{jk} \gamma_k^j \right) \rho_S^n(t) - i \sum_{k=1}^{N_R} c_k^R n_{Rk} \hat{L}^\times \rho_S^{n_{Rk}} \\ & + \sum_{k=1}^{N_I} c_k^I n_{Ik} \hat{L}^\circ \rho_S^{n_{Ik}}(t) - i \sum_{j=R,I} \sum_{k=1}^{N_j} \hat{L}^\times \rho_S^{n_{jk}^+}(t), \end{aligned} \quad (2.55)$$

The multi-index n is given by $n = (n_{R1}, n_{R2}, \dots, n_{RN_R}, n_{I1}, n_{I2}, \dots, n_{IN_I})$, where each component n_{jk} is an integer within the range $[0, N_c]$, N_c representing the cutoff order for convergence. The state corresponding to $(0, 0, \dots, 0)$ describes the system density matrix. Operators with non-zero indices, referred to as ADOs, have no direct physical interpretation. The notation $\rho_S^{n_{jk}^\pm}(t)$ indicates an ADO with a specific index either increased or decreased by one.

Using Eq. (2.55), the hierarchy can be truncated at certain level, allowing us to solve the resulting finite set of coupled differential equations through efficient numerical methods such as the Runge-Kutta method. Alternatively, the HEOM module in QuTiP provides a convenient way to simulate the dynamics, offering built-in tools for constructing and solving the hierarchy equations efficiently [129].

2.6 Conclusion

In this chapter, we introduced the essential concepts and formalism of open quantum system theory, focusing on the non-unitary evolution that arises from a system's interaction with its environment. We discussed quantum dynamical maps, which describe the time evolution of an open system, and serve as a foundation for defining CP divisibility. This concept is key in distinguishing between Markovian and non-Markovian dynamics, with the latter characterized by memory effects resulting from environmental backaction.

Given that this thesis centers on non-Markovian dynamics, we explored various methods to describe them. We systematically derived analytical techniques, starting with the Nakajima-Zwanzig projection method and followed by the time-convolutionless

master equation. These methods allow for approximations that lead to the quantum Redfield master equation, which is typically effective in describing dynamics in the weak-coupling regime. In addition, we introduced the numerical HEOM method, a powerful non-perturbative method capable of accurately capturing non-Markovian effects. These discussions set the stage for the upcoming chapters, where we examine both the theory and real-world applications of non-Markovian quantum dynamics.

Non-Markovian artificial giant atom dynamics

In this chapter, we explore the dynamics of few-level giant atoms, artificial atoms that interact with an acoustic waveguide at multiple points, focusing on two-level and Λ -type giant atom systems. We begin by deriving the exact solution for the non-Markovian dynamics of two-level giant atoms at zero temperature, providing a critical benchmark for evaluating the accuracy of standard methods commonly used in open quantum system studies. These methods, including the quantum Redfield master equation and the hierarchy equation of motion method, are widely applied to analyze open quantum dynamics across diverse regimes. By comparing their predictions with the exact zero-temperature solution, we assess their capability to capture non-Markovian effects arising from time-delayed self-interaction, rather than from a structured environment or strong coupling. Building on this comparison, we identify the effective approach from these methods and use it to investigate the finite-temperature dynamics of giant atoms. Additionally, we extend our study to three-level giant atom systems, offering deeper insights into their behavior, particularly with respect to the spontaneous emission process. This chapter is based on the Project [A].

3.1 Motivation

Superconducting qubits coupled to meandering transmission lines or surface acoustic waves (SAWs) enable the realization of giant artificial atoms. Unlike conventional atoms, which interact with a waveguide at a single localized point, giant atoms arise when the spatial extent of the qubit exceeds the wavelength of the acoustic waves, allowing them to couple to the waveguide at multiple distinct locations [4, 67, 119, 147, 211]. This spatially distributed coupling leads to several intriguing effects. For instance, it results in frequency-dependent decay rates and Lamb shifts [77], the formation of bound states in the continuum [91, 92, 234], and nonreciprocal single-photon scattering [235]. Moreover, giant atoms can be engineered to support decoherence-free interactions [66, 123] and facilitate entanglement generation [185, 229–231]. An essential consequence of this extended structure is the emergence of time-delayed self-interactions mediated by propagating phonons, leading to non-

Markovian dynamics. Experimental evidence of this behavior has been observed through non-exponential relaxation in these systems [4].

Despite the growing interest in giant atoms, accurately describing their dynamics remains a significant theoretical challenge. While exact solutions for the dynamics can be obtained under specific conditions, such as the rotating wave approximation and the single-excitation regime at zero temperature [90], these solutions are limited in their applicability. They cannot address more general cases involving thermal environments, multiple excitations, or the strong-coupling regime. Consequently, one of the primary objectives of this chapter is to find an efficient method capable of tackling these broader scenarios. Furthermore, we also aim to investigate the impact of memory effects on the spontaneous emission of higher-level giant atoms, such as Λ -type three-level giant atoms.

This chapter begins by introducing the giant atom platform in Section 3.1, offering a brief overview of its distinctive features and the physical model used to investigate its non-Markovian dynamics. Section 3.2 presents an exact solution for the dynamics of a two-level giant atom at zero temperature, derived under the single-excitation assumption. This solution serves as a benchmark for assessing the accuracy of various standard methods used to analyze open quantum system dynamics, including the quantum Redfield master equation and the HEOM method. Through a systematic comparison, we highlight the limitations of the Redfield approach in capturing non-Markovian effects and demonstrate the accuracy and robustness of the HEOM method. Section 3.3 expands the HEOM framework to explore the dynamics of giant atoms at finite temperatures, providing valuable insights into the intricate interplay between thermal effects and non-Markovian behavior. Lastly, Section 3.4 shifts the focus to the spontaneous emission dynamics of higher-level giant atoms, such as Λ -type three-level systems. This investigation delves deeper into the behavior of multi-level giant atoms, emphasizing the influence of their structure and environmental interactions on crucial processes like spontaneous emission. By examining these aspects, we aim to enhance our understanding of the complex dynamics exhibited by giant atoms in various settings.

3.2 The physical setup

In the experimental setup, the artificial atom is realized as a superconducting transmon qubit, which consists of a superconducting quantum interference device (SQUID) shunted by a large geometric capacitance. This configuration produces an anharmonic energy spectrum characteristic of atomic systems, with tunability achieved through the application of a magnetic flux [15, 122]. When coupled

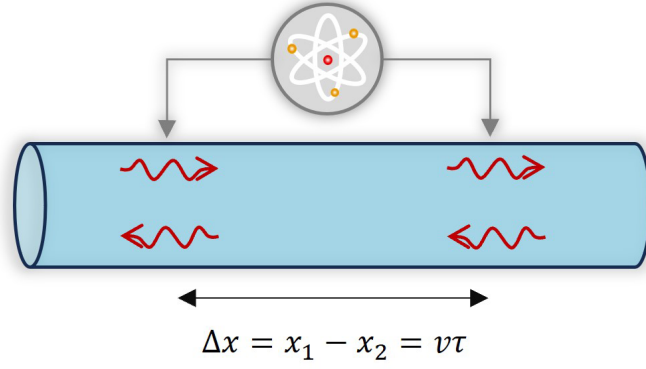


Fig. 3.1.: A giant atom couples to 1D surface acoustic waves via two contacts.

to surface acoustic waves (SAWs), the artificial atom is classified as a giant atom because its physical size spans several SAW wavelengths [4, 94]. This results in spatially distributed interactions, as opposed to the localized point-like coupling typically observed in photonic systems. SAWs are efficiently generated on piezoelectric substrates using interdigital transducers (IDTs), which convert electrical signals into acoustic waves, and propagate freely over long distances, before and after interacting with an atom in their path. With a propagation speed significantly slower than that of electromagnetic waves (e.g., approximately 2900 m/s on a GaAs substrate), SAWs allow for precise control in quantum experiments [95]. The coupling between the artificial giant atom and SAWs is mediated by piezoelectric interaction.

To study the dynamics of giant atom coupling to SAWs theoretically, one can model the setup as a few-level system couple to 1D transmission line or waveguide with left- and right- propagating waves via two contacts separated by a distance Δx , as illustrated in Fig. 3.1. We will first consider the case of the two-level giant atom consisting of states $|g\rangle, |e\rangle$, which was realized experimentally [4]. The total system Hamiltonian of atom and waveguide reads as

$$\hat{H} = \hat{H}_0 + \hbar \sum_{j=1,2} \int_0^\infty d\omega \sqrt{\frac{\gamma(\omega)}{\pi}} \cos\left(\frac{\omega\tau}{2}\right) [\hat{a}_{j\omega}^\dagger |g\rangle\langle e| + \hat{a}_{j\omega} |e\rangle\langle g|], \quad (3.1)$$

where the free Hamiltonian is given by

$$\hat{H}_0 = \hbar\omega_0 |e\rangle\langle e| + \sum_{j=1,2} \int_0^\infty d\omega \hbar\omega \hat{a}_{j\omega}^\dagger \hat{a}_{j\omega}. \quad (3.2)$$

The ω_0 is the transition frequency of the atom, $\gamma(\omega)$ is considered to be the frequency-dependent coupling strength per contact and $\tau = \Delta x/v$ is the delay time for memory

effects to occur, determined by the sound velocity v in the waveguide. The phonon mode operators at frequencies ω are denoted by $\hat{a}_\omega$, obeying $[\hat{a}_\omega, \hat{a}_{\omega'}^\dagger] = \delta(\omega - \omega')$.

3.3 Dynamics at zero temperature

SAWs typically have resonant frequencies in the gigahertz range, and achieving a zero-temperature environment can be realized by cooling the system down to temperatures on the order of tens of millikelvin [4, 94]. In this section, we investigate the dynamics of two-level giant atoms in an environment at zero temperature using different approaches and compare the outcomes. When the giant atom is resonantly coupled to the SAWs, it is possible to derive an exact solution under the assumption that only a single phonon is excited in the field.

3.3.1 Exact solution: probability amplitude method

To derive exact solution describing the dynamics of the giant atom system, we work in the interaction picture with respect to the free Hamiltonian $\hat{H}_0$. The interaction Hamiltonian in this picture is given by

$$\hat{H}_I(t) = \hbar \sum_{j=1,2} \int_0^\infty d\omega \sqrt{\frac{\gamma(\omega)}{\pi}} \cos\left(\frac{\omega\tau}{2}\right) \left[\hat{a}_{j\omega}^\dagger e^{-i(\omega_0-\omega)t} |g\rangle\langle e| + \hat{a}_{j\omega} e^{i(\omega_0-\omega)t} |e\rangle\langle g| \right] \quad (3.3)$$

Given that the SAW modes are initially in the vacuum state and interact resonantly with the atom, there can be at most a single phonon excitation present at any time t . The global pure state of thus be described by the ansatz

$$|\Psi(t)\rangle = \sum_{j=1,2} \int d\omega \alpha_{j\omega}(t) \hat{a}_{j\omega}^\dagger |g, 0\rangle + e(t) |e, 0\rangle + g(0) |g, 0\rangle, \quad (3.4)$$

with the initial condition $\alpha_\omega(0) = 0$. The amplitude of the $|g, 0\rangle$ component remains constant in time, as $\hat{H}_I(t)|g, 0\rangle = 0$. Using the Schrödinger equation $i\hbar\partial_t|\Psi(t)\rangle = \hat{H}_I(t)|\Psi(t)\rangle$, we obtain the coupled equations of motion for the probability amplitudes

$$\dot{e}(t) = -i \sum_{j=1,2} \int_0^\infty d\omega \sqrt{\frac{\gamma(\omega)}{\pi}} \cos\left(\frac{\omega\tau}{2}\right) \alpha_{j\omega}(t) e^{i(\omega_0-\omega)t}, \quad (3.5)$$

$$\dot{\alpha}_{j\omega}(t) = -i \sqrt{\frac{\gamma(\omega)}{\pi}} \cos\left(\frac{\omega\tau}{2}\right) e(t) e^{-i(\omega_0-\omega)t}. \quad (3.6)$$

By formally solving $\alpha_\omega(t)$ and substituting the result into Eq. (3.5), we obtain an integro-differential equation for the amplitude $e(t)$

$$\dot{e}(t) = - \int_0^t dt' C(t-t') e(t') e^{i\omega_0(t-t')}, \quad (3.7)$$

where $C(s)$ is the BCF of the SAW field at zero temperature, given by

$$C(s) = \frac{1}{\pi} \int_0^\infty d\omega 2\gamma(\omega) \cos^2\left(\frac{\omega\tau}{2}\right) e^{-i\omega s}, \quad (3.8)$$

This result is valid for a SAW field with a generic spectral density, as no restrictive assumptions have been made. The solution of $e(t)$ can be found through a Laplace transform or Fourier transform (need assume the boundary condition) and has the form $e(t) = G(t)e(0)$, where the function $G(t)$ satisfies the equation

$$\dot{G}(t) = - \int_0^t dt' C(t-t') G(t') e^{i\omega_0(t-t')}, \quad (3.9)$$

with initial condition $G(0) = 1$.

By means of the solution, the reduced density matrix of the giant atom can be obtained by tracing over the field

$$\rho_S(t) = \text{tr}_f\{|\Psi(t)\rangle\langle\Psi(t)|\} = \mathcal{E}(t) [\rho_s(0)] = \begin{pmatrix} \rho_{ee}(t) & \rho_{eg}(t) \\ \rho_{ge}(t) & \rho_{gg}(t) \end{pmatrix}, \quad (3.10)$$

with matrix elements have the following dynamics

$$\rho_{ee}(t) = |G(t)|^2 \rho_{ee}(0), \quad (3.11)$$

$$\rho_{eg}(t) = G(t) \rho_{eg}(0), \quad (3.12)$$

$$\rho_{ge}(t) = G^*(t) \rho_{ge}(0), \quad (3.13)$$

$$\rho_{gg}(t) = \rho_{gg}(0) + (1 - |G(t)|^2) \rho_{ee}(0). \quad (3.14)$$

These equations describe how the populations and coherences of the giant atom evolve over time, governed by the function $G(t)$. It is important to note that although these equations have been derived assuming a pure product state, they are valid for any initial state of the giant atom, whether pure or mixed. This generality arises from the fact that any mixed state can be represented as a convex linear combination of pure states, and the function $G(t)$ is independent of the initial

condition. Consequently, Eqs. (3.11)-(3.14) represent the exact dynamical map $\mathcal{E}(t)$, which transforms the initial state $\rho_S(0)$ into the state at time t

$$\mathcal{E}(t) : \rho_S(0) \mapsto \rho_S(t) = \mathcal{E}(t) [\rho_S(0)]. \quad (3.15)$$

Exact master equation in time-convolutionless form

The exact solution obtained in the previous section allows us to construct the exact generator $\mathcal{K}_{\text{TCL}}(t)$ of the time-convolutionless master equation (2.33)

$$\frac{d}{dt}\rho_S(t) = \mathcal{K}_{\text{TCL}}(t)\rho_S(t), \quad (3.16)$$

which governs the dynamics of the reduced density matrix. The generator $\mathcal{K}_{\text{TCL}}(t)$ can be obtained from the dynamical map $\mathcal{E}(t)$ using the following relation

$$\mathcal{K}_{\text{TCL}}(t) = \dot{\mathcal{E}}(t)\mathcal{E}^{-1}(t), \quad (3.17)$$

provided the inverse map $\mathcal{E}^{-1}(t)$ exists. Utilizing the expressions for the matrix elements given in Eqs. (3.11)-(3.14), one can show that the generator $\mathcal{K}_{\text{TCL}}(t)$ takes the form

$$\mathcal{K}_{\text{TCL}}(t)\rho_S(t) = -ih(t) [\hat{\sigma}_+\hat{\sigma}_-, \rho_S(t)] + \gamma_-(t)\mathcal{D}[\hat{\sigma}_-], \quad (3.18)$$

where $h(t) = -\text{Im} \left[\frac{\dot{G}(t)}{G(t)} \right]$ is the Lamb shift, which renormalizes the system energy, and $\mathcal{D}[\hat{\sigma}_-] = 2\hat{\sigma}_-\rho_S(t)\hat{\sigma}_+ - \{\hat{\sigma}_+\hat{\sigma}_-, \rho_S(t)\}$ is the dissipator describing the spontaneous emission of the giant atom with a time-dependent decay rate $\gamma_-(t) = -\text{Re} \left[\frac{\dot{G}(t)}{G(t)} \right]$. If the decay rate $\gamma_-(t)$ becomes negative at any point in time, it indicates that the system is exhibiting non-Markovian dynamics. Negative values of $\gamma_-(t)$ correspond to processes such as reabsorption of previously emitted phonons and recoherence of the giant atom. Transforming the master equation back to the Schrödinger picture, we obtain

$$\frac{d}{dt}\rho_S(t) = -i(\omega_0 + h(t)) [\hat{\sigma}_+\hat{\sigma}_-, \rho_S(t)] + \gamma_-(t)\mathcal{D}[\hat{\sigma}_-]. \quad (3.19)$$

In the subsequent analysis, we consider an Ohmic spectral density for the SAW environment, given by $\gamma(\omega) = \eta\omega e^{-\omega/\omega_c}$, where η is the coupling strength and ω_c is the cutoff frequency.

Figure 3.2(a) showcases the time-dependent decay rate as a function of time for various values of the time delay. In the Markovian limit (the time delay $\eta\tau = 0$), the decay rate initially depends on time but quickly settles to a constant value after

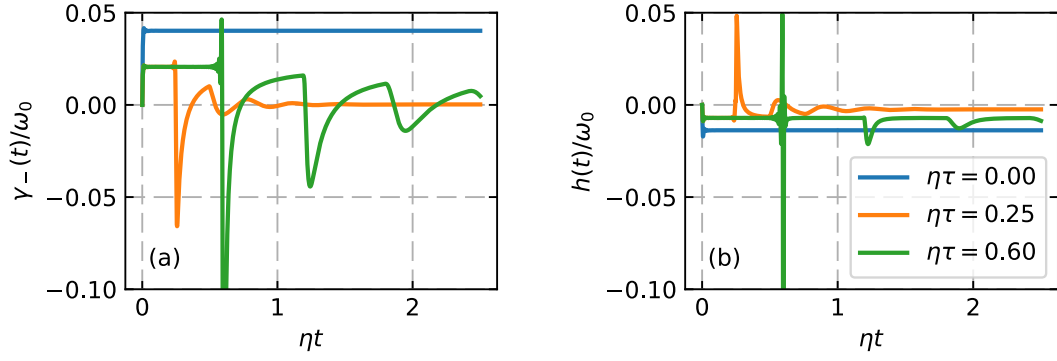


Fig. 3.2.: (a) Time-dependent decay rate and (b) Lamb shift as function of time. We consider an Ohmic spectral density of SAWs environment, $\gamma(\omega) = \eta\omega e^{-\omega/\omega_c}$ with the coupling strength η and cutoff frequency ω_c . The parameters are selected as $\eta/\omega_0 = 2.74 \times 10^{-3}$ and $\omega_c/\omega_0 = 1.2$ for consistency with following plots 3.3.

a brief transient period, resulting in a simple exponential decay of the giant atom's population. However, when $\eta\tau$ takes on non-zero values, such as 0.25 and 0.60, the decay rate exhibits a prolonged time-dependent behavior and displays pronounced oscillations. As the time delay increases, the non-Markovian effects become more significant. This is particularly evident in the case of $\eta\tau = 0.60$, where the decay rate assumes negative values at certain times, a hallmark of non-Markovian dynamics [20]. A negative decay rate indicates a temporary reversal of the information flow, from the SAW environment back to the giant atom, enabling a partial recovery of the atom's population. The non-Markovian behavior essentially arises from the fact that phonons emitted by the giant atom into the acoustic field at one coupling point propagate at the speed of sound and can be reabsorbed at another coupling point, introducing memory effects into the system's dynamics.

Figure 3.2(b) illustrates the temporal evolution of the Lamb shift, which represents the renormalization of the giant atom's energy levels due to its interaction with the SAW environment. In the Markovian case ($\eta\tau = 0$), the Lamb shift initially varies with time but quickly converges to a constant value after a short transient period. However, as $\eta\tau$ increases, the Lamb shift becomes increasingly time-dependent and exhibits more pronounced oscillations. The time-varying nature of the Lamb shift is a direct consequence of the non-Markovian character of the dynamics, reflecting the SAW environment's time-dependent influence on the giant atom's energy levels through memory effects.

Based on the observations discussed above, we conclude that the giant atom system exhibits significant non-Markovian dynamics arising from a time-delayed self-interaction or feedback mechanism, rather than from a structured bath or strong coupling. Remarkably, these non-Markovian effects persist even in the weak-coupling

regime. To further investigate the dynamics of this system and assess the applicability of standard open quantum system techniques, we will employ two widely recognized approaches: the quantum Redfield master equation [20, 222] and the HEOM method [205, 207]. They are standard tools for studying open quantum systems in the weak-coupling regime and strong-coupling regime, respectively. These approaches will be compared with the exact non-Markovian master equation (3.19) to evaluate their effectiveness in capturing the memory effects present in the giant atom system. By conducting this comparison, we aim to assess the applicability of these standard techniques in accurately describing the non-Markovian behavior of the giant atom.

3.3.2 Comparison with standard methods

We begin by applying the quantum Redfield master equation to model the dynamics of the giant atom. Following this, we discuss the HEOM method. While the theoretical foundations of both methods were presented in Chapter 2, this section focuses on their implementation in the context of the giant atom.

Redfield master equation

To derive the Redfield equation, we start from the interaction Hamiltonian (3.3) without applying the rotating wave approximation, $\tilde{H}_I(t) = \hbar \tilde{\sigma}_x(t) \otimes \tilde{B}(t)$, where the bath operator is given by

$$\tilde{B}(t) = \sum_{j=1,2} \int_0^\infty d\omega \sqrt{\frac{\gamma(\omega)}{\pi}} \cos\left(\frac{\omega\tau}{2}\right) (\hat{a}_{j\omega}^\dagger e^{i\omega t} + \hat{a}_{j\omega} e^{-i\omega t}), \quad (3.20)$$

and consider the SAWs field initialized in thermal state. The Redfield master equation, which describes the dynamics of the giant atom and is derived from Eq. (2.37), is expressed as

$$\frac{d}{dt} \rho_S(t) = -i\omega_0 [\hat{\sigma}_+ \hat{\sigma}_-, \rho_S(t)] - \int_0^t ds \{C(s) [\hat{\sigma}_x, \tilde{\sigma}_x(-s) \rho_S(t)] + \text{h.c.}\}. \quad (3.21)$$

The corresponding BCF for the initial thermal state is explicitly formulated as

$$\begin{aligned} C(s) &= \langle \tilde{B}(t) \tilde{B}(t+s) \rangle \\ &= \sum_{j=1,2} \int_0^\infty d\omega \frac{\gamma(\omega)}{\pi} \cos^2\left(\frac{\omega\tau}{2}\right) [2\bar{n}_j(\beta\omega) \cos \omega s + e^{-i\omega s}] \\ &= \frac{1}{\pi} \int_{-\infty}^\infty d\omega J(\beta, \omega) e^{-i\omega s}, \end{aligned} \quad (3.22)$$

where the effective SD is defined as

$$J(\beta, \omega) := \frac{2\gamma(\omega)}{1 - e^{-\beta\omega}} \cos^2\left(\frac{\omega\tau}{2}\right), \text{ with } \gamma(\omega) = -\gamma(-\omega) \text{ for } \omega < 0. \quad (3.23)$$

The BCF simplifies to its zero-temperature form as the inverse temperature β approaches infinity $\beta \rightarrow \infty$, in accordance with Eq. (3.8). In this limit, thermal contributions vanish, leaving only the zero-temperature components of the BCF. For an Ohmic spectral density, the BCF takes the following analytical form

$$\begin{aligned} C(s) = & \frac{\eta}{2\pi\beta^2} \left\{ 2\Psi^{(1)}\left[\frac{1 + is\omega_c}{\beta\omega_c}\right] + 2\zeta^{(2)}\left[-\frac{-\beta + is + 1/\omega_c}{\beta}\right] \right. \\ & + \zeta^{(2)}\left[-\frac{-i\tau - \beta + is + 1/\omega_c}{\beta}\right] + \zeta^{(2)}\left[-\frac{i\tau - \beta + is + 1/\omega_c}{\beta}\right] \\ & \left. + \zeta^{(2)}\left[\frac{1 - i\tau\omega_c + is\omega_c}{\beta\omega_c}\right] + \zeta^{(2)}\left[\frac{1 + i\tau\omega_c + is\omega_c}{\beta\omega_c}\right] \right\}. \end{aligned} \quad (3.24)$$

Here, the $\Psi^{(1)}(x)$ denotes the first-order Polygamma function, while $\zeta^{(2)}(x)$ represents the second-order Zeta function.

The integral in Eq. (3.21) can be simplified further by replacing the $\tilde{\sigma}_x(-s) = \hat{\sigma}_- e^{i\omega_0 s} + \hat{\sigma}_+ e^{-i\omega_0 s}$, which leads to the explicit form of Redfield master equation

$$\begin{aligned} \frac{d}{dt}\rho_S(t) = & -i\omega_0[\hat{\sigma}_+\hat{\sigma}_-, \rho(t)] + \{\Gamma_+(t)[\hat{\sigma}_+\rho(t), \hat{\sigma}_x] + \text{h.c.}\} \\ & + \{\Gamma_-(t)[\hat{\sigma}_-\rho(t), \hat{\sigma}_x] + \text{h.c.}\}, \end{aligned} \quad (3.25)$$

with the time-dependent coefficients (tdc)

$$\Gamma_{\pm}(t) = \int_0^t ds C(s) e^{\mp i\omega_0 s}. \quad (3.26)$$

For a sufficiently fast decaying BCF the asymptotic values $\Gamma_{\pm}(t \rightarrow \infty)$ may be used instead of the actual time dependent coefficients. This leads to the Redfield master equation with asymptotic coefficients (RF (asympt.))

To describe the dynamics of the giant atom under the Hamiltonian in Eq. (3.3), the RWA can be applied to Eq. (3.25). This leads to the evolution equation given by

$$\begin{aligned} \frac{d}{dt}\rho_S(t) = & -i[\omega_0\hat{\sigma}_+\hat{\sigma}_- + \text{Im}\{\Gamma_+(t)\}\hat{\sigma}_-\hat{\sigma}_+ + \text{Im}\{\Gamma_-(t)\}\hat{\sigma}_+\hat{\sigma}_-, \rho_S(t)] \\ & + \text{Re}\{\Gamma_+(t)\}\mathcal{D}[\hat{\sigma}_+] + \text{Re}\{\Gamma_-(t)\}\mathcal{D}[\hat{\sigma}_-], \end{aligned} \quad (3.27)$$

In the form, it is evident that the real and imaginary parts of $\Gamma_{\pm}(t)$ determine the dissipative and coherent contributions, respectively.

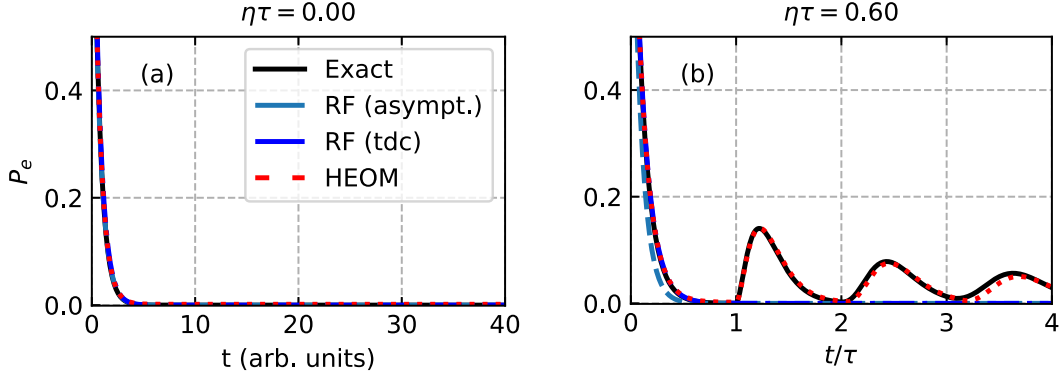


Fig. 3.3.: Spontaneous decay of an initially excited two-level giant atom in (a) the Markovian regime with zero time delay ($\eta\tau = 0$) and (b) the non-Markovian regime with a time delay ($\eta\tau = 0.6$), calculated using various methods. The parameters are set as $\eta/\omega_0 = 2.74 \times 10^{-3}$, $\omega_c/\omega_0 = 1.2$.

At zero temperature, the coefficient $\Gamma_+(t)$ decays rapidly to zero, effectively vanishing. As a result, the system's dynamics are primarily governed by the remaining terms, and the evolution equation simplifies to

$$\frac{d}{dt}\rho_S(t) = -i(\omega_0 + \text{Im}\{\Gamma_-(t)\})[\hat{\sigma}_+\hat{\sigma}_-, \rho_S(t)] + \text{Re}\{\Gamma_-(t)\}\mathcal{D}[\hat{\sigma}_-]. \quad (3.28)$$

This equation is used to compare with the exact solution (3.19) of the dynamics of giant atoms.

Figure 3.3 depicts the decay of the excited state population of a giant atom at zero temperature, calculated using various methods. The dynamics obtained from the Redfield master equation (3.28) with time-dependent and asymptotic coefficients are represented by the blue and light blue lines, respectively, while the exact dynamics derived from Eq. (3.19) are shown as a black solid line. In the Markovian limit ($\eta\tau = 0$), both versions of the Redfield master equation exhibit good agreement with the exact dynamics. However, when there is a non-zero time delay, the exact dynamics display strong non-Markovian behavior, characterized by revivals that reflect the memory effects of the SAWs environment. The Redfield master equation, whether employing asymptotic or time-dependent coefficients, is unable to capture the non-Markovian revivals observed in the exact dynamics, underscoring its limitations in accurately describing the memory effects arising from the SAW environment in giant-atom systems. Although the time-dependent coefficient variant aligns more closely with the exact dynamics at early times, its failure to describe non-Markovian behavior can be attributed to the assumption that the bath correlation time is negligible compared to the system's characteristic timescale. This assumption breaks down due to the interference of propagating acoustic modes at the contacts, which generates an oscillatory structure in the effective spectral density, as illustrated in

Fig. 3.4(a). Consequently, the bath correlation function persists during propagation time and exhibits a pronounced peak at τ , as shown in Fig. 3.4(b).

HEOM simulation

To employ the HEOM formalism to simulate giant atom dynamics, the BCF defined in Eq. (3.22) must be accurately represented using a minimal number of exponential terms, as described in Eq. (2.50). The accuracy of this decomposition and the number of terms significantly influence the performance and computational cost of HEOM simulations. Various numerical techniques have been developed to achieve this decomposition, broadly categorized into frequency-domain and time-domain approaches. In the frequency domain, methods such as Matsubara frequency decomposition (MSD) [61, 111, 205] and Padé spectral decomposition (PSD) [107, 108] are commonly applied to simple spectral densities. However, these methods often require numerous terms for convergence, particularly at low temperatures, where the Fano spectrum decomposition (FSD) [50, 233] is often more effective. Time-domain methods, including least squares fitting [5, 101, 213], and Prony's method [36, 186], excel in localized fitting and are well suited for short-to-medium time behavior. However, they may encounter difficulties when applied to highly structured BCFs.

As illustrated in Fig. 3.4(b), the BCF in our case exhibits two sharp peaks at distinct time points, with a flat region between them. This structure poses significant challenges for the aforementioned decomposition methods, particularly as larger time delays accentuate the distinctness of the peaks, making accurate representation more difficult.

In this work, we employ the estimation of signal parameters via rotational invariance techniques (ESPRIT) [182, 203] to efficiently model the BCF (3.22) as a sum of exponential functions. The ESPRIT method leverages the rotational invariance property of a Vandermonde matrix, which is constructed using time-domain samples of the BCF. The process begins with sampling the BCF on a discrete-time grid, followed by the formation of a Hankel matrix from these samples. Singular value decomposition (SVD) is then applied to estimate the number of exponential components, ensuring that the relative error between the fitted BCF and the original BCF satisfies the condition $\|C_{\text{fit}}(t) - C(t)\|_2 / \|C(t)\|_2 < \varepsilon_r$. Reducing the threshold ε_r improves the accuracy of the fit but requires a greater number of exponential functions to achieve this precision. Subsequently, the decay rates (frequencies) are determined by solving an eigenvalue problem, while the corresponding amplitudes are obtained via a least-squares fitting approach. By reconstructing the BCF as a sum of exponential functions, ESPRIT proves to be a robust and effective tool for time-domain analysis.

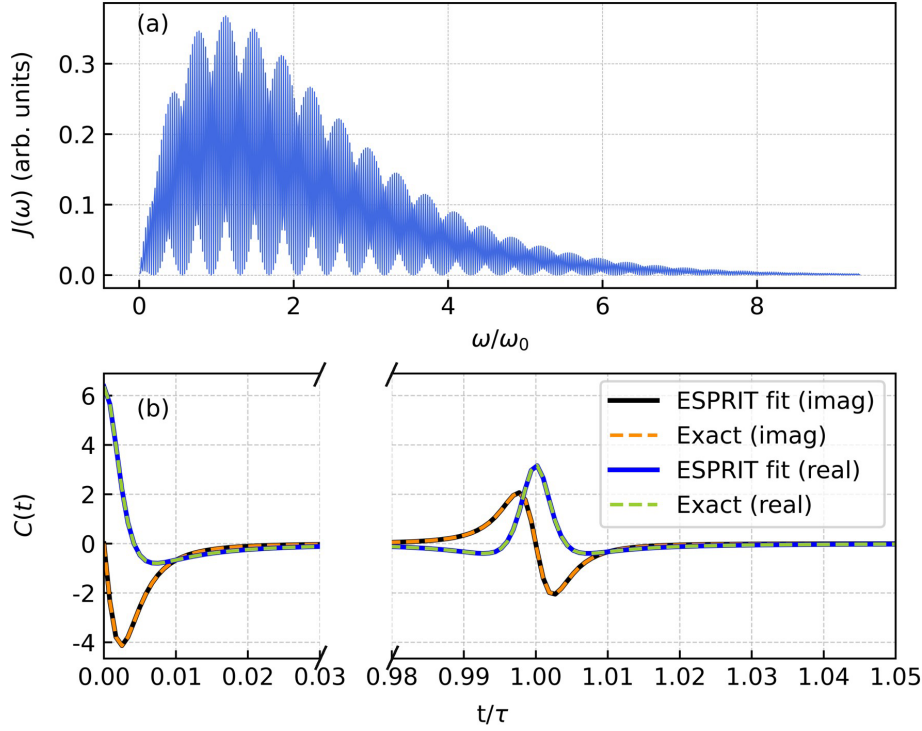


Fig. 3.4.: (a) Effective bath spectral density of the SAWs field at zero temperature; (b) The corresponding bath correlation function as function of time at zero temperature. The parameters are the same as in Fig. 3.3. The dashed lines represent fits based on the ESPRIT method, with a relative error threshold of $\varepsilon_r = 10^{-3}$.

This is demonstrated in Figure 3.4(b), where the real and imaginary components of the original and ESPRIT-fitted BCF show excellent agreement. The plot emphasizes the non-zero regions, focusing on the short-time decay and the oscillatory behavior near $t/\tau \approx 1$, excluding the intermediate flat region for visual clarity. For this fitting, we set the relative error threshold at $\varepsilon_r = 10^{-3}$, balancing accuracy and computational efficiency.

Table 3.1 also presents the number of exponential terms, N_I and N_R , required to fit the imaginary and real part of the BCF at different time delay $\eta\tau$, maintaining a relative error of 10^{-3} . Both N_I and N_R increase approximately linearly with $\eta\tau$, reflecting the growing complexity of the bath dynamics. This complexity arises from enhanced memory effects and richer interference patterns at longer time delays. Consequently, as the system retains memory over extended timescales, a more detailed representation of the bath correlation function becomes essential for accurately capturing its behavior. In the HEOM framework, the number of exponential terms directly determines the number of auxiliary density operators (ADOs). The size of the hierarchy scales combinatorially with both the number of

$\eta\tau$	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7
N_I	6	124	242	361	479	598	716	834
N_R	7	124	242	359	476	593	710	827

Tab. 3.1.: Number of exponential terms in the ESPRIT fit to the BCF for various time delays, given a relative error threshold $\varepsilon_r = 10^{-3}$.

exponential terms and the truncation level, leading to significantly higher memory and computational requirements as the number of exponential terms increases.

Using the fitted exponential functions, we implement the HEOM in QuTiP to simulate the dynamics of the giant atom. The decay of the excited-state probability is shown in Fig. 3.3 at zero temperature and compared with the exact solution, represented by the red dashed line. Our results demonstrate that the HEOM closely reproduces the exact solution in the weak coupling regime in both Markovian and non-Markovian cases. To ensure computational efficiency while accommodating the large number of exponential terms, we set the hierarchy depth or level to 2, which is sufficient for small coupling strength.

It is important to note that as the cutoff frequency of the Ohmic spectral density increases, the peaks of the BCF become sharper. This leads to more exponential terms in the ESPRIT fit, which can significantly increase the computational demands. Therefore, we set the cutoff frequency slightly above the resonance frequency to include the modes that interact resonantly with the atom. This consideration is justified because giant atoms and most optical systems predominantly couple to the environment through resonant interactions [4, 90, 190]. However, in solid-state environments, the assumption of setting the cutoff frequency just above the resonant frequency is no longer applicable. Solid systems often exhibit a broader spectral density, with notable coupling to both resonant and non-resonant modes [130]. As a result, the cutoff frequency must be selected carefully to encompass the relevant non-resonant modes that can affect the system's behavior.

Finally, we examine how the coupling strength affects the performance of HEOM. Fig. 3.5 shows the time evolution of the excited-state probability for different values of η/ω_0 , comparing results from HEOM (solid lines) with the exact solution (dashed lines). In the computation, the coupling strength η is held fixed and the system transition frequency ω_0 is varied. This allows us to explore the effects of entering the effective strong coupling regime (larger η/ω_0). Panels (a) and (b) correspond to the non-Markovian and Markovian regimes, respectively. In both cases, HEOM matches the exact solution well for small η/ω_0 , where the coupling is weak. However, as η/ω_0 increases (entering the effective strong coupling regime), deviations become evident. These discrepancies are likely due to the inclusion of counter-rotating terms

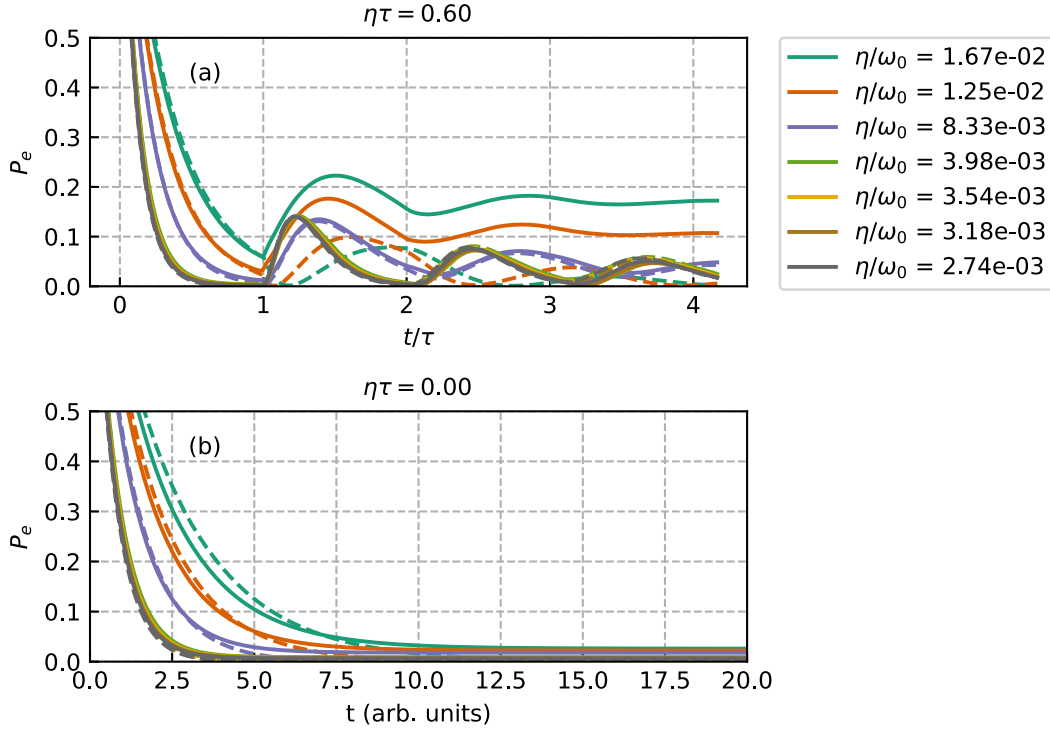


Fig. 3.5.: The spontaneous decay of a two-level giant atom in (a) Markovian regime with zero time delay ($\eta\tau = 0$) and (b) the non-Markovian regime with a time delay ($\eta\tau = 0.6$) with respect to different relative coupling strengths. The parameters are set as $\eta/\omega_c = 2.3 \times 10^{-3}$.

in HEOM, which are neglected in the exact solution under the RWA. The contribution of these terms becomes increasingly significant in the strong coupling regime.

To conclude the analysis of zero-temperature dynamics, we find that HEOM performs well in capturing the non-Markovian behavior of a giant atom at zero temperature. Building on this foundation, we now extend our study to finite temperatures, where thermal effects come into play. In this regime, the single-excitation assumption for the SAW field, as discussed in Section 3.3.1, is no longer valid, necessitating the use of HEOM to simulate the dynamics accurately.

3.4 Dynamics at finite temperature

To implement the HEOM approach at finite temperatures, it is essential to represent the thermal BCF with exponential functions. Fig. 3.6 shows the real part of the BCF, $C_R(t)$, as a function of time for various inverse temperatures. The imaginary part of the BCF, being temperature-independent, is not shown here for simplicity; please refer to Fig. 3.4(b). In the short-time regime, $C_R(t)$ exhibits an exponential-like decay, with the amplitude and decay rate significantly affected by temperature. At

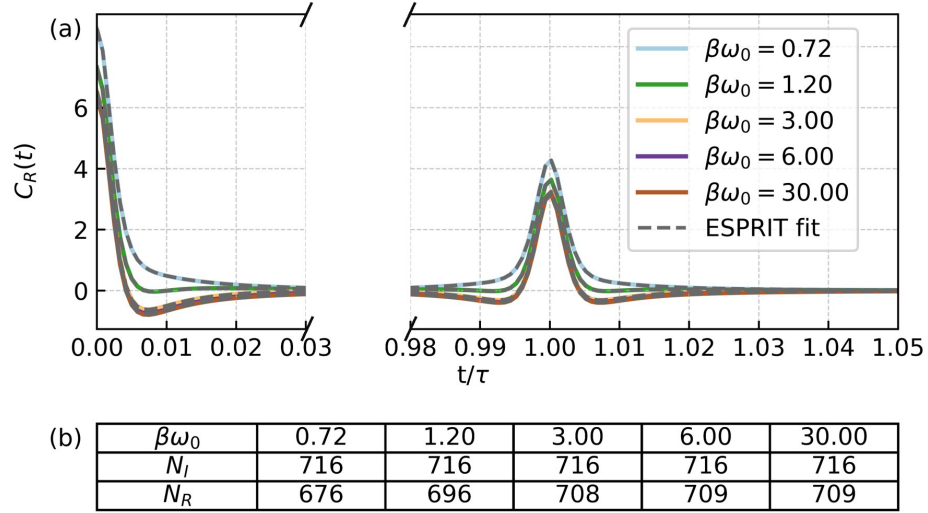


Fig. 3.6.: (a) The real part of thermal BCF for the SAWs field as function of time at various temperatures, along with their corresponding ESPRIT fittings. The parameters are chosen as $\eta/\omega_0 = 2.74 \times 10^{-3}$, $\omega_c/\omega_0 = 1.2$, $\eta\tau = 0.6$ and $\varepsilon_r = 10^{-3}$ for the fitting. (b) The number of exponential functions used in the ESPRIT fitting for the real and imaginary parts of the thermal BCF at different temperatures.

higher temperatures (lower $\beta\omega_0$), the initial amplitude is larger, and the decay is faster, driven by stronger thermal effects. Conversely, at lower temperatures, the initial amplitude decreases, and the decay slows, reflecting reduced thermal noise. Near $t/\tau \approx 1$, oscillatory behavior dominates. As the temperature increases, the peaks of the BCF become more pronounced and decay more quickly, despite the fact that their amplitudes grow larger. This behavior suggests that the memory effects in the thermal bath diminish as the temperature rises.

The dashed lines show the ESPRIT fitting results, which reliably replicate $C_R(t)$ across all temperature regimes, underscoring the accuracy and robustness of this fitting method. Additionally, as the temperature increases, the number of exponential terms required to fit the BCF decreases. This is due to the fact that higher temperatures simplify the structure of the BCF, reducing the need for additional components to capture its behavior.

Using the HEOM approach, we then simulate the dynamics of the giant atom, focusing on the spontaneous decay at various temperatures. The results, depicted in Fig. 3.7, show the excited-state probability P_e as a function of time for different inverse temperatures, with the time delay fixed at $\eta\tau = 0.6$. The non-Markovian behavior, indicated by the revival peaks, is caused by the interference between the atom's relaxation and the delayed feedback from the acoustic field. As the temperature increases (lower $\beta\omega_0$), the initial decay becomes faster, and the revival peaks also weaken and disappear more quickly. This is due to stronger interactions

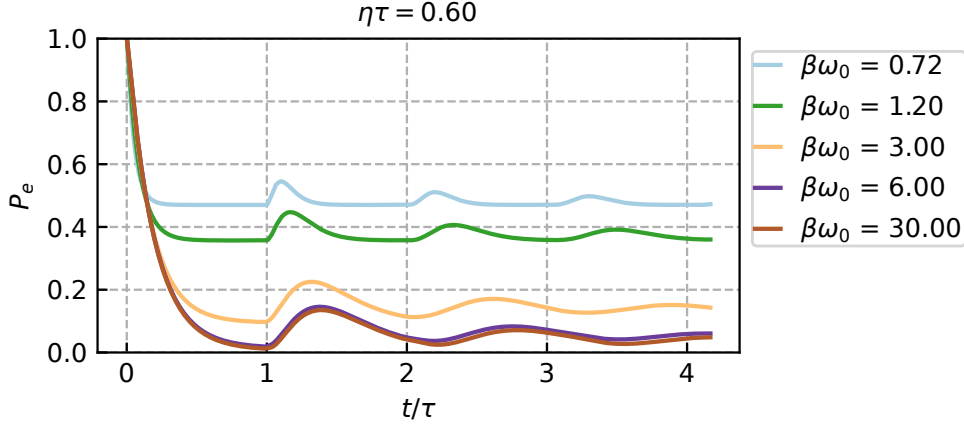


Fig. 3.7.: The spontaneous decay of a two-level giant atom at various temperatures. The parameters are set as $\eta/\omega_0 = 2.74 \times 10^{-3}$, $\omega_c/\omega_0 = 1.2$.

with thermal phonons at higher temperatures, which cause faster loss of coherence and energy. Despite the faster decay at higher temperatures, the system still shows non-Markovian features. The revival peaks become smaller and shorter but are still present even at elevated temperatures. However, at very high temperatures, the system approaches the Markovian regime, and the revival peaks fade completely.

3.5 Spontaneous emission in three-level giant atoms

Have examined the dynamics of two-level giant atoms, we now turn our attention to the more complex case of three-level giant atoms. The additional level structure introduces new interaction channels and dynamical features, motivating us to specifically investigate spontaneous emission in these systems. In this section, we derive the dynamics of a three-level Λ -type giant atom coupled to two 1D vacuum acoustic waveguides via two separated contacts each, as shown in Fig. 3.8. The Λ configuration comprises the states $|e\rangle$, $|s\rangle$, and $|g\rangle$, with associated energies $\omega_e > \omega_s > \omega_g \equiv 0$. We now assume that first waveguide addresses only the ω_e -transition between the ground state $|g\rangle$ and the excited state $|e\rangle$ at the single-contact coupling rate $\gamma_1(\omega)$, while the second waveguide addresses only the $(\omega_e - \omega_s)$ -transition between the metastable state $|s\rangle$ and $|e\rangle$ at the rate $\gamma_2(\omega)$. Direct transitions between ground and metastable state shall be forbidden, and the delay time τ between the contacts is considered to be different for both waveguides. (In practice, both transitions could be coupled to the same waveguide, and they would

still see spectrally non-overlapping, approximately independent vacua as long as the transition frequencies are clearly distinct.) The total Hamiltonian is given by

$$\begin{aligned}\hat{H} = & \hat{H}_0 + \hbar \sum_{j=1,2} \int_0^\infty d\omega \sqrt{\frac{\gamma_1(\omega)}{\pi}} \cos\left(\frac{\omega\tau_1}{2}\right) [\hat{a}_{j\omega}^\dagger |s\rangle\langle e| + \hat{a}_{j\omega} |e\rangle\langle s|] \\ & + \hbar \sum_{j=1,2} \int_0^\infty d\omega \sqrt{\frac{\gamma_2(\omega)}{\pi}} \cos\left(\frac{\omega\tau_2}{2}\right) [\hat{b}_{j\omega}^\dagger |g\rangle\langle e| + \hat{b}_{j\omega} |e\rangle\langle g|],\end{aligned}\quad (3.29)$$

with the free Hamiltonian

$$\hat{H}_0 = \hbar\omega_e |e\rangle\langle e| + \hbar\omega_s |s\rangle\langle s| + \sum_{j=1,2} \int_0^\infty d\omega \hbar\omega (\hat{a}_{j\omega}^\dagger \hat{a}_{j\omega} + \hat{b}_{j\omega}^\dagger \hat{b}_{j\omega}). \quad (3.30)$$

Once again, there can be at most one single photon excitation in each of the two baths at any time, which allows us to make the following ansatz for a general pure state of atom and field,

$$\begin{aligned}|\Psi(t)\rangle = & e(t)|0_1, 0_2, e\rangle + s(t)|0_1, 0_2, s\rangle + g(t)|0_1, 0_2, g\rangle \\ & + \sum_{j=1,2} \int_0^\infty d\omega (\alpha_{j\omega}(t) \hat{a}_{j\omega}^\dagger |0_1, 0_2, s\rangle + \beta_{j\omega}(t) \hat{b}_{j\omega}^\dagger |0_1, 0_2, g\rangle).\end{aligned}\quad (3.31)$$

Here, $|0_j\rangle$ denotes the vacuum state of the j -th waveguide. The solution can be obtained in the same manner as in the previous Section 3.3.1, which results in $g(t) = g(0)$, $s(t) = e^{-i\omega_s t} s(0)$, and $e(t) = G(t)e(0)$, with the decay factor satisfying the following equation

$$\dot{G}(t) = - \int_0^t dt' G(t') [C_1(t-t') e^{i(\omega_e - \omega_s)(t-t')} + C_2(t-t') e^{i\omega_e(t-t')}] , \quad (3.32)$$

where the $C_1(s)$ and $C_2(s)$ are the BCF of two acoustic baths at zero temperature, respectively,

$$C_{i=1,2}(s) = \frac{1}{\pi} \int_0^\infty d\omega 2\gamma_i(\omega) \cos^2\left(\frac{\omega\tau_i}{2}\right) e^{-i\omega s}. \quad (3.33)$$

We consider the scenario where each waveguide exhibits an Ohmic spectral density with distinct coupling strengths, denoted by η_1 and η_2 , and same cutoff frequency ω_c . Our aim is to investigate how the relative coupling strengths of the two waveguide mode continua and the time delays between the contacts affect the spontaneous emission dynamics of the giant atom. These factors influence the interference between emission pathways, ultimately determining the emission characteristics.

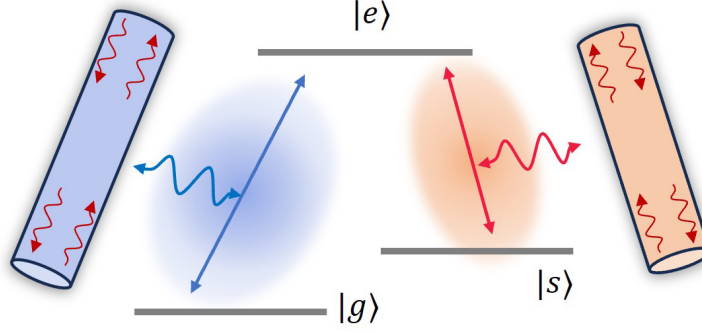


Fig. 3.8.: A Λ -type three-level giant atom coupled to two one-dimensional waveguides. The transition between excited state and ground state, $|e\rangle \leftrightarrow |g\rangle$, and the transition between excited state and metastable state, $|e\rangle \leftrightarrow |s\rangle$, are coupled to two distinct waveguide modes via two separate contact points, respectively.

Figure 3.9(a) presents the excited-state probability P_e of the Λ -type giant atom as a function of time and the time delay ratio τ_2/τ_1 . The color scale represents the magnitude of P_e , with brighter regions indicating higher probabilities. The horizontal dashed lines highlight specific values of τ_2/τ_1 , used to extract data for the corresponding lower plot (b). The atom is assumed to be initially in a fully excited state. The time delays introduce memory effects, reflected in the revivals of P_e over time. These revivals arise from delayed feedback loops in the waveguides, where part of the atom's emission is reflected and re-interacts with the atom after a finite delay. Periodic patterns of bright and dark bands emerge as the time delay ratio τ_2/τ_1 varies, corresponding to constructive and destructive interference of the feedback signals from two waveguides. The ratio τ_2/τ_1 governs the phase difference between these signals: constructive interference enhances the P_e revivals, while destructive interference diminishes them. Notably, when $\tau_2/\tau_1 = 1$, the delays create a resonant condition for optimal constructive interference, which results in the most pronounced revivals of P_e .

Figure 3.9(c) depicts the excited-state probability P_e as a function of time and the coupling strength ratio η_2/η_1 . The horizontal dashed lines correspond to specific values of η_2/η_1 , used to generate the lower plot (d). The plot demonstrates the double role of the coupling strength ratio in governing the atom's dynamics. As the coupling strength ratio η_2/η_1 increases, the initial decay of P_e becomes more rapid. This behavior arises from the stronger interaction between the atom and the waveguides, which facilitates enhanced energy dissipation into the environment. However, larger coupling also intensifies the interference effects of the feedback signals from the waveguides. This leads to more pronounced oscillations and revivals in P_e . The increased coupling amplifies the impact of delayed feedback on the atom's state, thereby strengthening memory effects.

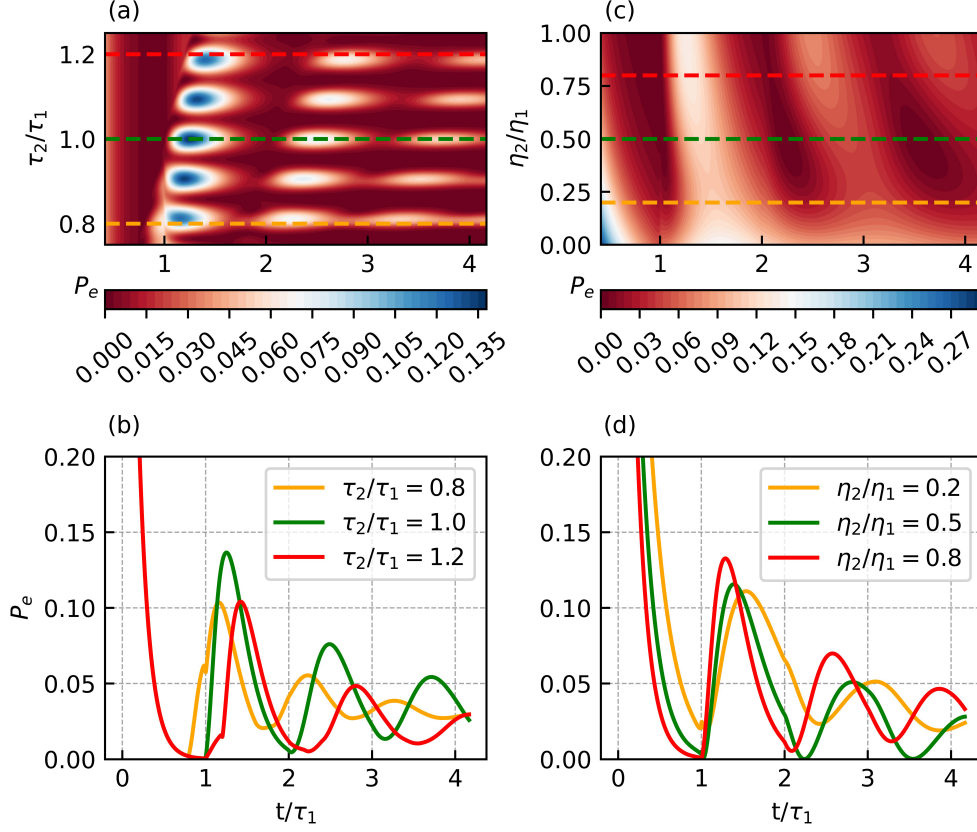


Fig. 3.9.: Excited-state probability P_e of the Λ -type giant atom as function of time and (a) the time delay ratio τ_2/τ_1 ; (c) the coupling strength ratio η_2/η_1 of two waveguides. The lower panels (b) and (d) correspond to the horizontal dashed lines in (a) and (c), respectively. The parameters are set as $\eta_2 = \eta_1$ in (a, b) and $\tau_2 = \tau_1$ in (c, b), respectively. The remaining parameters are chosen as $\omega_e/\omega_s = 2$, $\omega_c/\omega_s = 6.4$, $\eta_1/\omega_s = 0.016$, and $\eta_1\tau_1 = 0.6$.

In summary, by tuning the coupling strengths and time delays, it becomes possible to modulate the interference dynamics and, consequently, control the spontaneous emission of the three-level giant atom.

3.6 Conclusion

In this chapter, we began by investigating the non-Markovian dynamics of a two-level giant atom coupled to a SAWs field at zero temperature. By assuming a single excitation in the field and employing the RWA, we derived an exact solution that describes the dynamics of the giant atom. This solution served as a benchmark for evaluating the performance of two widely used methods: the Redfield master equation and the HEOM method. Our analysis revealed that the Redfield approach fails to accurately capture the non-Markovian effects stemming from time-delayed

self-interactions. In contrast, the HEOM method yielded relatively accurate results when the BCF is finely decomposed into exponential functions.

Additionally, we presented results in the strong coupling regime, where we observe that the HEOM starts to deviate from the exact solution under the RWA. This discrepancy may arise due to the counter-rotating terms in the HEOM simulation, as the current version of the QuTiP package used for HEOM implementation does not support dynamics under the RWA. Future work may involve the implementation of a non-Hermitian HEOM that incorporates the RWA in the system Hamiltonian [202].

We also extended the HEOM framework to explore the system's dynamics at finite temperatures, showing that non-Markovian effects persist even in the presence of thermal influence. This result offered new perspectives on the role of thermal effects in non-Markovian quantum systems. Finally, we investigated the impact of non-Markovian effects on the spontaneous emission of a three-level giant atom. Our findings demonstrate that by adjusting time delays and coupling strengths with the environment, spontaneous emission can be controlled or tuned. Additionally, it is worth investigating the influence of thermal effects on emission.

Looking ahead, future research could focus on studying memory effects in cooperative phenomena in giant atoms, such as superradiance and subradiance. These effects, driven by the collective interaction of multiple atoms with a shared environment [59, 120], may manifest in new ways due to the non-Markovian nature of giant atoms. Another potential direction is using giant atoms coupled to thermal baths in thermodynamic cycle designs. The non-Markovian dynamics of giant atoms could help improve the efficiency of thermal machines beyond the limits of standard Markovian systems. Moreover, giant atoms could be a useful platform for detecting quantum memory, which will be discussed in the next chapter.

Quantum memory detection using giant atom dynamics

In this chapter, we present a method for detecting quantum memory in non-Markovian dynamics, a property that precludes any simulation of the dynamics by a classical measurement-feedback process. In general, the time evolution of an open system can be described by a one-parameter family of CPTP maps $\{\mathcal{E}_n(t)\}$, which map the system's state from an initial time t_0 to a later time t_n . For any pair of consecutive time steps, one can define the amount of classical memory required to describe the transformation of the second time step based on the information attained in the first step. Our approach casts this definition as a convex optimization problem, where the set of two-step quantum dynamical maps attained by classical memory forms a convex set. Consequently, quantum maps outside this set are interpreted as requiring quantum memory. By introducing a distance measure between the quantum map and the convex set, we can quantify the degree of deviation from classical memory. Thus, this method not only differentiates between quantum and classical memory but also provides a way to quantify the extent of this distinction. We will demonstrate this approach using the dynamics of artificial giant atoms. As discussed in the previous chapter, these systems serve as an ideal physical platform for applying the proposed method to detect quantum memory in non-Markovian dynamics. This chapter is based on a collaborative project with Ties-A Ohst [B]. The method was primarily developed by Ties, while I focused on the dynamical process and other aspects.

4.1 Motivation

Non-Markovianity in quantum dynamics has become a pivotal focus in the study of open quantum systems [23, 30, 179, 214] and quantum information processing [145, 169, 220]. Unlike Markovian processes, where the system's evolution depends solely on its present state with no memory of the past, non-Markovian dynamics involve information backflow from the environment to the system [22, 180]. This backflow reflects the presence of memory effects, stemming from correlations between the system and its environment or the structured behavior of the environment itself.

An essential aspect of studying such memory effects is distinguishing whether they can be described classically or require intrinsically quantum degrees of freedom [208, 223, 224]. These two scenarios give rise to fundamentally different noise models and correction strategies. For instance, a scenario with classical memory can be seen as a process in which the system is continuously monitored and a classical feedback mechanism is applied to correct its evolution based on the measurement signal. However, this approach is ineffective for quantum temporal correlations mediated by the environment, where the interplay of coherence and entanglement demands fundamentally different techniques [223, 224]. Consequently, it is crucial to develop efficient methods to distinguish between quantum and classical memory. Such discrimination is not only vital for understanding the underlying physics but also for tailoring error mitigation strategies in quantum technologies, where the nature of memory plays a key role in determining performance and reliability [2, 175, 226].

Existing methods for characterizing quantum memory in dynamical processes are largely grounded in the process tensor framework [81, 154, 162, 208]. Within this framework, the classical nature of environmental memory can be associated with the separability of the process tensor [81]. While the process tensor framework is highly general and capable of describing a wide range of dynamics, including those beyond the traditional scope of open quantum systems, its application to the analysis of quantum memory presents significant experimental challenges. A thorough evaluation of quantum memory requires access to full multi-time correlations, which encode detailed information about the system's evolution across several time points. Achieving this demands precise experimental control and a large number of measurements, making the approach challenging to implement in practice.

An alternative approach focuses solely on the system's dynamics, requiring only the preparation of initial states and the performance of state tomography at two distinct time points [7]. While this method is experimentally viable for qubits, its reliance on computing the entanglement of assistance [193, 225] for Choi states renders it impractical for systems of higher dimensions.

In this chapter, we present our method, which builds upon the classical memory definition proposed in Ref. [7]. This approach not only measures the deviation of quantum memory from classical memory but also extends its applicability to higher-dimensional systems, going beyond two-level systems such as qubits or atoms. Finally, we employ this method to detect quantum memory in the non-Markovian dynamics of both two-level and three-level giant atoms.

4.2 Characterisation of quantum memory

Consider a one-parameter family of completely positive trace-preserving (CPTP) maps, $\{\mathcal{E}(t_n)\}$, describing the evolution of a quantum system from its initial state at $t_0 = 0$ to a later time t_n . We focus on the evolution maps $\mathcal{E}(t_1)$ and $\mathcal{E}(t_2)$ two distinct times, $t_1 < t_2$. The memory is classified as classical if the channel $\mathcal{E}(t_1)$ can be interpreted as a non-destructive measurement, where the measurement outcome $i \in \{1, 2, \dots, n\}$ influences the realization of the subsequent channel $\mathcal{E}(t_2)$. Formally, this means that $\mathcal{E}(t_1)$ can be decomposed into n subchannels $\mathcal{I}_i(t_1)$, referred to as instruments [52], such that $\mathcal{E}(t_1) = \sum_{i=1}^n \mathcal{I}_i(t_1)$. Each subchannel $\mathcal{I}_i(t_1)$ corresponds to a specific classical outcome i and a post-measurement state $\mathcal{I}_i(t_1)$. The classical outcome i then feeds back into the system dynamics by inducing a specific channel $\mathcal{K}_i(t_2, t_1)$. As a result, the overall dynamics at time t_2 can be expressed as

$$\mathcal{E}(t_2) = \sum_{i=1}^n \mathcal{K}_i(t_2, t_1) \mathcal{I}_i(t_1). \quad (4.1)$$

This relationship, described by Eq. (4.1), characterizes classical memory dynamics [7]. A natural example is pure dephasing dynamics. Notably, Markovian dynamics represent a special case of this framework, where with $n = 1$. If this condition is not satisfied, the process is said to require genuinely quantum memory.

We demonstrate that the condition in Eq. (4.1) can be formulated as a convex optimization problem as follows. For a given channel $\mathcal{E}(t_1)$ at time t_1 , we define its *classical future* $\mathcal{F}[\mathcal{E}(t_1)]$ as the set of all channels $\mathcal{G}$ obtained via $\mathcal{G} = \sum_{i=1}^n \mathcal{K}_i(t_2, t_1) \mathcal{I}_i(t_1)$, where $\{\mathcal{I}_i(t_1)\}_{i=1}^n$ is any instrument decomposition of $\mathcal{E}(t_1)$ and $\mathcal{K}_i(t_2, t_1)$ are valid channels. According to Eq. (4.1), the dynamics $\{\mathcal{E}(t)\}$ can be implemented with classical memory if and only if, for all two time points $t_1 < t_2$, the channel $\mathcal{E}(t_2) \in \mathcal{F}[\mathcal{E}(t_1)]$.

The classical future is proven to be a convex and compact set in Appendix A.1.2. With these properties, we begin by addressing the question of whether implementing dynamics with classical memory requires an infinite number of measurements—specifically, whether $n \rightarrow \infty$ in Eq. (4.1). In fact, we find that in any dynamics of a system of dimension d , the number of measurements is bounded by $d^4(d^4 + 1)$; see details in Appendix A.1.2.

4.2.1 Quantization of deviation from classical memory

The convexity of the classical future allows one to quantify the presence of quantum memory within a dynamical process by the various robustness measures derived

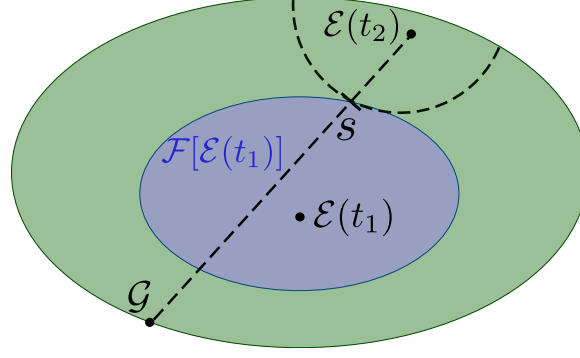


Fig. 4.1.: Sketch of the quantum memory robustness of a channel $\mathcal{E}(t_2)$ that lies outside of the classical future $\mathcal{F}(\mathcal{E}(t_1))$ of a channel $\mathcal{E}(t_1)$.

for convex programs [40, 198, 210, 218]. In particular, we consider the following constrained optimisation task, which constitutes a convex program:

$$\begin{aligned} s^* &= \max_{s, \mathcal{R}} s \\ \text{s.t. } & s\mathcal{E}(t_2) + (1-s)\mathcal{R} \in \mathcal{F}[\mathcal{E}(t_1)] \\ & \mathcal{R} \text{ is CPTP} \end{aligned} \quad (4.2)$$

The channel $\mathcal{E}(t_2)$ is in the classical future $\mathcal{F}[\mathcal{E}(t_1)]$ if and only if $s^* \geq 1$. Intuitively, if s^* is small, there is no channel in the vicinity of $\mathcal{E}(t_2)$ which lies in the classical future of $\mathcal{E}(t_1)$, see Figure 4.1. For convenience, we introduce the value $r^* = 1/s^* - 1$, which is referred to as the *robustness of quantum memory* with respect to the dynamics at two time points $(\mathcal{E}(t_1), \mathcal{E}(t_2))$.

4.2.2 Witnesses of quantum memory

The direct application of the convex program (4.2) for detecting quantum memory necessitates performing full process tomography on $\mathcal{E}(t_1)$ and $\mathcal{E}(t_2)$. However, leveraging the convex structure of the classical future enables quantum memory detection with only partial information about $\mathcal{E}(t_1)$ and $\mathcal{E}(t_2)$ using quantum memory witnesses. A quantum memory witness is typically defined by two sets of state preparations, ρ_k^1 and $\rho_{k'}^2$, along with corresponding sets of observables, O_l^1 and $O_{l'}^2$, such that

$$\sum_{kl} \text{tr} \left\{ O_l^1 \mathcal{E}(t_1) [\rho_k^1] \right\} + \sum_{k'l'} \text{tr} \left\{ O_{l'}^2 \mathcal{E}(t_2) [\rho_{k'}^2] \right\} \geq 0 \quad (4.3)$$

for all pairs of channels $(\mathcal{E}(t_1), \mathcal{E}(t_2))$ such that $\mathcal{E}(t_2) \in \mathcal{F}[\mathcal{E}(t_1)]$. A negative sum of expectation values on the left hand side of (4.3) henceforth implies the detection of quantum memory also when the set of prepared states and measured observables are not enough to reconstruct $\mathcal{E}(t_1)$ and $\mathcal{E}(t_2)$ in full; see Appendix A.1.4.

4.2.3 Choi representation and SDP relaxation

So far, the optimisation (4.2) and the construction of witnesses remain formal, and are difficult to implement in practice. Fortunately, one can also formulate a relaxation for (4.2) in terms of a semidefinite program (SDP), a concept that is often employed in quantum information theory [31, 212] familiar to quantum information theory. To this end, we employ the so-called Choi representation [42], where a quantum channel $\mathcal{R}$ over a system of dimension d is represented by the bipartite quantum state $R^{\text{AB}}(t_1) = 1/d^2 \sum_{i,j} |i\rangle\langle j| \otimes \mathcal{R}(|i\rangle\langle j|)$ which obeys $\text{tr}_B[R^{\text{AB}}(t_1)] = \mathbb{1}^{\text{A}}/d$. In this representation, the channel $\mathcal{E}(t_2)$ is in the classical future of $\mathcal{E}(t_1)$, if its associated Choi matrix $E^{\text{AB}}(t_2)$ can be written as $E^{\text{AB}}(t_2) = {}^{\text{DD}'}\langle\phi^+|X^{\text{ADD'B}}|\phi^+\rangle^{\text{DD}'}$, where

$$X^{\text{ADD'B}} = \sum_i I_i^{\text{AD}}(t_1) \otimes K_i^{\text{D'B}}(t_2, t_1), \quad (4.4)$$

$I_i^{\text{AD}}(t_1)$ and $K_i^{\text{D'B}}(t_2, t_1)$ are the Choi matrices of $\mathcal{K}_i(t_2, t_1)$ and $\mathcal{I}_i(t_1)$ in (4.1), respectively, and $|\phi^+\rangle_{\text{DD}'}$ is the maximally entanglement state over auxiliary system DD' ; see Appendix A.1.3 for the details.

Remarkably, Eq. (4.4) resembles the definition of separable states, with the additional constraints on the tensor factors

$$\text{tr}_B[K_i^{\text{D'B}}(t_2, t_1)] = \frac{\mathbb{1}^{\text{D}'}}{d} \quad (4.5)$$

required by Choi's representation [180]. This allows us to apply the various techniques for entanglement theory to that of quantum memory [39, 236]. In particular, the constraints for $X^{\text{ADD'B}}$ can be relaxed to those that are positive and has positive partial transposition (PPT), and

$$\text{tr}_B[X^{\text{ADD'B}}] = E(t_1)^{\text{AD}} \otimes \frac{\mathbb{1}^{\text{D}'}}{d} \quad (4.6)$$

This gives rise to the PPT-relaxation $\mathcal{F}_{\text{PPT}}[\mathcal{E}(t_1)]$ for the classical future $\mathcal{F}[\mathcal{E}(t_1)]$; see Appendix A.1.3 for the details. In the examples considered below, the PPT relaxation is close to be optimal. Moreover, the PPT relaxation $\mathcal{F}_{\text{PPT}}[\mathcal{E}(t_1)]$ also enables the explicit construction of PPT witnesses of quantum memory; see Appendix A.1.3.

4.3 Quantum memory in giant atom dynamics

In this section, we apply our method (4.2) to the dynamics of two-level and three-level giant atoms. These systems, distinguished by their spatially extended nature, offer an ideal platform for exploring memory effects. Building on the analysis

presented in the previous chapter, we aim to demonstrate how our method effectively identifies and characterizes the quantum memory effects in giant atom dynamics.

4.3.1 Two-level giant atom dynamics

Consider a two-level giant atom coupled to a one-dimensional acoustic waveguide through multiple interaction points. The system Hamiltonian is defined in Eq. (3.1), while the dynamics of the giant atom at zero temperature are described by Eqs. (3.11)-(3.14). Based on these equations, we determine the action of the one-parameter CPTP maps, which governs the evolution of the system from its initial state to its state at any time t , on the individual operator basis elements as follows

$$\mathcal{E}(t)[|e\rangle\langle e|] = |G(t)|^2|e\rangle\langle e| + (1 - |G(t)|^2)|g\rangle\langle g|, \quad (4.7)$$

$$\mathcal{E}(t)[|e\rangle\langle g|] = G(t)|e\rangle\langle g|, \quad (4.8)$$

$$\mathcal{E}(t)[|g\rangle\langle e|] = G^*(t)|g\rangle\langle e|, \quad (4.9)$$

$$\mathcal{E}(t)[|g\rangle\langle g|] = |g\rangle\langle g|. \quad (4.10)$$

The decay function $G(t)$ satisfies Eq. (3.9). Here, instead of assuming an Ohmic spectral density, a flat spectral density is considered, i.e., $\gamma(\omega) = \gamma$, resulting in an analytical expression for the decay function

$$G(t) = \sum_{n=0}^{\infty} \Theta(t - n\tau) \frac{[-\gamma(t - n\tau)]^n}{n!} e^{-i(\omega_0 - i\gamma)(t - n\tau)}. \quad (4.11)$$

The Heaviside step function is given by $\Theta(x) = 1$ for $x > 0$, and equals zero otherwise. This equation shows that the memory effect is encapsulated in the sum over past emission events occurring at times $t - n\tau$. These contributions are reabsorbed by the atom and interfere, leading to non-Markovian dynamics in which the atom's current state depends on its history.

The Choi state $E(t)$ associated with each map is obtained by applying the map $\mathcal{E}(t)$ to one half of a maximally entangled state, $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|gg\rangle + |ee\rangle)$, where the auxiliary system has the same dimension as the atom. The specific expression for the resulting Choi state is

$$E(t) = [\mathcal{E}(t) \otimes \mathbb{I}]|\psi^+\rangle\langle\psi^+| = \frac{1}{2} \begin{pmatrix} |G(t)|^2 & 0 & 0 & G^*(t) \\ 0 & 1 - |G(t)|^2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ G(t) & 0 & 0 & 1 \end{pmatrix}. \quad (4.12)$$

This state enables us to analyze the properties of the dynamical map.

For the quantum process under consideration, the dynamics between two time points t_1 and t_2 can be described using a classical memory if and only if the condition: $|G(t_2)| \leq |G(t_1)|$ is satisfied, as proven in Appendix A.2.1. Furthermore, if $(\mathcal{E}(t_1), \mathcal{E}(t_2))$ is classical, it is even Markovian (CP-divisible) in the sense that there exists a channel $\mathcal{K}(t_2, t_1)$ such that

$$\mathcal{E}(t_2) = \mathcal{K}(t_2, t_1)\mathcal{E}(t_1). \quad (4.13)$$

It is important to note that when $|G(t_2)| \leq |G(t_1)|$, the quantum dynamical maps $\mathcal{E}(G)$ exhibit a composition property: $\mathcal{E}(G)\mathcal{E}(G') = \mathcal{E}(GG')$. This property reveals that the mapping $G \mapsto \mathcal{E}(G)$ is a semigroup homomorphism, specifically, a homomorphism from the multiplicative semigroup of complex numbers within the unit disk to the semigroup of qubit quantum channels under the operation of composition.

Therefore, the condition $|G(t_2)| \leq |G(t_1)|$ directly implies that the two-point dynamics, represented by the pair of quantum dynamical maps $(\mathcal{E}(t_1), \mathcal{E}(t_2))$, displays Markovian behavior. In this scenario, the connecting quantum channel between the two time points is given by $\mathcal{K} = \mathcal{E}(G(t_2)/G(t_1))$, which depends solely on the ratio of the function $G(t)$ evaluated at the two time points t_1 and t_2 . As a result, if the dynamics governed by the function $G(t)$ shows monotonic decay, it is not only equivalent to a process with classical memory, but it even corresponds to a Markovian process (an extreme case of classical memory). On the other hand, non-monotonic decay of the dynamics necessitates a quantum memory.

Alternatively, it can be observed that $|G(t)|$ quantifies the concurrence of the Choi matrix in equation (4.12), serving as an entanglement measure of the Choi matrix [180]. The requirement of quantum memory for non-monotonic decay is in agreement with the finding in Ref. [7], which states that a zero-temperature non-Markovian amplitude damping channel cannot be simulated using only classical memory.

Using the SDP method (4.2), we evaluate the quantum memory robustness at two time points, t_1 and $t_2 = t_1 + \Delta t$, as illustrated in Fig. 4.2. The SDP implementation was carried out by the coauthor. In the figure, white regions represent Markovian two-step dynamics, whereas colored regions indicate non-Markovian dynamics that necessitate quantum memory. The robustness of quantum memory reaches its maximum when t_1 matches the time delay required for acoustic wave modes to propagate between two contact points, and t_2 aligns with the first peak of information backflow from the environment to the atom. Moreover, for a fixed t_1 , the robustness

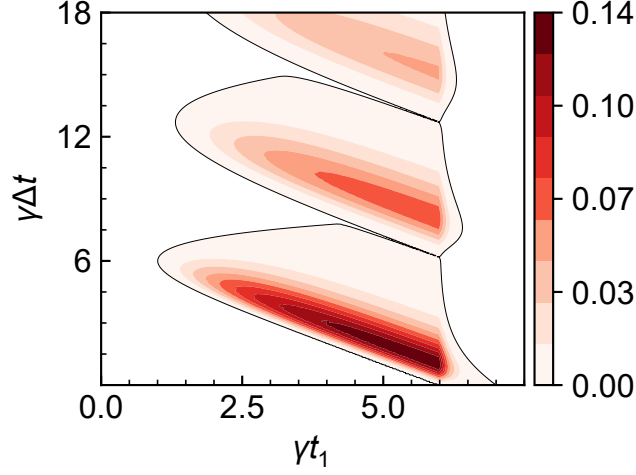


Fig. 4.2.: Quantum memory robustness of the two-level giant atom versus time γt_1 and $\gamma \Delta t$ with fixed parameters $\omega_0 \tau = 40\pi$, $\gamma \tau = 12$.

exhibits periodic decay as t_2 increases, reflecting oscillations in the quantum memory requirements over time.

From the analytical expressions (4.11), we also find that when $\omega_0 \tau = 2\pi k$ ($k \in \mathbb{N}$), all terms in $G(t)$ share the same phase factor $e^{-i\omega_0 t}$, leading to sharp peaks in $|G(t)|$. This alignment further implies that the system's robustness becomes periodic in ω_0 , with a period of $2\pi/\tau$. The periodicity arises because shifting ω_0 by $k2\pi/\tau$ transforms $G(t)$ into $e^{-ik2\pi t/\tau} G(t)$. For the Choi state $E(t)$, this corresponds to a local unitary transformation, $[\mathbb{I} \otimes U(t)] E(t)$, which leaves the quantum memory robustness unchanged.

To detect quantum memory in practice, we can construct a witness based on preparations of Pauli matrix eigenstates and Pauli measurements at times t_1 and t_2 . For the first time point it suffices to measure the correlations of $\hat{\sigma}_x$ and $\hat{\sigma}_y$ preparations and measurements as well as performing runs with $\hat{\sigma}_z$ preparations $\hat{\sigma}_z$ measurements. At the second time point one only needs to perform coinciding preparations and measurement for $\hat{\sigma}_x$ and $\hat{\sigma}_y$; see Appendix A.1.4 for details.

4.3.2 Three-level giant atom dynamics

We now extend our method to the dynamics of a three-level giant atom in a Λ -type configuration, consisting of an excited state $|e\rangle$, a metastable state $|s\rangle$, and a ground state $|g\rangle$, as depicted in Fig. 3.8. When this system is coupled to two one-dimensional waveguides via multiple contact points, its Hamiltonian is described by Eq. (3.29). At zero temperature, the atom undergoes non-exponential spontaneous decay, with the decay function determined by Eq. (3.32), previously analyzed in Section 3.5

for environments with an Ohmic spectral density. For simplicity, we assume that both waveguides have flat spectral densities, i.e., $\gamma_1(\omega) = \gamma_1$ and $\gamma_2(\omega) = \gamma_2$, as well as identical time delays $\tau_1 = \tau_2 = \tau$. Under these conditions, the decay function governing the population and coherence dynamics can be expressed as follows

$$G(t) = \sum_{n=0}^{\infty} \Theta(t - n\tau) \frac{[-\bar{\gamma}_2(t - n\tau)]^n}{n!} e^{-i(\omega_e - i\bar{\gamma}_1)(t - n\tau)},$$

given the collective damping parameters $\bar{\gamma}_1 = \gamma_1 + \gamma_2$, and $\bar{\gamma}_2 = \gamma_1 e^{-i\omega_s \tau} + \gamma_2$. Compared to the two-level giant atom, the three-level giant atom exhibits more intricate non-Markovian dynamics due to the interference effects arising from multiple emission pathways.

For this type of spontaneous emission process in a three-level system, we can construct the family of quantum channels $\mathcal{E}(t)$ that govern the time evolution of the atom's reduced state

$$\mathcal{E}(t)[|e\rangle\langle e|] = |G(t)|^2 |e\rangle\langle e| + (1 - |G(t)|^2 - S(t)) |s\rangle\langle s| + S(t) |g\rangle\langle g|, \quad (4.14)$$

$$\mathcal{E}(t)[|e\rangle\langle s|] = G(t) e^{i\omega_s t} |e\rangle\langle s|, \quad (4.15)$$

$$\mathcal{E}(t)[|e\rangle\langle g|] = G(t) |e\rangle\langle g|, \quad (4.16)$$

$$\mathcal{E}(t)[|s\rangle\langle s|] = |s\rangle\langle s|, \quad (4.17)$$

$$\mathcal{E}(t)[|s\rangle\langle e|] = G^*(t) e^{-i\omega_s t} |s\rangle\langle e|, \quad (4.18)$$

$$\mathcal{E}(t)[|s\rangle\langle g|] = e^{-i\omega_s t} |s\rangle\langle g|, \quad (4.19)$$

$$\mathcal{E}(t)[|g\rangle\langle g|] = |g\rangle\langle g|, \quad (4.20)$$

$$\mathcal{E}(t)[|g\rangle\langle e|] = G^*(t) |g\rangle\langle e|, \quad (4.21)$$

$$\mathcal{E}(t)[|g\rangle\langle s|] = e^{i\omega_s t} |g\rangle\langle s|. \quad (4.22)$$

The associated Choi states can be written as

$$E(t) = \frac{1}{3} \begin{pmatrix} 1 & 0 & 0 & 0 & e^{i\omega_s t} & 0 & 0 & 0 & G^*(t) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ e^{-i\omega_s t} & 0 & 0 & 0 & 1 & 0 & 0 & 0 & G^*(t)e^{-i\omega_s t} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & S(t) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Upsilon(t) & 0 \\ G(t) & 0 & 0 & 0 & G(t)e^{i\omega_s t} & 0 & 0 & 0 & |G(t)|^2 \end{pmatrix},$$

where $\Upsilon(t) = 1 - |G(t)|^2 - S(t)$ and the function $S(t)$ is given by

$$\begin{aligned} S(t) &= \sum_{j=1,2} \int_0^\infty d\omega |\beta_{j\omega}(t)|^2 \\ &= 2\gamma_2 \left[\int_0^t dt' |G(t')|^2 + \int_\tau^t dt' \operatorname{Re}\{G(t')G^*(t' - \tau)\} \right], \end{aligned} \quad (4.23)$$

which represents the probability of the single phonon in the second radiation field.

From the map (4.14)-(4.22), we derive the following criteria for Markovianity. The two-point dynamics of the process at times $t_1 \leq t_2$ is Markovian (CP-divisible) if and only if the following inequalities hold:

$$S(t_2) \geq S(t_1) \quad (4.24)$$

$$S(t_1) + |G(t_1)|^2 \geq S(t_2) + |G(t_2)|^2. \quad (4.25)$$

If either inequality is violated, the dynamics is not only non-Markovian, but also require quantum memory; see Appendix A.2.2 for the proof. Consequently, the spontaneous emission of the three-level giant atom, like that of the two-level giant atom, cannot be simulated using classical memory.

Figure 4.3 displays the quantum memory robustness at the two time points t_1 and $t_1 + \Delta t$ for an exemplary three-level parameter setting, computed using the SDP method. This plot can also be reproduced using the condition (4.24), further confirming that the non-Markovian spontaneous process in a three-level giant atom

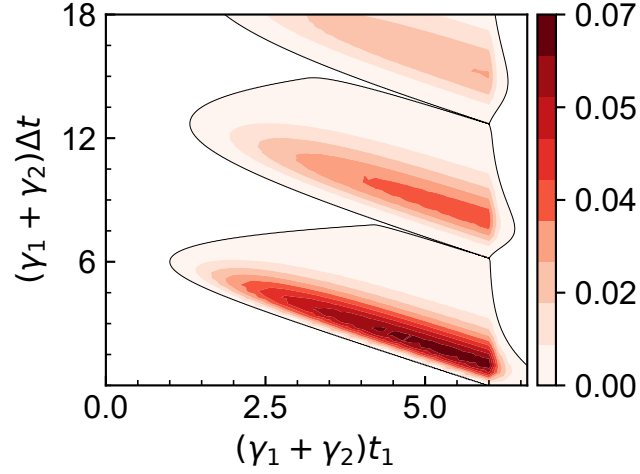


Fig. 4.3.: Quantum memory robustness of the three-level giant atom dynamics with fixed parameters $\omega_s\tau = 20\pi$, $\omega_e\tau = 40\pi$, $\gamma_1\tau = 4$, $\gamma_2\tau = 8$.

can only be achieved with quantum memory. A similar pattern to the two-level case emerges, but with a larger region where the dynamics are non-Markovian, requiring greater quantum memory for implementation. This is due to the constructive interference between the two emission channels in the three-level giant atom, which enhances the memory effects. Additionally, the quantum memory properties of the time evolution $\mathcal{E}(t)$ remain invariant under transformations of the form $\omega_s \mapsto \omega_s + 2\pi k_s/\tau$ and $\omega_e \mapsto \omega_e + 2\pi k_e/\tau$, where k_s and k_e are integers.

4.4 Conclusion

In this chapter, we presented a novel method for detecting quantum memory in quantum dynamics. This approach is based on defining non-Markovian dynamics implemented by classical memory, where the corresponding quantum dynamical maps are described by Choi states. We examined the separability of these Choi states, showing that channels implemented with classical memory form a set where the Choi states are separable. On the other hand, channels outside this set require quantum memory for their implementation, with the degree of this deviation quantified by the proposed notion of quantum memory robustness.

We applied our method to the dynamics of two-level and three-level giant atoms, as discussed in the previous chapter. Our analysis confirmed that quantum memory is always present whenever the dynamics of these systems at zero temperature are non-Markovian. In both cases, the quantum memory robustness of the two-step dynamics shows periodic decay, indicating oscillations in the quantum memory requirements over time. In particular, the three-level giant atom exhibits stronger

memory effects due to the interference of past interactions with the two waveguides, leading to higher quantum memory robustness.

This method can also be extended to study higher-dimensional system dynamics, though at the cost of increased computational complexity. Future research could apply this approach to systems with finite spin baths or finite temperatures, enabling the study of temperature effects on quantum memory. Based on the findings from Chapter 3, where non-Markovian behavior persisted in the dynamics of the giant atom even at relatively high temperatures, the proposed method could be used to determine whether these processes are still sustained by quantum memory. Additionally, developing quantum memory criteria for continuous systems instead of discrete ones would be a promising direction for further investigation.

Non-Markovian dynamics in finite spin baths

In this chapter, we present a spin-lattice model with Ising-type phase interactions, developed for quantum computing platforms such as Rydberg atom arrays, trapped polar molecules, and nuclear magnetic resonance (NMR) systems. This model facilitates the study of spin dephasing in a finite spin bath and provides exact solutions for the dynamics of the central spin system. With it, we first explore the dynamics of a single spin in both uncorrelated and correlated spin baths, and investigate how these environments influence the spin's behavior, particularly in terms of non-Markovian dephasing. Then we move on to study the behavior of two spins and how their entanglement is affected by the spin bath. We focus on two case studies: Entangled spins in a 2D lattice interacting with an evolving environment, and two nuclear spins in an organic molecule interacting with a thermal spin bath at finite temperatures. This chapter is based on the Project [C].

5.1 Motivation

Spin-based qubits, implemented on various platforms such as superconducting circuits [94, 121], semiconductor quantum dots [26], nitrogen-vacancy (NV) centers [112, 181], and trapped ions [16, 79], are promising candidates for scalable quantum computing due to their long coherence times and high degree of controllability. However, the interaction between these qubits and their environment, which consists of degrees of freedom such as phonons, nuclear spins, or electromagnetic fluctuations, leads to decoherence processes, including dephasing and energy relaxation. These decoherence mechanisms have a detrimental effect on the fidelity of quantum gates and consequently the performance of quantum algorithms [188].

Given the impact of decoherence on the practical realization of quantum technologies, it is crucial to investigate the decoherence dynamics of spin qubits from both fundamental and applied perspectives. By studying and modeling the effects of environmental noise, effective strategies can be developed to mitigate errors, such as dynamical decoupling [150], quantum error correction [175, 215], and engineered reservoir techniques [9].

Among the various decoherence processes, pure dephasing stands out as a dominant source of decoherence in several promising platforms for quantum information processing, including NV centers in diamond [1, 57, 89] and Rydberg atom arrays [8, 13, 24, 86]. Pure dephasing is also of great importance in nuclear magnetic resonance (NMR) experiments, as it directly influences the coherence of spin states and, consequently, the free induction decay signal [70]. In these systems, pure dephasing often exhibits non-Markovian behavior, which arises from the structured nature of the environment [65, 97] and their finite-size effects [69]. To gain a deeper understanding of these systems and design targeted strategies for enhancing their performance, it is essential to develop efficient models capable of simulating non-Markovian dynamics.

In this chapter, we introduce a spin lattice model to investigate spin dephasing in a finite spin bath and provide exact solutions for the dynamics of the central spins. We start by exploring the dynamics of a single spin interacting with uncorrelated and correlated spin baths to understand how the bath's nature influences dephasing. Next, we shift our focus to the behavior of two spins and their entanglement in the presence of a spin bath through two case studies. The first involves a 2D spin lattice with entangled spins interacting with an evolving environment. We examine non-Markovian dephasing, random reset operations, and three-body interactions. The second case study looks at two nuclear spins in an organic molecule interacting with a thermal spin bath at finite temperatures. It highlights the role of bath correlations in enhancing or reducing dephasing depending on temperature.

5.2 The spin-lattice model

To model spin dephasing in a finite-size environment, we consider a spin configuration, such as the periodic lattice model introduced in Refs. [27, 99] and illustrated in Fig. 5.1, where $N = N_A + N_B$ spins occupy some or all of the available sites. Among these spins, a subset of N_A spins (here, $N_A = 2$) constitutes the system of interest, while the remaining $N_B \gg 1$ spins form the environment. The environmental spins may either remain stationary or be allowed to hop between lattice sites. The motion of the spins is described by time-dependent discrete position vectors $\mathbf{r}_n(t)$, where $n = 1, \dots, N$. The Hamiltonian of the entire system, comprising local spin energies and Ising-like interactions energies, can be expressed as

$$\begin{aligned} \hat{H}(t) = & \hbar \sum_{i=1}^N \omega(\mathbf{r}_i(t)) \sigma_z^i + \hbar \sum_{i < j} g(\mathbf{r}_i(t), \mathbf{r}_j(t)) \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j \\ & + \hbar \sum_{i < j < k} h(\mathbf{r}_i(t), \mathbf{r}_j(t), \mathbf{r}_k(t)) \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j \otimes \hat{\sigma}_z^k, \end{aligned} \quad (5.1)$$

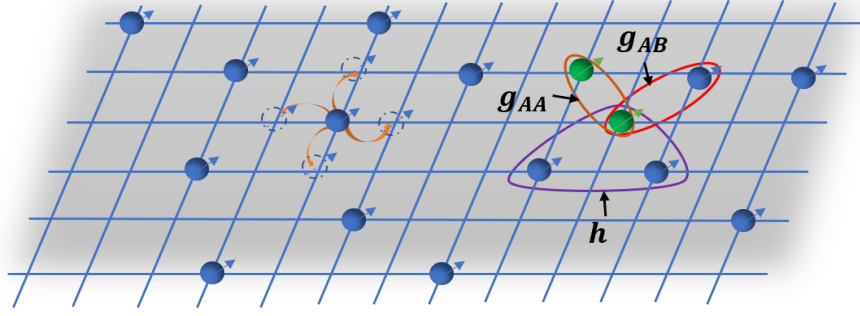


Fig. 5.1.: Sketch of a dynamical spin lattice model for non-Markovian dephasing, with N_A quantum spins (green, $N_A = 2$) surrounded by N_B environmental spins (blue) on a periodic lattice. The configuration can be static or dynamic, with phase exchange via Ising-type interactions. Intrasystem and system-environment couplings are represented by g_{AA} and g_{AB} , respectively. A three-body phase interaction of strength h is also considered between neighboring spins.

where $\omega(\mathbf{r}_i(t))$ represents the local spin frequency, $g(\mathbf{r}_i(t), \mathbf{r}_j(t))$ denotes the two-body Ising coupling strength that depends on the positions of the spins, and $h(\mathbf{r}_i(t), \mathbf{r}_j(t), \mathbf{r}_k(t))$ represents the three-body interaction strength, which also generally depends on the positions of the spins. Here, we primarily focus on homogeneous lattices, in which the local spin frequency $\omega(\mathbf{r}_i(t))$ are identical for all spins. As a result, these terms can be neglected by considering the system in a co-rotating frame. Next, we represent the Hamiltonian using the computational basis states, i.e., $|0_n\rangle$ and $|1_n\rangle$ for the n -th spin. By regrouping the terms and shifting the energy reference point, we obtain a simplified form of the Hamiltonian

$$\begin{aligned} \hat{H}(t) = & \hbar \sum_i \tilde{\omega}_i(t) |i_i\rangle \langle 1_i| + \hbar \sum_{i < j} \tilde{g}_{ij}(t) |1_i 1_j\rangle \langle 1_i 1_j| \\ & + \hbar \sum_{i < j < k} h_{ijk}(t) |1_i 1_j 1_k\rangle \langle 1_i 1_j 1_k|, \end{aligned} \quad (5.2)$$

with $h_{ijk}(t) = h(\mathbf{r}_i(t), \mathbf{r}_j(t), \mathbf{r}_k(t))$ and the renormalized one- and two-spin terms

$$\begin{aligned} \tilde{g}_{ij}(t) &= g(\mathbf{r}_i(t), \mathbf{r}_j(t)) - \frac{1}{2} \sum_{k \neq i, j} h(\mathbf{r}_i(t), \mathbf{r}_j(t), \mathbf{r}_k(t)), \\ \tilde{\omega}_i(t) &= \omega(\mathbf{r}_i(t)) - \frac{1}{2} \sum_{j \neq i} \left[g(\mathbf{r}_i(t), \mathbf{r}_j(t)) - \frac{1}{2} \sum_{k \neq i, j} h(\mathbf{r}_i(t), \mathbf{r}_j(t), \mathbf{r}_k(t)) \right]. \end{aligned} \quad (5.3)$$

Observe that the h_{ijk} and the $\tilde{g}_{ij}$ are symmetric under index permutation. As all terms in the Hamiltonian commute with one another, the associated unitary time evolution can be written as

$$\begin{aligned}\hat{U}(t) &= \prod_i e^{-i \int_0^t dt' \tilde{\omega}_i(t') |1_i\rangle\langle 1_i|} \prod_{i < j} e^{-i \int_0^t dt' \tilde{g}_{ij}(t') |1_i 1_j\rangle\langle 1_i 1_j|} \\ &\times \prod_{i < j < k} e^{-i \int_0^t dt' h_{ijk}(t') |1_i 1_j 1_k\rangle\langle 1_i 1_j 1_k|},\end{aligned}\quad (5.4)$$

where the one-, two-, and three-body phases accumulate based on the spin's hopping trajectory between sites. For static positions, all accumulated phases depend linearly on t . The first term represents local phase rotations that do not influence dephasing or entanglement among the system's spins. These rotations can be incorporated by moving to the rotating frame,

$$\hat{U}_t = \prod_{i < j} e^{-i \int_0^t dt' \tilde{g}_{ij}(t') |1_i 1_j\rangle\langle 1_i 1_j|} \prod_{i < j < k} e^{-i \int_0^t dt' h_{ijk}(t') |1_i 1_j 1_k\rangle\langle 1_i 1_j 1_k|} =: U_t^{(2)} U_t^{(3)}, \quad (5.5)$$

where $\hat{U}_t^{(2)}$ and $\hat{U}_t^{(3)}$ encompass the terms involving two- and three-body interactions, respectively. For clarity, we define binary arrays $\underline{a} = (a_1, \dots, a_{N_A}) \in \{0, 1\}^{\times N_A}$, $\underline{b} \in \{0, 1\}^{\times N_B}$, and their concatenated form $\underline{ab}$ to represent the spin configurations of the energy eigenstates for both the system and the environment.

$$|\underline{ab}\rangle = |\underline{a}\rangle|\underline{b}\rangle = |a_1, \dots, a_{N_A}, b_1, \dots, b_{N_B}\rangle \in \mathbb{C}^{2(N_A, N_B)}, \quad (5.6)$$

where the inner products $\underline{a} \cdot \underline{a}$ and $\underline{b} \cdot \underline{b}$ give the numbers of A and B spins in the state $|1\rangle$, respectively.

As the joint system, encompassing both the primary system and its environment, evolves, the phases induced by interactions between spin pairs can be represented by the adjacency matrix $\underline{\Gamma}(t)$ of a weighted graph. In this graph, vertices correspond to individual spins, and edges connecting spins represent the interaction. Each edge carries a weight representing the accumulated phase, $\Gamma_{ij}(t) = \int_0^t dt' \tilde{g}_{ij}(t') = \Gamma_{ji}(t)$ for $i \neq j$, with $\Gamma_{ii} = 0$. The elements of the adjacency matrix capture the history of interactions between spins i and j [98, 103]. In this context, a state $|\underline{ab}\rangle$ accrues the corresponding phase from these pairwise interactions

$$\hat{U}_t^{(2)} |\underline{ab}\rangle = e^{-\frac{i}{2} \underline{ab} \cdot \underline{\Gamma}(t) \underline{ab}} |\underline{ab}\rangle = e^{-\frac{i}{2} \underline{a} \cdot \underline{\Gamma}_{AA}(t) \underline{a} + 2 \underline{a} \cdot \underline{\Gamma}_{AB}(t) \underline{b} + \underline{b} \cdot \underline{\Gamma}_{BB}(t) \underline{b}} |\underline{ab}\rangle. \quad (5.7)$$

Expressions like $\underline{\Gamma} \underline{v}$ and $\underline{w} \cdot \underline{v}$ denote the standard real-valued matrix-vector multiplication and scalar product, respectively. The coefficient $1/2$ ensures that each interaction pair is accounted for precisely once. Furthermore, the global interaction matrix

can be partitioned into submatrices: $\underline{\Gamma}_{AA}(t)$ with dimensions $N_A \times N_A$, $\underline{\Gamma}_{AB}(t)$ with dimensions $N_A \times N_B$, and $\underline{\Gamma}_{BB}(t)$ with dimensions $N_B \times N_B$. These submatrices represent the phases associated with internal system interactions, system-environment interactions, and interactions within the environment, respectively.

Including arbitrary interactions among three spins introduces significant complexity to the graphical model, requiring the use of hyperedges connecting three nodes and managing a substantially larger matrix to track the history of spin triplets' interactions. Given that physical three-body interactions are generally weak and short-ranged, we restrict our focus to spin triplets where at least two of the three pairs are direct neighbors, assigning a uniform coupling strength h to such interactions. If all three spins are mutual nearest neighbors, the coupling strength is increased to $2h$ for simplicity. To represent these interactions, we define a second time-dependent matrix $\underline{\Lambda}(t)$, where each binary entry $\Lambda_{ij}(t) \in \{0, 1\}$ indicates whether spins i and j are connected as neighbors at a given time t . For a system with $N_A = 2$ adjacent spins, two distinct categories of neighbor triplets are relevant: (i) both system spins and a single spin from the environment, and (ii) one system spin along with two spins from the environment. The resulting three-body phases are captured using the submatrices $\underline{\Lambda}_{AB}(t)$ and $\underline{\Lambda}_{BB}(t)$, which describe system-environment and environment-environment neighbor relationships, respectively, at each moment in time

$$\hat{U}_t^{(3)}|\underline{ab}\rangle = e^{-ih \int_0^t dt' \left\{ a_1 a_2 (1,1) \cdot \underline{\Lambda}_{AB}(t') \underline{b} + \underline{a} \cdot \underline{\Lambda}_{BB}(t') [\underline{b} \circ \underline{\Lambda}_{BB}(t') \underline{b}] \right\}} |\underline{ab}\rangle. \quad (5.8)$$

here the $\circ$ operator represents the Hadamard product, which refers to the element-wise multiplication of two arrays or matrices of the same dimensions. The initial term in the exponent corresponds to interaction type (i), which only has a non-zero contribution when $\underline{a} = (a_1, a_2) = (1, 1)$. This can also be generalized for larger systems where $N_A > 2$. When focusing on the dynamics of an individual system spin while still considering three-body interactions, the contribution from type (i) will be zero.

We assume that the N_A system spins are fully controllable and can be initialized in a pure reference state $\rho_A = |\Psi_A\rangle\langle\Psi_A|$, whereas the environment is in a predetermined state, typically an uncontrolled one such as a thermal state ρ_B . When tracing over the N_B environment spins, the evolution of the reduced system state only depends on the diagonal elements $p(\underline{b}) = \langle \underline{b} | \rho_B | \underline{b} \rangle$, so the off-diagonal coherences of ρ_B do

not need to be considered. Therefore, the global initial state can be taken as this form

$$\rho_{AB}(0) = \sum_{\underline{a}, \underline{a}', \underline{b}} \langle \underline{a} | \rho_A | \underline{a}' \rangle p(\underline{b}) | \underline{a} \rangle \langle \underline{a}' | \otimes | \underline{b} \rangle \langle \underline{b} |. \quad (5.9)$$

The system evolves according to the general Hamiltonian (5.2) over a time interval t . At the end of this evolution, we can obtain the reduced state of the two-spin system as

$$\begin{aligned} \rho_A(t) &= \text{tr}_B [\hat{U}_t \rho_{AB}(0) \hat{U}_t^\dagger] \\ &= \sum_{\underline{a}, \underline{a}'} \langle \underline{a} | \rho_A(t) | \underline{a}' \rangle D_t(\underline{a}, \underline{a}') e^{\frac{i}{2} (\underline{a}' \cdot \underline{\Gamma}_{AA}(t) \underline{a}' - \underline{a} \cdot \underline{\Gamma}_{AA}(t) \underline{a})} | \underline{a} \rangle \langle \underline{a}' |, \end{aligned} \quad (5.10)$$

with the decoherence factor

$$\begin{aligned} D_t(\underline{a}, \underline{a}') &= \sum_{\underline{b}} p(\underline{b}) e^{i(\underline{a}' - \underline{a}) \cdot \underline{\Gamma}_{AB}(t) \underline{b}} e^{ih \int_0^t dt' (\underline{a}' a'_2 - \underline{a} a_2) (1,1) \cdot \underline{\Lambda}_{AB}(t') \underline{b}} \\ &\times e^{ih \int_0^t (\underline{a}' - \underline{a}) \cdot \underline{\Lambda}_{AB}(t') [\underline{b} \circ \underline{\Lambda}_{BB}(t') \underline{b}]}. \end{aligned} \quad (5.11)$$

The decoherence factor $D_t(\underline{a}, \underline{a}')$ plays a crucial role in system evolution and is determined by several factors, including the properties of the environment, the coupling strength between the system and environment, and the interaction history.

5.3 Non-Markovian pure dephasing of single spin

In the previous section, we presented a spin lattice model and derived a general solution for the decoherence of system spins within finite spin baths. While we obtained the reduced two-spin state at time t in Eq. (5.10), which will later be used to analyze the entanglement dynamics of two spins in a shared bath, the framework can be easily extended to larger system sizes. Before delving into the two-spin entanglement study, it is worthwhile to first examine the dynamics of a single spin. In this section, we focus on a single system spin, which interacts with the environment spins exclusively through pairwise phase interactions. This simplified interaction model allows us to derive a more straightforward expression for the decoherence dynamics, offering a clearer understanding of the underlying mechanisms.

An arbitrary initial state of a single spin will undergo pure dephasing with the simplified decoherence factor

$$D_t = \sum_{\underline{b}} p(\underline{b}) e^{-i \underline{\Gamma}_{AB}(t) \underline{b}}, \quad (5.12)$$

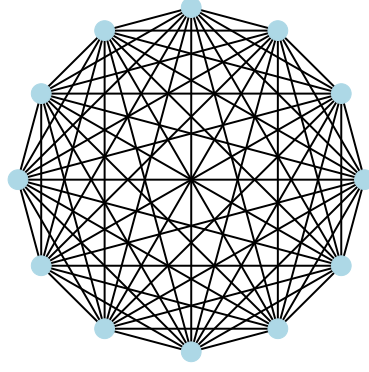


Fig. 5.2.: Curie-Weiss spin bath: Every spin interacts uniformly with all others, represented by a complete graph. In this graph, vertices correspond to spins, and edges between vertices i and j denote the coupling term $-(J/N_B)\hat{\sigma}_z^i \otimes \hat{\sigma}_z^j$ in the total interaction energy, where J is the coupling rate and N_B is the total number of bath spins.

where the adjacency matrix $\underline{\Gamma}_{AB}(t)$ is a matrix of size $1 \times N_B$. In the following, we consider two simple bath examples of spin baths for which the decoherence of the system spin can be given analytically and its non-Markovian nature can be identified straightforwardly.

Finite bath of static spins at infinite temperature

In the simplest case, we assume the environment is in the maximally mixed state, i.e., $p(\underline{b}) = 1/2^{N_B}$. Consequently, the decoherence factor takes the form

$$\begin{aligned}
 D_t &= \frac{1}{2^{N_B}} \sum_{\underline{b}} e^{-i \underline{\Gamma}_{AB}(t) \underline{b}} \\
 &= \prod_{n=1}^{N_B} \frac{1}{2} \left(1 + e^{-i \Gamma_{AB,n}(t)} \right) \\
 &= e^{-\frac{i}{2} \sum_{k=1}^{N_B} \Gamma_{AB,n}(t)} \prod_{k=1}^{N_B} \cos \left(\frac{\Gamma_{AB,n}(t)}{2} \right). \tag{5.13}
 \end{aligned}$$

The equation reveals that the decoherence factor exhibits an oscillatory behavior when N_B has a finite value, indicating that coherence information lost from the system to the environment can partially return. Consequently, the single-spin dynamics displays clear signatures of non-Markovianity.

Infinite fully connected bath of thermal spins

As another bath example, we choose the Curie-Weiss model [76] in which each spin couples uniformly to all the other spins through an Ising-type pairwise interaction, representing a fully connected graph as illustrated in Fig. 5.2. This simple model

admits an analytical treatment in the thermodynamical limit and has been used to illustrate the phase transition [76]. The bath Hamiltonian reads

$$\begin{aligned}\hat{H}_B^{cw} &= -\frac{J}{2N_B} \sum_{i,j=1}^{N_B} \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j - h \sum_{i=1}^{N_B} \hat{\sigma}_z^i \\ &= -\frac{J}{2N_B} \left(\sum_{i=1}^{N_B} \hat{\sigma}_z^i \right)^2 - h \sum_{i=1}^{N_B} \hat{\sigma}_z^i.\end{aligned}\quad (5.14)$$

The coupling energy between two spins is given by J/N_B , where we divide by N_B to account for the number of spins in the system, ensuring a proper scaling of the interaction strength. The prefactor $1/2$ is included to prevent double counting of spin pairs. The h represents the individual spin energy in the external magnetic field. Suppose the bath is in the thermal equilibrium and the probability distribution of each spin configuration reads

$$p(\underline{b}) = e^{-\beta E(\underline{b})}/Z_B, \quad (5.15)$$

where $E(\underline{b})$ is the energy of spin configuration $\hat{H}_B^{cw}|\underline{b}\rangle = E(\underline{b})|\underline{b}\rangle$ and the β denotes the inverse temperature. In the thermodynamical limit, we show that the bath will experience a phase transition as temperature varies at zero magnetic field in Appendix. B.1. With $\hat{\sigma}_z^i|\underline{b}\rangle = (1 - 2b_i)|\underline{b}\rangle = m_i|\underline{b}\rangle$, where $m_i = 1 - 2b_i \in \{-1, 1\}$ represents the magnetization of i -th spin, the partition function Z_B is given by

$$\begin{aligned}Z_B &= \text{tr}[e^{-\beta \hat{H}_B^{cw}}] \\ &= \sum_{m_1=-1}^1 \dots \sum_{m_{N_B}=-1}^1 e^{(J/2N_B)\beta (\sum_{i=1}^{N_B} m_i)^2 + h\beta \sum_{i=1}^{N_B} m_i} \\ &= \sum_{M=-N_B}^{N_B} \binom{N_B}{\frac{N_B+M}{2}} e^{(J/2N_B)\beta M^2 + h\beta M},\end{aligned}\quad (5.16)$$

where $M = \sum_{i=1}^{N_B} m_i$ is the total magnetization. To derive the partition function, we start by approximating the binomial coefficient with the Stirling formula, which is valid for $N_B \rightarrow \infty$ and typically holds well for N_B on the order of hundreds. Next, the discrete summation over M is approximated as an integral over the continuous magnetization density $m = M/N_B \in [-1, 1]$ per spin. Thus the Eq. (5.16) then becomes

$$Z_B \approx \int_{-1}^1 e^{-N_B f(m)} dm, \quad (5.17)$$

with the free energy approximately given by

$$f(m) \approx \frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} - \frac{\beta J m^2}{2} - \beta h m. \quad (5.18)$$

For large N_B , the integral (5.17) is dominated by the region around the minimum of $f(m)$, referred to as the saddle point, which is determined by the condition $f'(m_0) = 0$. This results in a self-consistent equation

$$\tanh(J\beta m_0 + h\beta) = m_0. \quad (5.19)$$

Further, we can perform the saddle-point approximation and obtain

$$Z_B = e^{-N_B f(m_0)} \sqrt{\frac{2\pi}{N_B f''(m_0)}}, \quad (5.20)$$

with the second derivative of system's free energy $f''(m_0) = 1/(1 - m_0^2) - J\beta$, which vanishes at the critical point ($J\beta_c = 1$).

The decoherence factor (5.12) for a single spin in this environment is given by

$$D_t = \frac{1}{Z_B} \sum_{m_1=-1}^1 \dots \sum_{m_{N_B}=-1}^1 e^{(J/2N_B)\beta (\sum_{i=1}^{N_B} m_i)^2 + h\beta \sum_{i=1}^{N_B} m_i - i g t \sum_{i=1}^{N_B} m_i}. \quad (5.21)$$

For simplicity, we assumed that the system spin couples equally to all bath spins with a coupling strength g . As a result, the system-environment adjacency matrix is given by $\Gamma_{AB}(t) = g t (1, 1, \dots, 1)$. Applying the same procedure and approximations used in the partition function derivation, the equation simplifies to

$$D_t = e^{-i\tilde{g} t m_0 - (\tilde{g} t)^2 / [2N_B f''(m_0)]}, \quad (5.22)$$

with $\tilde{g} = g N_B$.

Figure 5.3 shows the time-dependent decoherence factor at various temperatures, comparing cases with and without a magnetic field in the bath. In both cases, the coherence decay deviates from exponential decay seen in Markovian environments, signaling non-Markovian behavior. At higher temperatures, we observe that the mean magnetization vanishes ($m_0 = 0$) from Fig. B.1, and the second derivative of system's free energy is $f''(m_0) = 1 - J\beta$. As a result, the decoherence takes the simple form $D_t = e^{-(\tilde{g} t)^2 / [2N_B(1-J\beta)]}$, which shows a Gaussian decay. In contrast, at lower temperatures, the system displays oscillatory behavior, a clearer indication of non-Markovian dynamics.

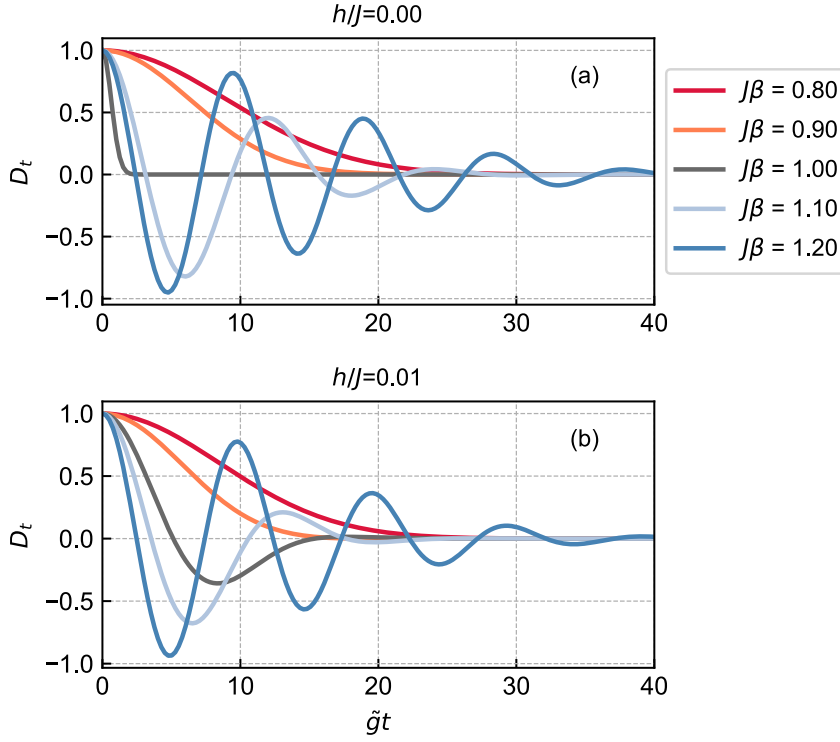


Fig. 5.3.: The decoherence factor (5.22) as a function of time at various temperatures for two scenarios: (a) in the absence of a magnetic field ($h = 0$) and (b) in the presence of a magnetic field. Different colors correspond to different temperature values.

One particularly interesting observation is that the initial decay of coherence increases as the temperature decreases. This can be explained by the fact that at lower temperatures, the environmental spins become more correlated due to interactions between neighboring spins. As the temperature decreases, thermal fluctuations decrease, causing the spins to align and minimize the system's energy, which leads to stronger collective interactions between the system and the bath. The increased coherence of the bath spins enhances the system-environment interactions, resulting in faster decoherence in the early stages.

Furthermore, in the absence of a magnetic field ($h = 0$), the bath undergoes a phase transition at the critical point $J\beta_c = 1$, as shown in Fig. B.1. Near this critical point, the system coherence undergoes a rapid decay, with the decay rate approaching infinity. This can be observed directly from Eq. (5.22), where $f''(m_0)$ vanishes at this point. This transition signifies a sharp change in the bath's dynamics, where the bath spins become highly correlated.

5.4 Entanglement dynamics of two spins

In this section, we examine the dephasing dynamics of two entangled spins, which correspond to the behavior of two qubits in quantum information processing. Two-qubit phase gates play a fundamental role in quantum algorithms, serving as essential components for universal quantum computation. In particular, these gates are crucial for generating entanglement, a key resource for achieving quantum advantage [84, 88].

However, their performance is often compromised by decoherence, particularly dephasing, which can arise due to interactions with surrounding qubits [43, 188]. To investigate this effect, we consider a system of two qubits with a fixed Ising-like coupling strength. Under such interactions, these qubits form a phase gate, leading to entanglement that evolves over time. We specifically analyze how dephasing impacts the entangling power of this phase gate, focusing on two prominent physical platforms for quantum simulation: 2D Rydberg atom arrays [8, 13, 24, 86] and molecular systems [3, 58, 110, 165, 221, 228]. Both 2D Rydberg atom arrays and molecular systems can be effectively described using spin lattice models due to their intrinsic spin-like interactions and spin representations [184].

5.4.1 2D lattice structure bath—Rydberg atoms

For our first case study of the two-spin system, we consider a model where both the system and its surrounding spins form a two-dimensional Rydberg atom array [8, 13, 24, 87]. In this setting, each atom acts as a qubit or spin and interacts with its nearest neighbors via dipole-dipole coupling. The surrounding spins can either stay fixed or move randomly, resulting in dephasing processes that range from nearly Markovian to non-Markovian behavior. This enables us to study the effects of both Markovian and non-Markovian dephasing on the fidelity and entangling power of a phase gate between two system spins. We also examine how random reset operations—where spins are randomly reset to a specific state—can help preserve entanglement, as well as the potential role of three-body interactions in reducing dephasing.

The entire system is modeled as a two-dimensional lattice with a Hamiltonian (5.3). The system consists of two distinct, strongly interacting atoms that exchange phase information via nearest-neighbor Rydberg blockade interactions with strength $g_{AB} > 0$, coupled to an environment of N_B atoms distributed across the lattice. In the worst-case scenario, the environment is at infinite temperature, with a uniform

excitation probability $p(b) = 2^{-N_B}$, which can also be described by the pure state $\rho_B = (|+\rangle\langle+|)^{\otimes N_B}$, as described in Refs. [27, 99].

In our example, we start from a bath configuration in which each lattice site of a 10×10 lattice hosts a single B -atom in the $|+\rangle$ state. Environmental fluctuations are simulated by allowing atoms to hop randomly to neighboring sites at a probability rate $\eta_B > 0$. For simplicity, multiple atoms are allowed to occupy the same site, and we assume periodic boundary conditions, i.e., a toroidal lattice topology. Atoms on a site and its eight adjacent sites are treated as nearest neighbors, interacting at a fixed rate g_{BB} . Two scenarios are compared: (i) a highly non-Markovian regime where the two system atoms are placed on top of B atoms at neighboring sites in the center of the lattice and remain fixed, and (ii) an almost Markovian regime where the positions (and consequently the neighboring environment) of the system spins change randomly at each simulation step. In an infinite lattice, the random movement in scenario (ii) prevents the system from encountering the same environmental spins more than once, resulting in a memoryless evolution describable by a Markovian sequence of completely positive (CP) maps. In contrast, in scenario (i), the stationary system interacts persistently with the same environment, leading to evolution that cannot be expressed as a chain of CP maps—a defining feature of non-Markovianity [23, 180]. However, in a finite lattice, the relocating system in scenario (ii) will eventually revisit previous environmental spins, causing non-Markovian behavior to emerge over extended periods.

Since the coupling strength between the two system spins ($N_A = 2$) is assumed to be constant at g_{AA} , the $N_A \times N_A$ submatrix $\underline{\Gamma}_{AA}(t)$ is expressed as follows

$$\underline{\Gamma}_{AA}(t) = \begin{pmatrix} 0 & g_{AA}t \\ g_{AA}t & 0 \end{pmatrix}. \quad (5.23)$$

In the absence of three-body interactions, the reduced two-spin system state evolves as

$$\rho_A(t) = \sum_{\underline{a}, \underline{a}'} \langle \underline{a} | \rho_A | \underline{a}' \rangle D_t(\underline{a}, \underline{a}') e^{ig_{AA}t(a'_1 a'_2 - a_1 a_2)} | \underline{a} \rangle \langle \underline{a}' |. \quad (5.24)$$

For an infinite-temperature lattice environment, the decoherence factor (5.11) simplifies considerably, reducing to

$$D_t(\underline{a}, \underline{a}') = \prod_{n=1}^{N_B} e^{\frac{i}{2}(\underline{a}' - \underline{a}) \cdot \underline{\Gamma}_{AB}(t) \cdot \underline{b}^{(n)}} \cos \left[\frac{1}{2} (\underline{a}' - \underline{a}) \cdot \underline{\Gamma}_{AB}(t) \cdot \underline{b}^{(n)} \right], \quad (5.25)$$

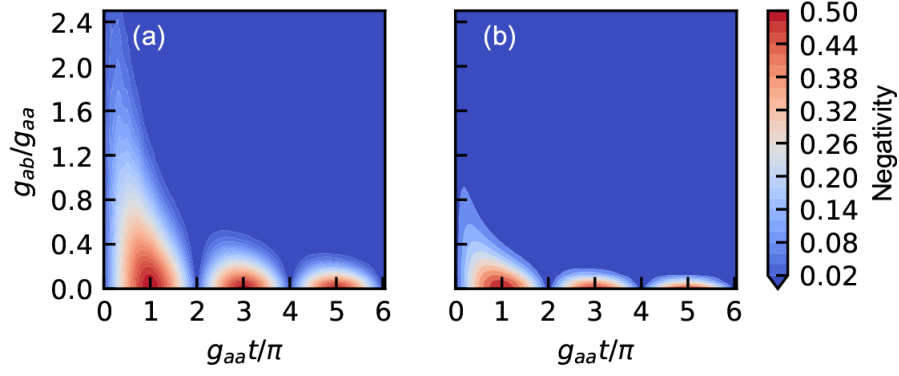


Fig. 5.4.: Entanglement negativity between system spins as a function of normalized time g_{AB}/π and system-environment coupling g_{AB}/g_{AA} . become entangled through their phase interaction, with $g_{AA}\Delta t = 0.05$, while experiencing (a) nearly Markovian and (b) non-Markovian dephasing induced by an infinite-temperature spin environment. The hopping rate of environmental spins is $\eta_B = 1/5$. In (a), undergo random jumps between lattice sites at each time step Δt . Entanglement negativity is computed for ensemble-averaged states over 2×10^5 trajectories.

with the neighbour adjacency matrix between system and environment spins is given by $\underline{\Gamma}_{AB}(t) = g_{AB} \int_0^t \underline{\Lambda}_{AB}(t') dt'$. The $\underline{b}^{(n)}$ denote the N_B basis vectors, where the n -th atom is in the state $|1_n\rangle$ and all other atoms are in the $|0\rangle$ state. The decoherence factor (5.25) can be efficiently calculated for large environments, where $N_B \gg 1$, and will form the foundation for our subsequent evaluation of an entangling phase gate under the influence of environmental dephasing. Our simulations are carried out with discrete time steps Δt and random hopping events of the environment spins occurring at every $1/\eta_B$ -th step.

Entangling power of a two-qubit phase gate

Consider the two system spins are initially prepared in the product state $|\psi_A\rangle = |+\rangle|+\rangle$, which stay in close proximity with a constant interaction rate of g_{AA} . When isolated, the Rydberg interaction generates entanglement periodically, leading to a maximally entangled Bell state at odd multiples of $g_{AA}t = (2n+1)\pi$. This interaction effectively performs a perfect controlled phase (c-phase) gate, which is essential for enabling universal quantum computation with qubit arrays [184]. However, the presence of additional surrounding spins induces dephasing, which rapidly reduces the gate fidelity. A useful measure of this effect is the evolution of system entanglement over time, which can be quantified using the negativity [173, 217].

$$\mathcal{N}(t) = \frac{\|\rho^{TA}\| - 1}{2}, \quad (5.26)$$

which ranges from zero to its maximum value 0.5.

In Fig. 5.4, we illustrate the effects of (a) nearly Markovian and (b) non-Markovian dephasing on the c-phase gate negativity as a function of time t and the relative coupling strength g_{AB}/g_{AA} . The system state ρ was averaged over 2×10^5 simulated trajectories on a representative 10×10 lattice with $N_B = 100$ spins, where each spin hops to a random neighboring site every 5 time steps. Panels (a) and (b) correspond to the nearly Markovian regime, where the system spins relocate randomly at each step, and the non-Markovian regime, where the system spins remain fixed at specific lattice positions (both spins placed on the third site from the left and second from the top).

In an ideal scenario, the negativity would exhibit periodic oscillations, as observed in the lower regions of the plots. However, it is evident that the non-Markovian case presented in (b) leads to a more rapid deterioration of entanglement compared to the Markovian case. Negativity values greater than 0.1 are only observed for weak coupling strengths, where $g_{AB} \lesssim 0.5g_{AA}$. Furthermore, in the non-Markovian case, the periodic revival of entanglement is almost absent, emphasizing the detrimental impact of non-Markovian effects on the maintenance of entanglement.

Additionally, as the environment coupling increases, the time at which maximum entanglement occurs shifts to earlier values, which is a result of an effective Lamb shift in the system's energies given by the complex phase of Eq. 5.25. These findings suggest that, for a given two-spin coupling, phase coherence and entanglement are more robust in a dynamic Markovian environment compared to a static non-Markovian one.

One might question whether the observed behavior and differences can be captured by strictly Markovian, CP-divisible dephasing processes with adjusted effective coupling rates [46]. To investigate this, we introduce a discrete-time Markovian chain model for the dephasing of the two system spins, where they interact with the same local environment in the interaction picture. At each time step Δt , the state of the system updates to $\rho_{A,j} = \rho_A(t = j\Delta t)$ following the rule

$$\rho_{A,j} = \text{tr}_B \left[\hat{V}_{AB} \hat{U}_A \left(\rho_{A,j-1} \otimes \left(\frac{\mathbb{1}}{2} \right)^{\otimes n_B} \right) \hat{U}_A^\dagger \hat{V}_{AB}^\dagger \right], \quad (5.27)$$

where the system evolution is described by the unitary $\hat{U}_A = e^{ig_{AA}\Delta t|1_1 1_2\rangle\langle 1_1 1_2|}$ and the system-environment coupling by

$$\hat{V}_{AB} = \prod_{n=1}^{n_B} e^{-ig_{AB}\Delta t(|1_1\rangle\langle 1_1| + |1_2\rangle\langle 1_2|) \otimes |1_n\rangle\langle 1_n|}. \quad (5.28)$$

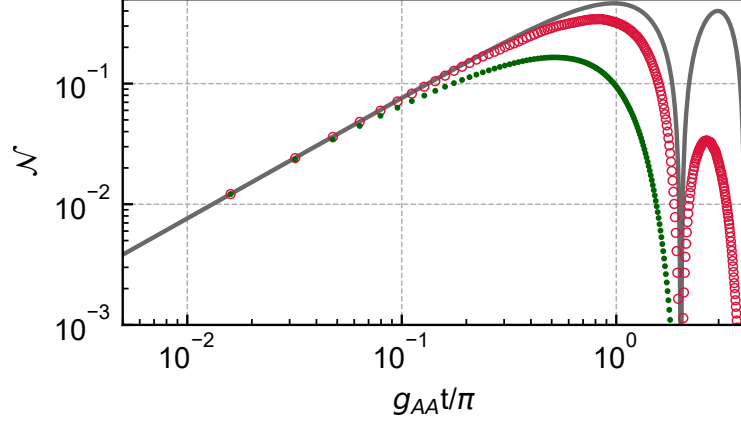


Fig. 5.5.: Entanglement negativity as a function of time at $g_{AB}\Delta t = 0.05$ and $g_{AB}/g_{AA} = 0.5$. We compare the almost Markovian (red circles) and the non-Markovian case (green dots) from Fig. 5.4 against the strictly Markovian collision model based Eq. 5.29 with $n_B = 8$ (solid line).

The update rule (5.27) describes the discrete-time evolution of the system within the context of collision models [45], where each step involves both system spins interacting with an independent set of n_B maximally mixed environment spins. In the computational basis $|\underline{a}\rangle$, this Markovian update rule can be rewritten in terms of a Hermitian coefficient matrix

$$\langle \underline{a} | \rho_{A,j} | \underline{a}' \rangle = D_M(\underline{a}, \underline{a}') \langle \underline{a} | \rho_{A,j-1} | \underline{a}' \rangle. \quad (5.29)$$

The diagonal elements of this matrix are all $C_M(\underline{a}, \underline{a}) = 1$, while the off-diagonal elements are given by

$$\begin{aligned} D_M(00, 01) &= D_M(00, 10) = e^{i\frac{1}{2}n_B g_{AB}\Delta t} \cos^{n_B} \left(\frac{g_{AB}\Delta t}{2} \right), \\ D_M(00, 11) &= e^{i(g_{AA} + n_B g_{AB})\Delta t} \cos^{n_B} (g_{AB}\Delta t), \\ D_M(01, 10) &= 1, \\ D_M(01, 11) &= D_M(10, 11) = e^{ig_{AA}\Delta t} D_M(00, 01), \end{aligned} \quad (5.30)$$

and the respective Hermitian conjugates. A straightforward calculation starting from the initial product state then yields the entanglement negativity in each time step.

In Fig.5.5, we compare the negativity decay results from Fig.5.4 at fixed $g_{AB} = 0.5g_{AA}$ and $g_{AA}\Delta t = 0.05$ to the Markovian collision model (5.29) with $n_B = 8$ (solid line), which represents the average expected number of neighboring environment spins in a fully populated lattice. The results from the almost Markovian regime (red circles) show good agreement with the Markovian model for approximately the

first 15 random hopping steps. After this point, however, deviations increase due to the finite lattice size. The Markovian model (5.29) continually subjects the system to an independent set of n_B environment spins at each step, while in the actual simulation, the system spins eventually encounter the same neighboring particles again, violating the Markov assumption. In line with this, the negativity from the static non-Markovian simulation (green dots) decays more rapidly, deviating much sooner from the simple collision model.

Reset-based entanglement preservation

In the above, we examined the entangling power of the c-phase gate between two spins subjected to dephasing from surrounding spins. Our findings revealed that a dynamically varying, nearly Markovian local environment is less harmful than a static non-Markovian one. However, in both cases, the entanglement (and gate fidelity) decays exponentially on short timescales $g_{AB}t \lesssim 1$, which are governed by the system-environment coupling. To address this, we propose a straightforward repeated intervention method to generate and maintain a non-vanishing average level of entanglement for use at long times. A similar, but less pronounced entanglement-preserving effect was noticed previously [100] for random single-spin reset interventions, starting from a maximally entangled state.

Consider an operation that resets the two system spins to their initial or any other pure product state $|\psi_1\psi_2\rangle$, which is a CPTP map with Kraus representation

$$\Phi_r(\rho_A) = |\psi_1\psi_2\rangle\langle\psi_1\psi_2| = \sum_{a_1, a_2=0}^1 |\psi_1\psi_2\rangle\langle a_1 a_2| \rho_A |a_1 a_2\rangle\langle\psi_1\psi_2|. \quad (5.31)$$

By performing this local operation at regular or random intervals, with an probability per time step $\kappa\Delta t$ comparable to the environment coupling strength, one can partially counteract dephasing and drive the system toward an ensemble-averaged steady state with a finite amount of entanglement for times $\kappa t > 1$. For this approach, the reset states should be chosen along the equator of each spin's Bloch sphere.

To demonstrate the effect, we performed simulations using a Poisson process to introduce reset interventions at varying rates of $\kappa\Delta t$ within our lattice dephasing model. In each trajectory, the waiting times between reset events are drawn from an exponential distribution, and the system evolves according to our decoherence model (5.25) between events. We observed that the highest amount of entanglement is preserved when resetting to the initial state $|\psi_1\psi_2\rangle = |++\rangle$.

Figure 5.6 presents the results averaged over 2×10^5 simulated trajectories for each parameter set. Panel (a) illustrates the rapid equilibration to a steady-state

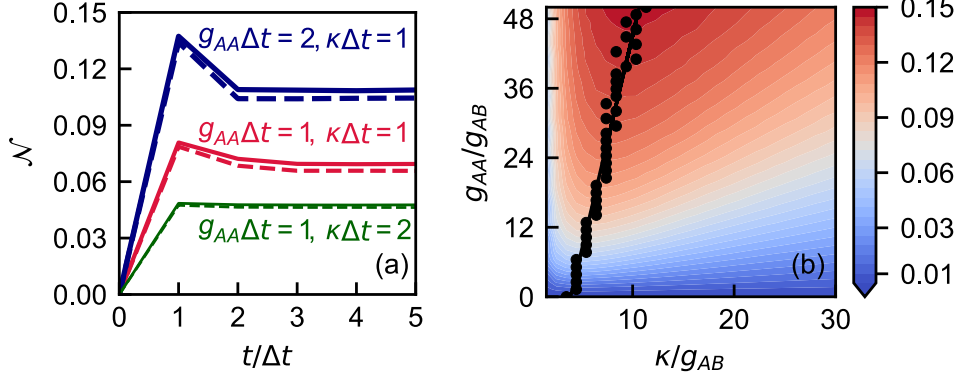


Fig. 5.6.: Entanglement negativity versus time in the presence of dephasing and random simulation reset operations on the two system spins. The solid and dashed lines represent the almost Markovian and the non-Markovian case, respectively; the colors represent different combinations of intrasystem coupling and reset rate. (b) Steady-state negativity versus reset rate κ and intrasystem coupling g_{AA} , as evaluated at $t = 15\Delta t$. The dots show the maximum negativity with respect to $\kappa/g_{AA} = 7$. We fix $g_{AB}\Delta t = 0.1$ and average over 2×10^5 trajectories.

entanglement negativity as a function of time for various intra-system coupling rates g_{AA}/g_{AB} and reset rates κ/g_{AB} . Both the almost Markovian environment (solid line) and the static non-Markovian environment (dashed line) yield nearly identical results. In panel (b), the steady-state negativity is shown as a function of these two rates, demonstrating that the maximum entanglement is achieved when resetting at a rate of $\kappa \sim 7g_{AA}$. Generally, when the system-environment coupling is weak ($g_{AA} \gg g_{AB}$), a significant portion of the entanglement can be preserved on average. A similar, albeit less pronounced, entanglement-preserving effect was previously observed for random single-spin reset interventions starting from a maximally entangled state [100]. The reset protocol considered here requires synchronized single-qubit control at a rate comparable to the c-phase gate timescale, which is feasible on current spin array platforms for quantum information processing [16, 156, 184].

Three-body interaction curbing dephasing

In Rydberg atom systems, there can also be three-body phase interactions on top of the pairwise [78, 79]. These interactions, which can be either repulsive or attractive, are typically weaker than two-body interactions and emerge as higher-order corrections to the dominant pairwise couplings. In this context, we examine the influence of three-spin interactions on entanglement decay under dephasing, demonstrating that even weak three-body couplings of opposite sign to the two-body terms can significantly mitigate dephasing effects. This improvement enhances both the achievable entanglement and the fidelity of a controlled-phase (c-phase) gate between two system spins.

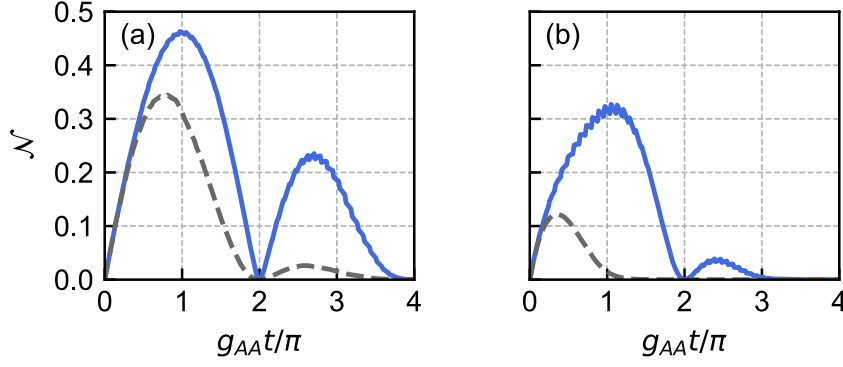


Fig. 5.7.: Entanglement negativity as function of time with and without three-body coupling effect. We choose the same parameters setting as in Fig. 5.5 (dashed line), with an additional three-body coupling of strength $h = -0.015g_{AB}$ (solid). The comparison is made for (a) the almost Markovian case and (b) the non-Markovian case, with results averaged over 10^5 trajectories.

By introducing three-body interactions with a fixed rate $h < 0$ between nearest neighbors in the lattice model, the decoherence factor for the worst-case scenario, where the environment spins are maximally mixed, is given by

$$D_t(\underline{a}, \underline{a}') = \prod_{n=1}^{N_B} e^{\frac{i}{2}(\underline{a} - \underline{a}') \cdot \left[\underline{\Gamma}_{AB}(t) \cdot \underline{b}^{(n)} + h \underline{\Lambda}_{AB}(t) \cdot \left(\underline{b}^{(n)} \circ \underline{\Lambda}_{BB}(t) \cdot \underline{b}^{(n)} \right) \right]} \quad (5.32)$$

$$\cos \left(\frac{1}{2}(\underline{a} - \underline{a}') \cdot \left[\underline{\Gamma}_{AB}(t) \cdot \underline{b}^{(n)} + h \underline{\Lambda}_{AB}(t) \cdot \left(\underline{b}^{(n)} \circ \underline{\Lambda}_{BB}(t) \cdot \underline{b}^{(n)} \right) \right] \right).$$

Figure 5.7 compares the c-phase entanglement negativity with and without three-body coupling, based on an average over 1×10^5 simulated trajectories within our lattice model. Panels (a) and (b) represent the almost Markovian and static non-Markovian regimes, respectively. In these simulations, the two-body environment coupling is fixed at $g_{AB} = 0.5g_{AA}$, consistent with the setup in Fig. 5.5, where the gray curves replicate the simulated results from that figure. Introducing a weak three-body coupling with strength $h = -0.015g_{AB}$ leads to a notable increase in the achievable entanglement, as seen in the blue curves. This enhancement is particularly significant in the non-Markovian case (b), where there is also a shift toward longer gate times for achieving maximum entanglement. Therefore, considering such three-spin interactions could improve the stability of local gate operations on qubit array platforms, boosting the potential for quantum computing.

5.4.2 Organic molecule as a finite correlated spin bath

Molecules with individually addressable and controllable nuclear spins offer a promising foundation for scalable quantum technologies [3, 136, 233]. However, the coherence times of quantum operations are constrained by dephasing effects, which result from magnetic dipole-dipole interactions with nearby spins in the surrounding environment. For example, the decoherence of a single central spin in a triphenylphosphine (PPh₃) molecule and the propagation of multispin correlations have been studied theoretically and validated experimentally [165]. These studies were conducted in a high-temperature regime where the bath spins were effectively modeled as uncorrelated maximally mixed states.

We extend the analysis to a system with two central spins within a different molecule, which are used to implement a controlled-phase (c-phase) gate. In this setup, we investigate the dephasing effects caused by interactions with the surrounding spin bath and assess the role of bath correlations at finite temperature. The dynamics of the two central spins are analyzed in the presence of a thermal spin bath. We will show that bath correlations significantly enhance the decoherence effect at low temperatures, where these correlations become non-negligible.

The exemplary molecule under consideration is 1,2-Bis(dimethylphosphino)ethane (dpme), with the chemical formula C₆H₁₆P₂, as depicted in Fig. 5.8. The two nuclear spins of the phosphorus atoms (yellow) constitute the system of interest, while the $N = 16$ surrounding hydrogen spins (light gray) form the thermal bath. To utilize our framework for examining dephasing at finite temperature, we consider a scenario in which the spin bath is assumed to be in thermal equilibrium at ultralow temperatures, extending down to the nanokelvin range. This stands in contrast to conventional NMR experiments, which are usually carried out at room temperature. By exploring this ultralow temperature regime, we can gain a more precise understanding of how temperature influences dephasing processes in a more controlled setting. We model the interactions in the system using a simple Ising-type dipole-dipole interaction, which is valid when the molecule is placed in a strong magnetic field along the z -direction [71].

The Hamiltonian of the global system is given by (5.1) without the three-body interaction term, where the quantization axis e_z for the spin states is aligned with the external homogeneous magnetic field of strength B_z . The bare resonance frequencies of the hydrogen spins are uniform and expressed as $\omega_H = g_H \mu_N B_z / \hbar$, where $g_H = 5.585$ is the hydrogen atom g -factor, and μ_N is the nuclear magneton. Since we work in the co-rotating frame of the system spin, its bare resonance

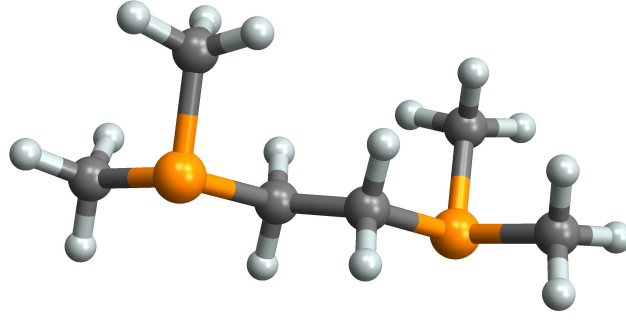


Fig. 5.8.: Structure of the 1,2-Bis(dimethylphosphino)ethane (dpme) molecule $C_6H_{16}P_2$ possesses C_2 molecular symmetry, with the two phosphorus atoms (yellow) occupying symmetry-equivalent positions.. The nuclear spins of the two phosphorus atoms (yellow) act as the quantum system subject to non-Markovian dephasing from the 16 surrounding hydrogen spins (light grey) via magnetic dipole interactions. We average over random orientations of the molecule with respect to the external magnetic field axis.

frequencies can be neglected. The magnetic dipole-dipole interaction between any two spins, as represented in Eq. (5.2), takes the following form [131]

$$\tilde{g}_{kn} = g_{kn} = \frac{\mu_0 \mu_N^2 g_k g_n}{4\pi \hbar |\mathbf{r}_k - \mathbf{r}_n|^3} \left[1 - 3 \frac{(z_k - z_n)^2}{|\mathbf{r}_k - \mathbf{r}_n|^2} \right]. \quad (5.33)$$

Here, μ_0 is the magnetic constant, and $g_H = 5.585$ and $g_P = 2.261$ are the g -factors for the hydrogen and phosphorus spins, respectively. As usual, we set $\tilde{g}_{kk} = 0$. The interaction between two spins depends on the angle between their distance vector and the magnetic field. To account for this, we average over random orientations of the molecule relative to the external magnetic field. In NMR experiments, powdered samples are typically employed at low temperatures, so we model an ensemble of molecules with randomly distributed orientations. The two phosphorus spins are prepared in the maximally entangled state $|\Phi_A\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$ and now undergo dephasing due to interactions with the hydrogen spin bath.

The hydrogen spins are assumed to be in thermal equilibrium at an inverse temperature $\beta = \hbar/k_B T$ and the corresponding thermal state reads

$$\rho_B = \sum_{\underline{b}} p(\underline{b}) |\underline{b}\rangle \langle \underline{b}| = \frac{1}{Z_B(\beta)} \sum_{\underline{b}} e^{-\beta \left(\tilde{\omega}_B \cdot \underline{b} + \frac{1}{2} \underline{b} \cdot \tilde{g}_B \cdot \underline{b} \right)} |\underline{b}\rangle \langle \underline{b}| \quad (5.34)$$

with the partition function

$$Z_B(\beta) = \text{tr} \left(e^{-\beta H_B} \right) = \sum_{\underline{b}} e^{-\beta \left(\tilde{\omega}_B \cdot \underline{b} + \frac{1}{2} \underline{b} \cdot \tilde{g}_B \cdot \underline{b} \right)} \quad (5.35)$$

where $\underline{\tilde{g}}_B$ is the 16×16 matrix of homonuclear H-H coupling frequencies (5.33) with zeros on the diagonal. The renormalized hydrogen eigenfrequencies in $\underline{\tilde{\omega}}_B$ are given by

$$\tilde{\omega}_k = \omega_H - \frac{1}{2} \sum_{n_A=1}^2 g(\mathbf{r}_k, \mathbf{r}_{n_A}) - \frac{1}{2} \sum_{\substack{n=1 \\ n \neq k}}^{16} g(\mathbf{r}_k, \mathbf{r}_n). \quad (5.36)$$

The renormalized frequency array already incorporates the heteronuclear coupling with the two P spins and the homonuclear coupling from the other H spins. The orientation independent prefactors in (5.33) determine the magnitude of the coupling frequencies, which, in this case, range from $2\pi \times 27.5$ Hz to $2\pi \times 3.52$ kHz. The bare H-spin resonance frequency ω_H is approximately $2\pi \times 42.5$ kHz/mT. Consequently, bath correlations become significant only at relatively weak magnetic fields, $B_z \lesssim 0.1$ mT. In contrast, at high magnetic fields, the local spin energies dominate, allowing us to approximate the thermal state as a product of local Gibbs states.

$$p(\underline{b}) \approx \prod_{n=1}^{N_B} \frac{e^{-\beta \tilde{\omega}_n b_n}}{1 + e^{-\beta \tilde{\omega}_n}} \approx \frac{e^{-\beta \omega_H \underline{b} \cdot \underline{b}}}{(1 + e^{-\beta \omega_H})^{N_B}}, \quad (5.37)$$

regardless of the molecular orientation. This approximation will no longer be valid for the correlated thermal state. In either case, the thermal populations $p(\underline{b})$ and the decoherence factor followed for the two P spins will depend on the orientation of the molecule.

To represent an ensemble of randomly distributed static orientations in thermal equilibrium, the decoherence factor is determined by averaging uniformly over a sphere characterized by two key Euler angles: the inclination angle $\theta \in [0, \pi]$ relative to the z -axis of the field and the azimuthal angle $\gamma \in [0, 2\pi]$ around the molecule's principal axis. The third Euler angle, corresponding to a rotation around the molecule's own symmetry axis, is irrelevant to the averaging. This leads to

$$D_t(\underline{a}, \underline{a}') = \iint \frac{\sin \theta}{4\pi} d\theta d\gamma \sum_{\underline{b}} p(\underline{b}|\theta, \gamma) e^{it(\underline{a}-\underline{a}') \cdot \underline{\tilde{g}}_{AB}(\theta, \gamma) \cdot \underline{b}}. \quad (5.38)$$

It is important to note that for a correlated thermal state, the summation over all 2^{N_B} binary vectors $\underline{b}$ cannot be simplified into a product of N_B terms, resulting in an exponential increase in computational cost as the bath size grows. Based on the decoherence factor, we will examine how the entanglement between two P spins decays, following the same procedure as outlined in the previous section.

In Figure 5.9, the entanglement negativity between two P spins is presented as a function of time. Panels (a) and (b) illustrate results for a single fixed molecular orientation under different magnetic fields, $B_z = 0.05$ mT and $B_z = 1$ mT, respec-

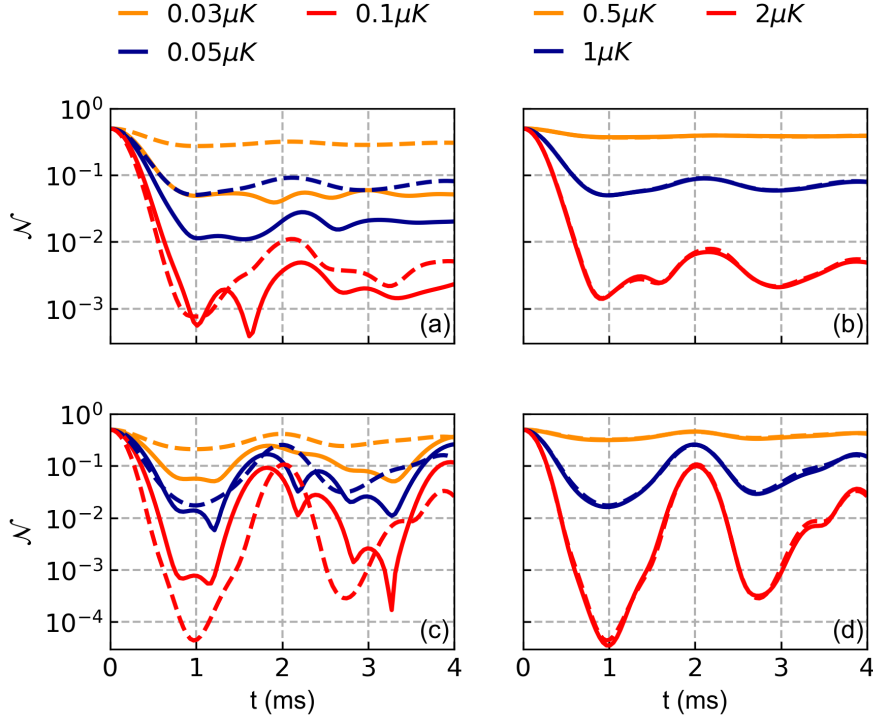


Fig. 5.9.: The decay of entanglement negativity over time for two nuclear P-spins, initially in a Bell-entangled state, subjected to dephasing by the surrounding H-spins of the dpme molecule under a magnetic field of (a, c) $B_z = 0.05$ mT and (b, d) 1 mT. The molecule is oriented (a, b) at a fixed configuration with $\theta = \pi/2$ and $\gamma = 0$, and (c, d) averaged over 5000 random orientations relative to the magnetic field axis. The dephasing dynamics are compared for an interacting (solid line) and a non-interacting (dashed line) thermal environment across different temperatures.

tively. In contrast, panels (c) and (d) show the corresponding averaged values over 5000 random orientations of the damped molecule relative to the fixed magnetic axis. Each panel compares the negativity for a thermal state with (solid line) and without (dashed line) correlation. The uncorrelated case is obtained by setting $\tilde{g}_{AB} = 0$. Different curve colors correspond to different temperatures. As anticipated, in the strong-field scenario, the correlated and uncorrelated baths produce nearly identical results. This occurs because the local spin energies dominate, and the spin-spin couplings are weak enough to be negligible. In contrast, under the weak field shown in panel (a), a significant difference emerges. The correlated bath induces much faster decay at lower temperatures. This phenomenon arises from dipole couplings within the bath, which generate thermally accessible low-energy excitation modes that interact with the system to acquire phase information. Due to the limited number of thermally excited modes, noticeable revivals are observed at approximately 2 and 4ms of evolution time.

Building on the above observation, we further investigate the relationship between the initial decay of entanglement and thermal excitations in the bath under a weak magnetic field. The initial entanglement decay is defined as the difference between the entanglement negativity at a small time interval τ and its initial value for the Bell state, which has a maximum of $\mathcal{N}(0) = 1/2$. To calculate the negativity at τ , the states of the two system spins at this time must be determined. The initial Bell state $|\Psi_A\rangle$ evolves as

$$\rho_A(\tau) = \frac{1}{2} \left[|00\rangle\langle 11| + |11\rangle\langle 00| + D_\tau(00, 11)|00\rangle\langle 11| + D_\tau(11, 00)|11\rangle\langle 00| \right], \quad (5.39)$$

with the coefficients $D_\tau(\underline{a}, \underline{a}')$ obtained from Eq. (5.38). The negativity (5.26) of this state assumes the simple form

$$\mathcal{N}(\tau) = \frac{\sqrt{D_\tau(00, 11)D_\tau(11, 00)}}{2} = \frac{|D_\tau(00, 11)|}{2}. \quad (5.40)$$

Expanding the coefficient D_τ to second order in τ results in a quadratic initial decay of negativity,

$$\begin{aligned} \mathcal{R} &:= \mathcal{N}(0) - \mathcal{N}(\tau) \\ &\approx \frac{1}{2} - \frac{1}{2} \sqrt{1 - \tau^2 \text{Var}[(1, 1) \cdot \underline{\tilde{g}}_{AB} \cdot \underline{b}]}, \\ &\approx \frac{\tau^2}{4} \text{Var}[(1, 1) \cdot \underline{\tilde{g}}_{AB} \cdot \underline{b}]. \end{aligned} \quad (5.41)$$

For the uncorrelated bath based on the orientation-independent probabilities (5.37), the initial decay of negativity factorizes and simplifies to

$$\begin{aligned} \mathcal{R} &\approx \frac{\tau^2}{4} \frac{1}{1 + e^{\beta\omega_H}} \left[\sum_{n=1}^{N_B} \left\langle \left((1, 1) \cdot \underline{\tilde{g}}_{AB} \cdot \underline{b}^{(n)} \right)^2 \right\rangle_{\theta, \gamma} \right. \\ &\quad \left. - \frac{1}{1 + e^{\beta\omega_H}} \left\langle \sum_{n=1}^{N_B} (1, 1) \cdot \underline{\tilde{g}}_{AB} \cdot \underline{b}^{(n)} \right\rangle_{\theta, \gamma}^2 \right], \end{aligned} \quad (5.42)$$

where $\langle \cdot \rangle_{\theta, \gamma}$ denotes the orientation average.

Figure 5.10(a) illustrates the initial entanglement decay $\mathcal{R}$ at $\tau = 10 \mu s$ as a function of temperature for both the correlated (solid line) and uncorrelated H-spin bath (dashed line), averaged uniformly over molecular orientations. The results reveal that at lower temperatures, the correlated bath induces greater decoherence and faster entanglement decay, while at higher temperatures, the uncorrelated bath

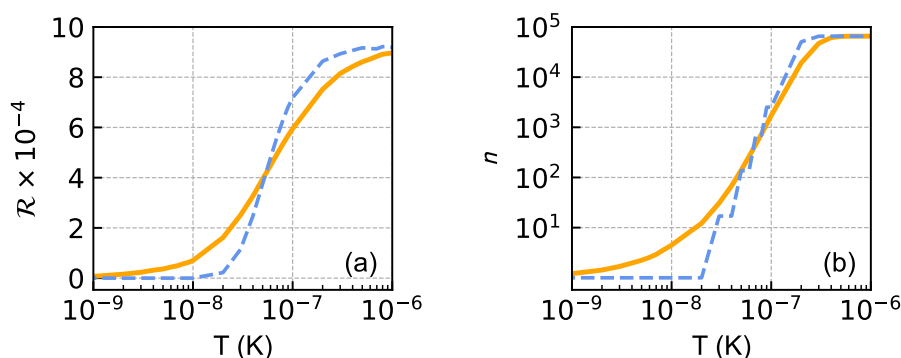


Fig. 5.10.: (a) Initial rate of entanglement negativity decay $\mathcal{R}$ at $\tau = 10 \mu\text{s}$ as a function of temperature, comparing the correlated (solid line) and uncorrelated (dashed line) spin baths in the Gibbs state. (b) Number of bath spin states occupied by 99% of the Gibbs distribution. The results were obtained for a weak magnetic field of $B_z = 0.05 \text{ mT}$, averaged over 5×10^3 random orientations of the molecule.

becomes dominant. This crossover behavior is attributed to the number of thermally accessible spin states since the variance of the P-H coupling in (5.41) increases with the population of different H-spin configurations. Panel (b) displays the 99 quantile of thermally occupied spin levels, representing the number of spin configurations b , ordered by ascending energy, that collectively account for 99% of the Gibbs distribution at each orientation within the uniform average. The crossover region aligns with the behavior observed in the entanglement decay in (a). The uncorrelated bath shows a stepwise increase due to the high degeneracy of its spin states.

5.5 Conclusion

In this chapter, we introduced a lattice model to describe the pure dephasing dynamics of central spins. Using this model, we first analyzed a single spin interacting with two types of spin baths: uncorrelated and correlated. Our analysis revealed that in both cases, the single spin can exhibit non-Markovian dynamics. Notably, for the correlated thermal bath, we demonstrated that the initial coherence decays more rapidly at lower temperatures.

The model was also employed to study the dephasing effects on the entangling power of a two-spin across different physical platforms. In the Rydberg atom system, we implemented both nearly Markovian and non-Markovian dephasing. It was observed that non-Markovian dephasing accelerates the decay of entanglement. By leveraging a random reset mechanism, we found that entanglement could be maintained in a stationary state. Additionally, introducing a weak three-body phase interaction proved effective in mitigating dephasing. In the case of organic molecules subjected to a magnetic field, we explored the effects of bath correlations

and thermal fluctuations on two-spin entanglement decay. Our findings showed that thermal effects enhance the initial entanglement decay in both correlated and uncorrelated baths as the temperature increases. At stronger magnetic fields, the correlated and uncorrelated baths result in similar entanglement decay behavior across different temperatures. However, as the magnetic field weakens and coupling effects dominate, the correlated bath leads to significantly faster initial decay at low temperatures.

Future research involves leveraging the insights gained from understanding non-Markovian dephasing dynamics to develop more effective and efficient decoupling schemes that preserve coherence and entanglement in quantum systems [143]. Moreover, local spin measurements can be utilized as phase probes to investigate many-body correlations or estimate temperature in finite interacting baths.

Non-Markovian phase thermometry

In this chapter, we investigate how critical phenomena in quantum many-body systems can be used to enhance the precision of temperature estimation. We focus on phase thermometry, a non-invasive technique where a quantum spin probe interacts with a small region of a system, such as a two-dimensional Ising spin lattice, and measures temperature by monitoring its dephasing dynamics. The unique property of systems near phase transitions is their heightened sensitivity to changes in temperature, which can significantly improve the accuracy of thermometric measurements. To quantify this sensitivity, we use the quantum Fisher information (QFI), a key metric that reveals how precisely temperature can be estimated. We find that QFI peaks near the critical temperature of the system, highlighting the enhanced precision achievable at phase transitions. Through theoretical modeling and simulations, we explore how factors like the probe's interaction range and the size of the measured region affect the results. We also compare these findings with analytical methods, including the mean-field theory, and high-temperature expansions, identifying their limitations in accurately describing critical behavior. This chapter is based on the Project [D].

6.1 Motivation

Quantum thermometry is a rapidly advancing discipline within quantum metrology that aims to achieve high-precision temperature measurements using quantum systems [54, 152]. The field is driven by the demand for accurate thermal sensing in experiments and technologies that rely on quantum effects, such as quantum sensors [55], quantum computing [128, 164], and ultracold atomic gases [80, 109, 157, 158, 161, 189, 227].

A standard approach in quantum thermometry involves employing a quantum probe—acting as a thermometer—coupled to a system at temperature T . By performing measurements on the probe, either by preparing multiple independent copies in parallel or by using a single continuously interacting probe sequentially, temperature estimates can be extracted from the statistical properties of the mea-

surement outcomes. One commonly used strategy is to analyze the probe after it has reached thermal equilibrium with the system [47, 96, 151]. While this method has been successfully implemented in several recent experiments [105, 138, 149, 160, 166, 178, 194], it encounters difficulties at extremely low temperatures, where equilibration times become prohibitively long and precise tuning of the probe's energy levels is required [28, 47, 53, 106, 118, 170, 174].

To overcome these challenges, an alternative approach utilizes the nonequilibrium dynamics of the probe for temperature estimation [17, 32, 74, 96, 104, 114, 146]. A particularly notable example is the pure dephasing regime, where the probe's energy remains unchanged, thereby inhibiting conventional thermalization. However, despite the absence of energy exchange, coherences between the probe's energy eigenstates can still develop over time, forming correlations with the surrounding environment that encode temperature information [25, 117, 176, 183].

In this chapter, we utilize this approach to estimate the temperature of systems that can be effectively represented by a two-dimensional (2D) Ising lattice of spins, such as ferromagnetic systems [76], spin-polarized Fermi gases [33, 34], systems of nitrogen-vacancy centers [1, 57, 89, 112, 113, 181], and Rydberg atom arrays [8, 13, 24, 86]. These systems are assumed to be in thermal equilibrium with a reservoir at temperature T . When coupled to a probe spin, they can induce non-Markovian pure dephasing on the probe. Furthermore, we take advantage of the fact that the system undergoes a phase transition with respect to temperature [76], which helps improve the precision of the temperature estimation.

6.2 Phase thermometry

In quantum thermometry, the primary task is to estimate the temperature T of a system that is in thermal equilibrium with a reservoir. This system, often referred to as the sample, is typically modeled as a subsystem of a larger thermal bath [55, 152]. A quantum probe—ranging from a two-level system (such as a qubit or atom) to a harmonic oscillator or even a more complex many-body system—interacts with the sample and acquires temperature-dependent information through its steady-state properties or dynamical evolution. The manner in which this information is encoded depends on the probe's structure and the interaction regime. By measuring the probe's state, one can infer the temperature of the sample. Among various probe choices, two-level systems are the most fundamental and extensively studied in quantum thermometry [47, 104, 114]. In this work, we focus on thermometry using a two-level quantum probe.

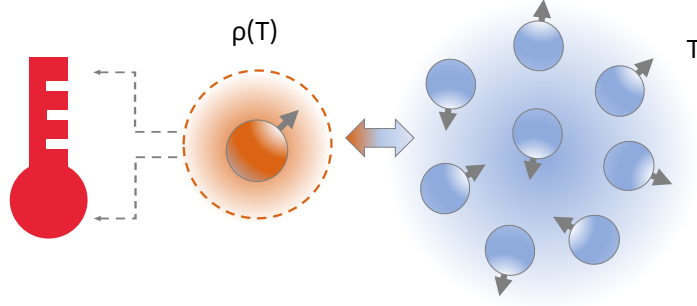


Fig. 6.1.: Qubit phase thermometry scheme: A two-level system couples to a sample system in thermal equilibrium with a reservoir at temperature T . The temperature information is encoded in the probe state and can be estimated by measuring the probe state.

Consider a general setup where a two-level quantum probe interacting with a thermalized sample system at temperature T , as illustrated in Fig. 6.1. Assuming that the probe-sample interaction commutes with the probe Hamiltonian, the total Hamiltonian takes the form

$$\hat{H} = \hat{H}_s + \hat{H}_p + \hat{H}_I = \hat{H}_s + \frac{1}{2}\hbar\omega_p\hat{\sigma}_z + \hbar\hat{\sigma}_z \otimes \hat{B},$$

where ω_p is the transition frequency of the probe system, and $\hat{B}$ is the sample system operator through which the probe interacts with the sample. As the combined system evolves, the probe undergoes pure dephasing while its energy population remains conserved over time. Starting from a generic initial probe state uncorrelated with the Gibbs state $\rho_s(T)$ of the sample,

$$\rho_p = \begin{pmatrix} p & c \\ c^* & 1-p \end{pmatrix}, \quad c = q\sqrt{p(1-p)}e^{-i\phi}, \quad (6.1)$$

where $p, q \in [0, 1]$ to ensure positivity. The reduced probe state evolves as

$$\begin{aligned} \rho_p(t, T) &= \text{tr}_s \left\{ e^{-i\hat{H}t/\hbar} [\rho_p \otimes \rho_s(T)] e^{i\hat{H}t/\hbar} \right\} \\ &= \begin{pmatrix} p & ce^{-i\omega_p t} D_t(T) \\ c^* e^{i\omega_p t} D_t^*(T) & 1-p \end{pmatrix} \end{aligned} \quad (6.2)$$

with the decoherence function

$$D_t(T) = \text{tr}_s[e^{-i\hat{B}t}\rho_s(T)]. \quad (6.3)$$

For a sample system consisting of spins, the bath coupling operator has $\hat{B} = \sum_i g_i \hat{\sigma}_z^i$. The decoherence function, which was described in Chapter 5, takes the form of Eq. (5.12).

The sample temperature enters as a parameter in the probe state by virtue of the decoherence function $D_t(T)$. Hence, by understanding the precise dependence of $D_t(T)$ on T , the sample's temperature can be inferred through statistical analysis of measurements on a large ensemble of identically prepared probes. To estimate the temperature, we utilize quantum estimation theory [152, 171].

A measurement can be represented by a positive operator-valued measure (POVM) $\{\Pi_x\}$ that satisfies the relationship $\int dx \Pi_x = \mathbb{1}$. Each outcome is labeled by x , occurring with a probability described by $p(x|t, T) = \text{tr}[\rho_p(t, T) \Pi_x]$. The experimental procedure involves M distinct measurements on identically prepared probes, yielding a dataset $\mathbf{x} = \{x_1, x_2, \dots, x_M\}$ collected at chosen times $\mathbf{t} = \{t_1, t_2, \dots, t_M\}$. From this data, we can estimate the temperature using a function $\tilde{T}(\mathbf{x}|\mathbf{t})$. The estimator is considered unbiased when its expectation value equals the actual temperature T , expressed mathematically as $\mathbb{E}[\tilde{T}(\mathbf{x}|\mathbf{t})] = T$ [19, 75]. However, any such temperature estimate carries an unavoidable uncertainty due to the random character of quantum measurement and the finite data size M . The statistical uncertainty can be quantified by the dimensionless mean-square error, expressed as $\mathbb{E}[(\tilde{T} - T)^2]/T^2$, and the error obeys the quantum Cramér-Rao bound [19, 49]

$$\frac{\mathbb{E}[(\tilde{T} - T)^2]}{T^2} \geq \frac{1}{MT^2 \mathcal{F}_T(t)} \geq \frac{1}{MT^2 \mathcal{F}_T^Q(t)}. \quad (6.4)$$

The first inequality depends specifically on the quantum measurement we choose and is expressed using the Fisher information (FI), which we calculate from the temperature-dependent likelihood function

$$\mathcal{F}_T(t) = \int dx p(x|t, T) \left[\frac{\partial \ln p(x|t, T)}{\partial T} \right]^2. \quad (6.5)$$

This FI tells us how sensitively the likelihood function responds to tiny temperature changes at a given interrogation time t . When we maximize this FI across all possible POVMs, that is, $\mathcal{F}_T^Q(t) = \max_{\{\Pi_x\}} \mathcal{F}_T(t)$, we obtain the second inequality, yielding what's known as the QFI. This QFI represents the fundamental limit of measurement precision that can be achieved.

Alternatively, the QFI can be obtained explicitly by using the symmetric logarithmic derivative (SLD) operator $\hat{L}_T(t)$, which is defined as the self-adjoint solution of the following Lyapunov equation [171]

$$\frac{\partial \rho_p(t, T)}{\partial T} = \frac{1}{2} [\rho_p(t, T) \hat{L}_T(t) + \hat{L}_T(t) \rho_p(t, T)]. \quad (6.6)$$

This solution varies based on the probe state. To achieve the maximum precision specified by the QFI bound at a given temperature, one should use the optimal projective measurement defined by the eigenbasis of $\hat{L}_T(t)$. The QFI takes the form

$$\mathcal{F}_T^Q(t) = \text{tr} [\rho_p(t, T) \hat{L}_T^2(t)] = 2 \sum_{nm} \frac{|\langle \psi_m | \partial_T \rho_p(t, T) | \psi_n \rangle|^2}{\rho_n + \rho_m}. \quad (6.7)$$

The second equation is derived when we express the probe state in terms of its eigenstate decomposition as $\rho_p(t, T) = \sum_n \rho_n |\psi_n\rangle \langle \psi_n|$, which leads to

$$\hat{L}_T(t) = 2 \sum_{nm} \frac{\langle \psi_m | \partial_T \rho_p(t, T) | \psi_n \rangle}{\rho_n + \rho_m} |\psi_m\rangle \langle \psi_n|. \quad (6.8)$$

For a two-level phase probe, the QFI associated to the probe state (6.1) is given as

$$\mathcal{F}_T^Q(t) = 4q^2 p(1-p) \frac{|\partial_T D_t(T)|^2 - q^2 (\text{Im}[D_t(T) \partial_T D_t(T)^*])^2}{1 - q^2 |D_t(T)|^2}. \quad (6.9)$$

The expression increases monotonically with q^2 , as evidenced by the inequality $\text{Im}[D \partial_T D^*]^2 \leq |D|^2 |\partial_T D(T)|^2$. This mathematical relationship shows that to achieve maximum QFI, we need the initial probe state to be pure (where $q = 1$). We must also maximize the term $p(1-p)$, which reaches its peak value when $p = 1/2$, regardless of what value ϕ takes. These conditions tell us that the optimal probe state for phase thermometry can be any quantum state lying on the equator of the Bloch sphere, resulting in QFI

$$\mathcal{F}_T^Q(t) = \frac{|\partial_T D_t(T)|^2 - (\text{Im}[D_t(T) \partial_T D_t(T)^*])^2}{1 - |D_t(T)|^2}. \quad (6.10)$$

We start from the $\hat{\sigma}_x$ -eigenstate $\rho_p = |+\rangle \langle +|$ with $p, c = 1/2$. The projective measurement that saturates the QFI bound at some (t, T) corresponds to the eigenbasis of the SLD operator (6.6), given by the state

$$|\psi_T(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta} \\ 1 \end{pmatrix}, \quad \theta = \omega_p t + \arg [\partial_T D_t(T) + i D_t(T) \text{Im}(D_t(T) \partial_T D_t(T)^*)], \quad (6.11)$$

and its orthogonal complement. For the results presented in the following, we evaluate the maximum of the QFI (6.10) with respect to t , $\mathcal{F}_T^{\text{opt}} = \max_t \mathcal{F}_T^Q$, showing the highest attainable phase thermometry precision in our setting. For convenience, we express the temperature in terms of the inverse temperature rescaled in units of inverse energy, $\beta = 1/k_B T$. This reparameterization preserves the relative Cramér-Rao bound in Eq. (6.4), such that $T^2 \mathcal{F}_T = \beta^2 \mathcal{F}_\beta$ and $T^2 \mathcal{F}_T^Q = \beta^2 \mathcal{F}_\beta^Q$.

6.3 Thermometric performance in physical models

We consider a finite two-dimensional (2D) Ising lattice spin system with nearest-neighbor interactions as the thermal sample, aiming to estimate its temperature. The 2D Ising model is a widely adopted framework for representing systems with discrete binary states, including magnetic spins in ferromagnetic systems [76], spin-polarized Fermi gases [33, 34], systems of nitrogen-vacancy centers [1, 57, 89, 112, 113, 181], and Rydberg atom arrays [8, 13, 24, 86]. The Hamiltonian of this model is given by

$$\hat{H}_s = -J \sum_{\langle ij \rangle} \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j - h \sum_{i=1}^N \hat{\sigma}_z^i, \quad (6.12)$$

where J and h represent the nearest-neighbor interaction energy and the single-site energy due to an external field, respectively. The notation $\langle ij \rangle$ denotes all possible pairs of nearest neighbors, and N is the total number of spins in the system. The spin operator $\hat{\sigma}_z^i$ describes the Z -component of a spin-1/2 at the i -th lattice site, with eigenvalues $m_i = \pm 1$. The 2D lattice is assumed to have periodic boundary conditions. The system is in thermal equilibrium at temperature T , and its state is described by the Gibbs state $\rho_s = e^{-\beta \hat{H}_s} / \mathcal{Z}$, with the partition function $\mathcal{Z} = \text{tr}(e^{-\beta \hat{H}_s})$.

This type of system is known to exhibit a critical phenomenon, undergoing a phase transition from a paramagnetic phase at high temperatures to a ferromagnetic phase at low temperatures in the absence of an external field [76]. Near the phase transition point, the system's sensitivity to temperature variations increases significantly, enabling more precise temperature sensing. A central theme of this chapter is the exploration of phase transitions as a tool to enhance the precision of temperature estimation.

To evaluate the maximum sensitivity of a phase probe to the temperature of an Ising lattice sample with N spins in thermal equilibrium, we begin by examining the Curie-Weiss model, which provides a mean-field approximation of the Ising model. We then proceed to assess the exact results for the Ising lattice and compare these

with the sensitivity predicted by the mean-field approximation and high-temperature expansion. Additionally, we compare the phase thermometric precision of both models to that of equilibrium thermometry, where the temperature is inferred by allowing the probe to reach thermal equilibrium with the sample and measuring its mean energy [47, 48, 53, 96, 104, 114, 146, 151, 152, 155, 195]. In our analysis, we consider a fraction of the thermalized sample system as the probe for equilibrium thermometry.

6.3.1 Curie-Weiss model

The Curie-Weiss model is grounded in the idea that, in a ferromagnetic lattice, all spins align in response to a collective magnetization or an external magnetic field [76]. Unlike models with nearest-neighbor or more general site-specific interactions, each spin $\hat{\sigma}_z^i$ in the lattice interacts only with the collective spin of the entire lattice, $\sum_j \hat{\sigma}_z^j$, as depicted in Fig. 5.2 of Section 5.3. The system Hamiltonian is given by

$$\hat{H}_s^{\text{cw}} = -\frac{J}{2N} \sum_{i,j=1}^N \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j - h \sum_{i=1}^N \hat{\sigma}_z^i. \quad (6.13)$$

For a single spin probe uniformly interacting with such system, the dephasing has been analyzed in Section 5.3 of Chapter 5 with the decoherence function

$$D_t(\beta) = e^{-i\tilde{g}tm_0 - (\tilde{g}t)^2/[2Nf''(m_0)]}, \quad (6.14)$$

where $\tilde{g} = Ng$, with g representing the coupling strength between the probe and sample spins, and temperature-dependent m_0 being the mean magnetization per site, determined by the self-consistent equation (5.19). For $h = 0$, the mean magnetization m_0 undergoes a temperature-dependent phase transition at the critical point $J\beta_c = 1$. It vanishes in the paramagnetic phase above the critical temperature ($J\beta < 1$) and approaches 1 in the ferromagnetic phase at low temperatures ($J\beta > 1$), as illustrated in Fig. B.1. The quantity $f''(m_0) = 1/(1 - m_0^2) - J\beta$ denotes the second derivative of the system's free energy and vanishes at the critical point ($J\beta_c = 1$). The free energy is expressed in Eq. (5.18), with additional details provided in Section 5.3. To study temperature sensitivity, we introduce the coherence decay timescale $\tilde{g}\tau(\beta) = \sqrt{Nf''(m_0)}$, which highlights that coherence decays more rapidly as the lattice size N increases.

In Fig. 5.3, we have already illustrated that the probe exhibits non-Markovian dynamics. Specifically, for temperatures above the critical point, where the sample system is in the paramagnetic phase ($J\beta < 1$), the probe exhibits Gaussian decay.

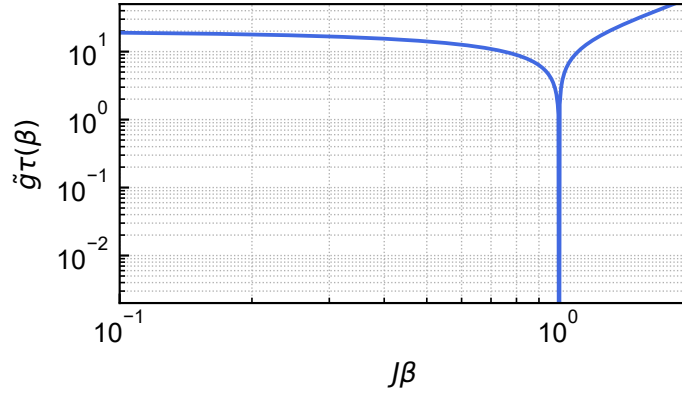


Fig. 6.2.: Coherence decay time as a function of inverse temperature, as predicted by the Curie-Weiss model in the thermodynamic limit. The parameters are set to $N = 400$ and $h = 0$.

Conversely, in the ferromagnetic phase, the decay features damped oscillations with a Gaussian envelope. The decay time is shortest at the critical point (indicated by the gray line in Fig.5.3(a)) and increases as the system moves further from the critical temperature in either direction, as also shown in Fig. 6.2. In the zero-temperature limit, there is no decay as $m_0 \rightarrow 1$, resulting in $\tau(\beta) \rightarrow \infty$. In the paramagnetic phase, m_0 remains zero, and at high temperatures, $\tau(0) \approx 1/g\sqrt{N}$. For the following analyzation near the critical point in the ferromagnetic phase, we can expand the tanh function in Eq. (5.19) in Section 5.3 of Chapter 5 for small $m_0 > 0$ and introduce the dimensionless scale variable $\epsilon = 1 - \beta/\beta_c < 0$, yielding $m_0 \approx \sqrt{-3\epsilon}$.

Phase thermometric performance at criticality

At the phase transition point, the fluctuations in the sample system lead to the divergence of the second moment of its magnetization $\langle (\sum_i \hat{\sigma}_z^i)^2 \rangle = N/f''(m_0)$, and thus its magnetic susceptibility and heat capacity [83]. Eq. (6.14) shows that the probe decoherence function also depends on the higher moments of the lattice magnetization, and thus exhibits a critical damping at criticality. Therefore, a temperature change can be sensed very precisely around the transition by measuring the probe in the SLD operator basis (6.11). As discussed before, the temperature estimation precision is quantified by the QFI $\mathcal{F}_\beta^Q$. The greater it is at a given temperature, the higher the estimation precision. The QFI can be obtained by inserting the decoherence function (6.14) into the Eq. (6.10)

$$\begin{aligned} \mathcal{F}_\beta^Q = & \frac{J^2 [(1 - m_0^2)^2 f''(m_0) - 2m_0^2]^2}{4 (1 - m_0^2)^4 [f''(m_0)]^4} \frac{t^4/\tau^4(\beta)}{e^{t^2/\tau^2(\beta)} - 1} \\ & + N J^2 \frac{m_0^2}{f''(m_0)} \frac{t^2}{\tau^2(\beta)} e^{-t^2/\tau^2(\beta)}, \end{aligned} \quad (6.15)$$

see Appendix B.2 for details on the derivation. The optimal temperature sensitivity is attained at the time t that maximizes the QFI, i.e., $\mathcal{F}_\beta^{\text{opt}} = \max_t \mathcal{F}_\beta^Q$ at $t_\beta^{\text{opt}} = \arg \max_t \mathcal{F}_\beta^Q$. The following analysis aims to investigate how the optimal quantum QFI of the phase probe scales with temperature near the critical point.

In the paramagnetic phase ($\beta < \beta_c$, $\epsilon > 0$), where $m_0 = 0$ and $f''(0) = 1 - \beta/\beta_c = \epsilon > 0$, the QFI simplifies to

$$\mathcal{F}_{\beta < \beta_c}^Q = \frac{J^2}{4\epsilon^2} S\left(\frac{\tilde{g}^2 t^2}{N\epsilon}\right), \quad S(x) = \frac{x^2}{e^x - 1}. \quad (6.16)$$

Optimal sensitivity is achieved at the time t that maximizes the function S , which yields the numerical values $\mathcal{F}_{\beta \leq \beta_c}^{\text{opt}} \approx 0.162J^2/\epsilon^2$ at $(\tilde{g}t_\beta^{\text{opt}})^2 \approx 1.594N\epsilon$.

In the ferromagnetic phase ($\beta > \beta_c$, $\epsilon < 0$) near the critical temperature, the magnetization is also small, $m_0 \approx \sqrt{-3\epsilon} \ll 1$, and we have $f''(m_0) \approx -2\epsilon$. Hence, to leading order in the temperature deviation ϵ ,

$$\mathcal{F}_{\beta > \beta_c}^Q \approx \frac{J^2}{\epsilon^2} S\left(-\frac{\tilde{g}^2 t^2}{2N\epsilon}\right). \quad (6.17)$$

This analysis reveals consistent scaling behavior for the optimal QFI and the measurement time near the critical point. Specifically, the critical exponents are as follows: the optimal QFI diverges as $\mathcal{F}_\beta^{\text{opt}} \propto \epsilon^{-2}$, and the optimal time to measure the probe scales as $t_\beta^{\text{opt}} \propto |\epsilon|^{1/2}$ as $\epsilon \rightarrow 0$ in the thermodynamic limit.

For finite N , however, an exact computation of the probe decoherence factor $D_t(\beta)$ —without relying on the continuum approximation in Eq. (6.14)—yields a QFI that remains finite across all temperatures.

To better understand the performance of phase probe method, we compare it to an alternative estimation scheme based on equilibrium thermometry, where the focus is on directly probing the local magnetization of a single lattice spin. In this scheme, one measures $\hat{\sigma}_z^i$ at a random lattice site i and estimates the temperature based on statistical analysis of repeated measurements. The temperature sensitivity in this approach is quantified by the FI in Eq. (6.5), which depends on the probabilities of the magnetization outcomes ± 1 . In the thermodynamic limit, the probabilities for these outcomes are given by $p_\pm = (1 \pm m_0)/2$. Consequently, the FI of this measurement, referred to as the local FI, has the following form

$$\mathcal{F}_\beta^{(\text{lc})} = \frac{(\partial_\beta m_0)^2}{1 - m_0^2} \xrightarrow[\epsilon < 0]{\epsilon \rightarrow 0} -\frac{3J^2}{4\epsilon}. \quad (6.18)$$

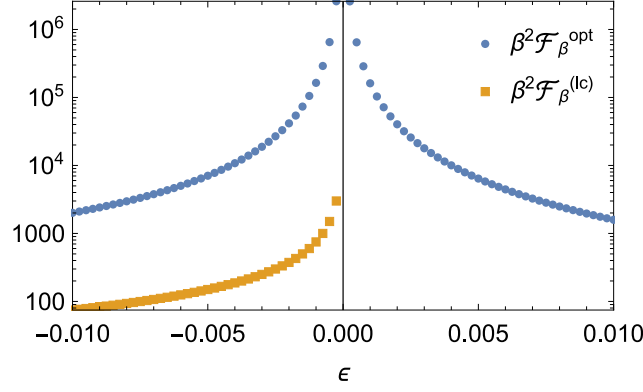


Fig. 6.3.: The optimal QFI of the phase probe (maximized in Eq. (6.15) with respect to time) and local FI (6.18) for direct lattice spin measurement are shown as functions of the relative temperature deviation ϵ from the critical point. We consider the probe-lattice coupling $\hbar g/J = 0.4$ and lattice coupling $J = 1/4$ in arbitrary energy units.

At temperatures above the critical point, the average magnetization vanishes ($m_0 = 0$) leading to a local FI of zero. This indicates that this scheme is ineffective for estimating high temperatures in such sample system. In contrast, just below the critical point, the FI diverges as $|\epsilon|^{-1}$ albeit more slowly than the QFI of the phase probe.

The comparison between the local FI and the optimal phase probe QFI $\mathcal{F}_\beta^{\text{opt}}$ near the phase transition is shown in Fig. 6.3. While both approaches involve measuring a single spin degree of freedom, the phase probe's interaction with the entire lattice allows it to sense correlated thermal fluctuations around the mean magnetization m_0 via the dephasing function (6.14). This results in substantially enhanced temperature sensitivity. In the subsequent sections, we will identify a related but less significant benefit of the phase probe in the context of the Ising lattice.

6.3.2 2D Ising model at zero field

The Curie-Weiss model, as a simplified version of the Ising model, provides an analytical solution for temperature sensitivity and its behavior near the critical point in the thermodynamic limit. We now shift our focus to phase thermometry for a finite ferromagnetic Ising lattice in the absence of an external field, as described by the Hamiltonian (6.12) with $h = 0$ and $J > 0$. Rather than assuming the probe interacts with all sample spins, we consider the case where the probe couples only to a subset of the system consisting of a local n -spin cluster. Additionally, this cluster is treated as the probe for equilibrium thermometry. We could compare the optimal phase probe QFI with the FI of the local cluster probe under these conditions.

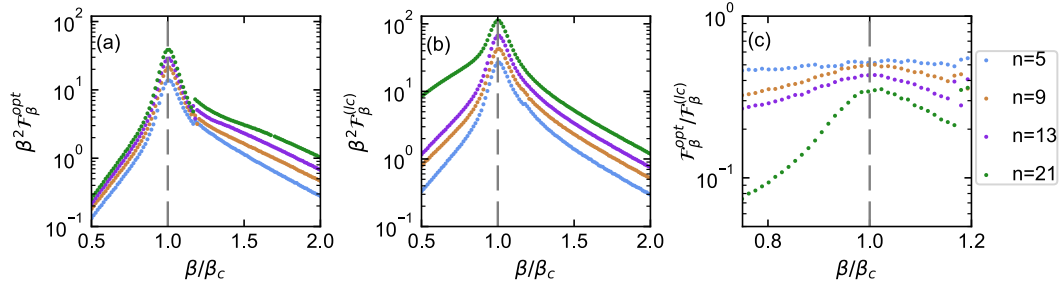


Fig. 6.4.: (a) Optimal QFI of the phase probe (optimized over time) interacting with spin clusters of varying size n in a 20×20 Ising lattice, as a function of inverse temperature relative to the critical point (vertical dashed line). (b) local FI from Eq. (6.20) associated to a direct local measurement of the configuration of the n cluster spins. (c) Ratio of optimal probe QFI and direct local FI close to the critical point. We use the probe-cluster coupling strength $\hbar g/J = 0.4$ and set $J = 1/4$ (in arbitrary reference units).

When the probe is coupled to an n -spin cluster, the resulting decoherence function is expressed as

$$D_t(\beta) = \sum_{\underline{b}'} \left(\sum_{\underline{b}''} p(\underline{b}', \underline{b}'') \right) e^{-it \underline{\Gamma}' \cdot \underline{b}'}. \quad (6.19)$$

The binary array $\underline{b}$ describes the spin configuration of the sample system, where each binary value $b_i \in 0, 1$ represents the spin state at the i -th lattice site; refer to Chapter 5 for further discussion. We partition $\underline{b}$ into $\underline{b} = (\underline{b}', \underline{b}'')$, where $\underline{b}'$ corresponds to the configuration of the n -spin cluster interacting with the probe, and $\underline{b}''$ corresponds to the configuration of the remaining $N - n$ spins. The $1 \times n$ adjacency matrix $\underline{\Gamma}'$ encodes the probe-cluster interaction, which simplifies in the uniform coupling model to $\underline{\Gamma}' = g(1, 1, \dots, 1)$.

To compute Eq. (6.19) and sample the thermally occupied spin configurations, we carried out a Monte Carlo simulation on a lattice of size 20×20 ($N = 400$) with periodic boundary conditions. The probability $p(\underline{b})$ of each spin configuration was simulated by the relative frequency over 1.2×10^7 instances. Using the decoherence function of the phase probe (6.19), we computed the QFI (6.10) at arbitrary times and determined its maximum value $\mathcal{F}_\beta^{\text{opt}} = \max_t \mathcal{F}_\beta^Q(t)$ with respect to time.

Figure 6.4(a) presents simulation results for the maximum QFI in relative units as a function of the inverse temperature β , for various cluster sizes n with which the probe interacts. The cluster sizes n correspond to the total number of spins within a circle centered on a lattice point, with radii $r = 1, \sqrt{2}, 2$, and $\sqrt{5}$ times the lattice spacing, respectively (refer to Fig. 6.7 for the case of $r = 2$). The inverse temperature β is scaled relative to the critical value $\beta_c = \ln(1 + \sqrt{2})/2J$ for the 2D Ising model

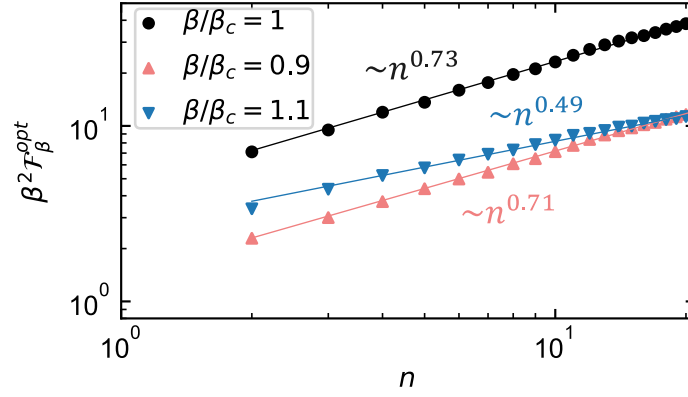


Fig. 6.5.: The scaling of the optimal probe QFI with the size n of the lattice spin cluster, based on the parameters in Fig. 6.4. The rightmost data points represent $n = 21$, with smaller cluster sizes obtained by sequentially removing outer spins. Scaling is compared at the critical point, at 10 % above ($\beta = 0.9\beta_c$), and at 10 % below the critical temperature. Solid lines represent linear fits on a double-logarithmic scale, with slopes of 0.73, 0.71, and 0.49, respectively.

in the thermodynamic limit [168], which aligns with the QFI peaks observed in this 20×20 simulation. The sharp transitions around $\beta \sim 1.2\beta_c$ arise from numerical instabilities in the Monte Carlo algorithm near the phase transition point, where spontaneous symmetry breaking occurs. The phenomenon can be attributed to the fact that, below the phase transition point, a zero-field Ising system with a finite size may still randomly select one of the two opposing ferromagnetic states, a behavior that arises due to its finite nature [11, 83].

Moreover, we observed sublinear scaling of the optimal QFI with cluster size n , following $n^{0.73}$, $n^{0.71}$, and $n^{0.49}$ at criticality and 10 % above and below it, respectively, as shown in Fig. 6.5. This sublinear behavior reflects the strong correlations among the cluster spins. Strong correlations reduce the marginal information gain because they create redundancy: spins share fluctuations and do not contribute independent pieces of information.

In an alternative scheme, temperature estimation relies on direct measurement of the local cluster configuration $\underline{b}'$ in the Ising lattice, thermally distributed with marginal probability $p_n(\underline{b}') = \sum_{\underline{b}''} p(\underline{b}', \underline{b}'')$. The temperature sensitivity of this n -bit measurement is determined by the local FI, expressed as

$$\mathcal{F}_\beta^{(\text{lc})} = \sum_{\underline{b}'} \frac{1}{p_n(\underline{b}')} \left[\frac{\partial p_n(\underline{b}')}{\partial \beta} \right]^2 = \sum_{\underline{b}'} \frac{1}{p_n(\underline{b}')} \left[\sum_{\underline{b}''} E(\underline{b}) p(\underline{b}) \right]^2 - \langle \hat{H}_s \rangle^2. \quad (6.20)$$

We sampled results from our Monte Carlo simulation for moderate cluster sizes $n \lesssim 30$. Fig. 6.4(b) shows these results for the same temperature range and

cluster sizes as before. A peak is again observed at the phase transition, with a less steep decay into the paramagnetic phase. As expected, the local FI for this n -bit measurement exceeds the QFI of the phase probe, but near the critical point, their ratio increases only sublinearly with n , as shown in Fig. 6.4(c). Deep in the ferromagnetic phase, the strong alignment (correlation) of lattice spins allows the phase probe to capture nearly all temperature information within the cluster. In contrast, in the paramagnetic phase, broken correlations lead to a larger disparity between the two measurements.

The results presented above are exact but obtained numerically. Next, we introduce approximate analytical models for sensitivity based on the widely used mean-field theory (MFT) [11] and a high-temperature expansion (HTE) of the Gibbs state [196]. These models provide accurate predictions for temperatures deep in the ferromagnetic and paramagnetic phases, respectively, but fail to capture the critical behavior observed in our exact numerical simulations.

Mean-field approximation In this theory, thermal fluctuations are assumed to be relatively small and can be partially neglected [11]. Under this assumption, the spin operator $\hat{\sigma}_z^i$ is expressed as the sum of its mean value and a fluctuation term. Thermal fluctuations, represented by the second-order term, are disregarded. As a result, the system Hamiltonian (6.12) with $h = 0$ simplifies to a decoupled form

$$\hat{H}_s^{(\text{MFT})} \approx -J \sum_{\langle i,j \rangle} m_0 (\hat{\sigma}_z^i + \hat{\sigma}_z^j - m_0) = \frac{NJqm_0^2}{2} - Jqm_0 \sum_{i=1}^N \hat{\sigma}_z^i, \quad (6.21)$$

where m_0 is the mean value and q is the number of nearest neighbors per spin ($q = 4$ here). The Hamiltonian describes spins that no longer interact directly with each other but instead feel an effective mean field $h_{\text{MFT}} = Jqm_0$, which simply reflects the average alignment of all their neighbors. In thermal equilibrium, the thermal occupation probability is given by

$$p(b) = \frac{e^{-2Jqm_0\beta \sum_i b_i}}{(1 + e^{-2Jqm_0\beta})^N}. \quad (6.22)$$

The mean magnetization per spin is given by the self-consistency equation $m_0 = \tanh[Jqm_0\beta]$. This approach also predicts a critical temperature of $J\beta_c = 1/q = 0.25$, which is higher than the exact value $J\beta_c = 0.44$ obtained from our simulation.

Using the approximation, the decoherence function (6.19) of the phase probe can be calculated

$$D_t(\beta) = \left[1 - \frac{1 - e^{-igt}}{1 + e^{2Jqm_0\beta}} \right]^n \approx e^{(1 - \cos gt - i \sin gt)np_1}, \quad (6.23)$$

with the single-spin excitation probability $p_1 = 1/(1 + e^{2Jqm_0\beta})$. The approximation holds for cluster sizes $n > 10$ in the ferromagnetic phase. From this, we arrive at an analytic expression for the QFI,

$$\mathcal{F}_\beta^{(\text{MFT})} = \frac{J^2 q^2 n^2 (m_0 + \beta \partial_\beta m_0)^2}{4 \cosh^4(Jqm_0\beta)} e^{-2\gamma(1-p_1)} \left[\sin^2(gt) + \frac{(1 - \cos gt)^2}{1 - e^{-2\gamma(1-p_1)}} \right]. \quad (6.24)$$

The derivative $\partial_\beta m_0$ diverges at the (overestimated) critical temperature, leading to a divergence in the approximated QFI. Beyond this temperature, both the mean-field magnetization and the approximated QFI drop to zero.

In Fig.6.6(a)-(d), the MFT approximation for the QFI (black solid line) is compared with exact Monte Carlo simulation results for four different cluster sizes. One can see that Eq. (6.24) accurately predicts temperature sensitivity for subcritical temperatures but fails at and above the phase transition, as magnetization vanishes beyond the critical point. To analyze the QFI in the paramagnetic phase, we employ a high-temperature expansion [196].

High-temperature expansion

Unlike in MFT, where thermal fluctuations are neglected, they dominate at high temperatures in the paramagnetic phase, causing the lattice spins to orient randomly. To analyze the properties of such systems, it is common to expand the relevant physical quantities in terms of the inverse temperature, $\beta \ll 1/J$. Here, we expand the thermal occupation probability and partition function up to second order in $\tanh \beta J$, see derivation details in Appendix B.3. Again, we obtain the decoherence function (6.19) for the phase probe, having the form

$$D_t(\beta) = \cos^n(gt) \left\{ 1 - \tanh(\beta J) \tan^2(gt) \times \left[K_{12} - \tanh(\beta J) (K_{22} + K_{23} - \tan^2(gt) K_{24}) \right] \right\}, \quad (6.25)$$

where K_{12} denote the number of intracluster pair bonds, K_{22} counts the number of pair bond doublets with two spins inside and one mutual spin outside the cluster, K_{23} counts doublets of intra-cluster pair bonds with one mutual spin, and $K_{24} =$

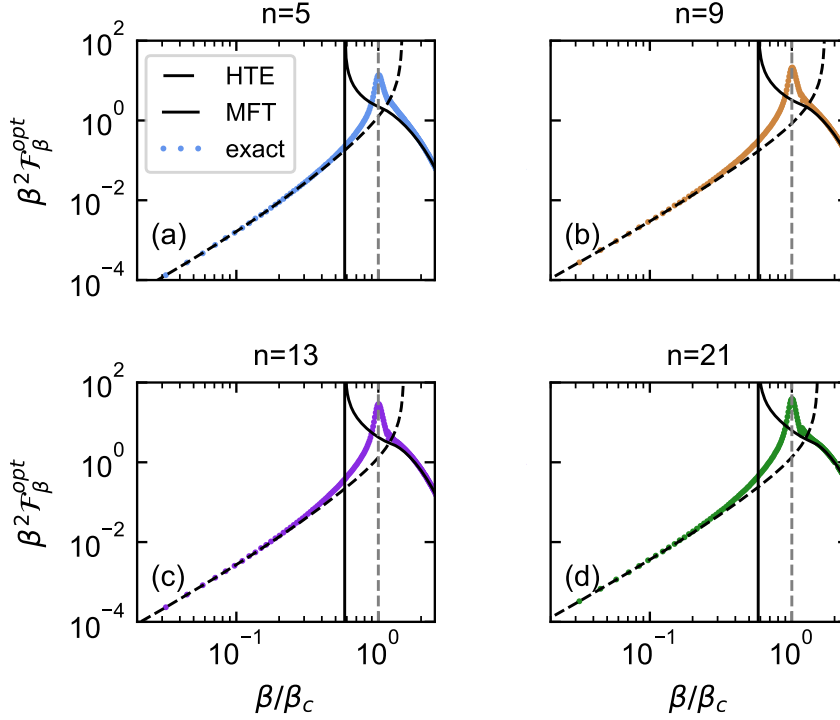


Fig. 6.6.: Optimal QFI of the phase probe as a function of inverse temperature relative to the critical point (vertical dashed line), extending the results in Fig. 6.4(a). We separate the four cases corresponding to different cluster sizes n into different diagrams (a)-(d), comparing the exact Monte-Carlo simulation data to the approximate predictions of the mean-field theory (solid lines) and the high-temperature expansion (dashed).

$K_{12}(K_{12} - 1)/2 - K_{23}$ counts doublets of intra-cluster pair bonds with no mutual spin, as illustrated in Fig. 6.7. Furthermore, the QFI of the phase probe is given by

$$\begin{aligned} \mathcal{F}_\beta^{(\text{HTE})} &= \frac{J^2 \Lambda^2(t) \tan^4(gt) \cos^{2n}(gt)}{1 - [J\beta \Lambda(t) \tan^2(gt) - 1]^2 \cos^{2n}(gt)}, \\ \Lambda(t) &= K_{12} + 2J\beta [K_{22} + K_{23} - K_{24} \tan^2(gt)]. \end{aligned} \quad (6.26)$$

To derive this compact expression, we approximate $\tanh(J\beta) \approx J\beta$. This shows that the phase probe extracts temperature information through correlations involving up to four lattice spins. In Fig. 6.6, the dashed lines represent the high-temperature expansion (HTE) (6.26) of the QFI, which aligns with the exact results for $\beta \ll \beta_c$ in the paramagnetic phase.

From the above observations, we conclude that neither analytical approximation of the QFI accurately captures the true critical behavior or the peak value of the phase probe's temperature sensitivity. The MFT fails due to the emergence of strong long-range thermal fluctuations, while the HTE fails because of the development

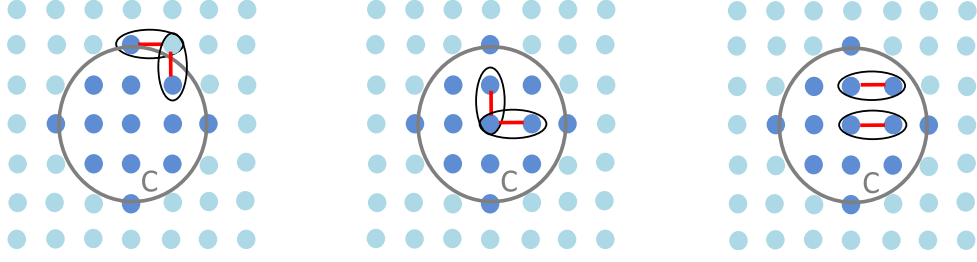


Fig. 6.7.: Construction of pair bond doublets in the Ising lattice. The cluster C of spins interacting with the probe (dark blue) are contained in a circle. Exemplary red lines symbolize pair bonds due to the Ising interaction between any two neighbouring lattice spins. From left to right, each marked doublet of pair bonds represents one possible contribution that is counted by the numbers K_{22} , K_{23} , K_{24} , respectively. In the depicted configuration there are $n = 13$ cluster spins, $K_{12} = 16$ intra-cluster bonds, and one obtains $(K_{22}, K_{23}, K_{24}) = (8, 34, 86)$.

of long-range multi-spin correlations in the critical Ising lattice. Furthermore, the finite peak value of the QFI cannot be captured by continuous models describing the phase transition in the thermodynamic limit, highlighting the need for numerical simulations.

6.4 Conclusion

In this chapter, we formulated the framework for phase thermometry, which leverages the measurement of the phase of a probe interacting with a sample system to estimate its temperature. Using this framework, we analyzed the thermometric performance in the 2D Ising lattice model, focusing particularly on the system's behavior near its phase transition point, as quantified by the QFI. We began with the Curie-Weiss model as an instructive example, where the phase probe uniformly couples to all spins in the system. In this scenario, we derived an analytical expression for the QFI in the thermodynamic limit. Our analysis revealed that the temperature estimation precision achieved using a single phase probe diverges at the critical point and significantly surpasses that of direct energy measurements on a single spin within the sample. Moreover, we demonstrated that direct energy measurement becomes inefficient in the high-temperature regime.

For the 2D Ising model, we numerically calculated the exact QFI. Instead of coupling the phase probe to all spins, we examined its interaction with local spin clusters of varying sizes. For comparison, we also considered direct measurements of local clusters to estimate the temperature. The results showed that as cluster size increases, the direct measurement scheme outperforms the single-phase-probe approach. However, in both methods, temperature sensitivity peaks at the critical point.

Additionally, we employed the mean-field approximation and high-temperature expansion to approximate the QFI in the 2D Ising model. These methods were shown to yield accurate results deep within the ferromagnetic and paramagnetic phases, respectively, neither accurately described the critical behavior or the peak value of the phase probe's temperature sensitivity. Therefore, it would be valuable to develop an analytical method that goes beyond these approximations and accurately captures the QFI at criticality.

Future research could involve enhancing phase thermometry by optimizing time-dependent couplings and investigating the use of phase probes for temperature estimation in finite Heisenberg-type spin systems. On the experimental side, promising routes include the use of trapped ions and Rydberg atom arrays, where spin–spin interactions can be engineered to emulate Ising or Heisenberg models with tunable parameters, and where coherent phase control of probe qubits is already well established. Similarly, superconducting qubit platforms and solid-state spin defects, such as nitrogen-vacancy centers in diamond, offer natural candidates for implementing local probe–cluster couplings and phase-sensitive readout. Ultracold atomic gases in optical lattices also provide a versatile setting in which both global and local probe couplings can be realized and controlled with high precision. Demonstrating phase-based thermometry in these platforms would not only validate the theoretical framework presented here but also open new opportunities for noninvasive temperature sensing in strongly correlated quantum systems.

Conclusion

In this thesis, we aimed to investigate non-Markovian behaviors in a range of physical systems by integrating established methods. Furthermore, we explored the potential of these dynamic models to improve the precision of temperature measurements and aid in quantum memory detection.

To summarize, we have first examined the dynamics of few-level giant atoms coupled to SAWs, focusing on two-level and Λ -type three-level systems in Chapter 3. We began by deriving the exact solution for the non-Markovian dynamics of two-level giant atoms at zero temperature, using it as a benchmark to evaluate conventional methods for modeling open quantum systems. By comparing these methods to the exact solution, we assessed their ability to capture non-Markovian effects arising from time-delayed self-interactions, as opposed to those resulting from strong coupling or structured environments. From this comparison, we identified the most effective method and applied it to study the finite-temperature dynamics of giant atoms, revealing that non-Markovian effects remain robust against thermal fluctuations. Additionally, we extended our analysis to three-level giant atoms, with a particular focus on spontaneous emission. In this case, we demonstrated that the memory effect in three-level giant atoms can be utilized to control spontaneous emission through the interference of multiple emission pathways.

Building on our solution of non-Markovian dynamics in two- and three-level giant atom systems, we applied these results to quantum memory detection in Chapter 4. We proposed a novel approach based on the classical memory concept, reformulating it as a convex optimization problem. Moreover, we introduced a metric to quantify the deviation between the quantum memory required for a process and its classical memory counterpart. We showed that this approach can be extended to high-dimensional systems beyond qubits or two-level atom systems. In this study, we demonstrated the detection of quantum memory within the non-Markovian dynamics of two- and three-level giant atoms, finding that neither the spontaneous emission from two-level nor three-level systems at zero temperature could be described by classical memory.

In Chapter 5, we introduced a spin-lattice model to study non-Markovian pure dephasing in central spins embedded in finite spin baths. Using this model, we

initially examined the dynamics of a single spin interacting with two types of spin baths: uncorrelated and correlated. Our analysis revealed that the single spin could exhibit non-Markovian behavior in both cases. Specifically, for the correlated thermal bath, we showed that the initial coherence decays more rapidly at lower temperatures. The model was further applied to study the entanglement dynamics of two spins in the presence of a spin bath through two case studies. In the first case, we considered a 2D spin lattice with entangled spins interacting with a time-evolving environment. We analyzed both nearly Markovian and non-Markovian dephasing effects. Our observed that non-Markovian dephasing accelerated the loss of entanglement. However, by implementing a random reset mechanism, we were able to preserve the entanglement in a steady state. Additionally, we introduced a weak three-body phase interaction to effectively reduce the impact of dephasing. In the second case, we examined two nuclear spins in an organic molecule interacting with a thermal spin bath at finite temperatures, where the organic molecule was subjected to a magnetic field. We investigated the effects of bath correlations and thermal fluctuations on the decay of two-spin entanglement. At higher magnetic fields, our results showed both correlated and uncorrelated baths exhibited similar entanglement decay behaviors across different temperatures. However, when the magnetic field weakened and coupling effects became more dominant, the correlated bath caused a significantly faster initial decay at low temperatures.

In Chapter 6, we applied the spin-lattice model to study non-Markovian phase thermometry, a non-invasive technique where a quantum spin probe interacts with a system, such as a two-dimensional Ising spin lattice, to estimate its temperature through dephasing dynamics. We analyzed the thermometric performance near the phase transition, using the QFI to measure precision. For the Curie-Weiss model, we derived an analytical expression for QFI in the thermodynamic limit and found that temperature estimation improves significantly at the critical point compared to direct energy measurements, especially at lower temperatures. In the 2D Ising model, we numerically calculated the exact QFI and compared local spin cluster measurements to single-phase-probe measurements, showing that larger clusters outperform the phase probe as cluster size increases. Temperature sensitivity peaked at the critical point in both methods. We also used mean-field and high-temperature approximations, which accurately described the system away from the critical point but missed the peak sensitivity at criticality.

Each chapter discussed the open problems. We also hope that the findings and approaches presented in this thesis will contribute to future research in the field.

List of Publications

- [A] M. Yu, H. C. Nguyen, V. Link, W. Strunz, and S. Nimmrichter
Giant atom dynamics at finite temperature
in preparation.
- [B] M. Yu, T. Ohst, H. C. Nguyen, and S. Nimmrichter
Quantum memory in spontaneous emission processes
arXiv:2504.08605.
- [C] M. Yu, O. Gühne, and S. Nimmrichter
Exact entanglement dynamics of two spins in finite baths
Phys. Rev. A **108**, 022415 (2023).
- [D] M. Yu, H. C. Nguyen, and S. Nimmrichter
Criticality-enhanced precision in phase thermometry
Phys. Rev. Research **6**, 043094 (2024).

Bibliography

- [1] M. H. Abobeih, J. Cramer, M. A. Bakker, et al., “One-second coherence for a single electron spin coupled to a multi-qubit nuclear-spin environment”, *Nat. Commun.* **9**, 2552 (2018) (cit. on pp. 2, 52, 77, 81).
- [2] D. Ahn and B. Park, *Non-markovian noise sources for quantum error mitigation*, 2023 (cit. on p. 40).
- [3] L. Anderegg, L. W. Cheuk, Y. Bao, et al., “An optical tweezer array of ultracold molecules”, *Science* **365**:6458, 1156–1158 (2019) (cit. on pp. 61, 69).
- [4] G. Andersson, B. Suri, L. Guo, T. Aref, and P. Delsing, “Non-exponential decay of a giant artificial atom”, *Nature Physics* **15**:11, 1123–1127 (2019) (cit. on pp. 2, 19–22, 31).
- [5] T. Aushev, A. N. Kozhinov, and Y. O. Tsybin, “Least-squares fitting of time-domain signals for fourier transform mass spectrometry”, *Journal of the American Society for Mass Spectrometry* **25**:7, PMID: 24789745, 1263–1273 (2014) (cit. on p. 29).
- [6] A. Auza, A. Youssry, G. Paz-Silva, and A. Peruzzo, *Quantum control in the presence of strongly coupled non-markovian noise*, 2024 (cit. on p. 2).
- [7] C. Bäcker, K. Beyer, and W. T. Strunz, “Local disclosure of quantum memory in non-markovian dynamics”, *Phys. Rev. Lett.* **132**, 060402 (2024) (cit. on pp. 2, 40, 41, 45).
- [8] D. Barredo, V. Lienhard, S. de Léséleuc, T. Lahaye, and A. rowaey, “Synthetic three-dimensional atomic structures assembled atom by atom”, *Nature* **561**, 79 (2018) (cit. on pp. 2, 52, 61, 77, 81).
- [9] D. Basilewitsch, F. Cosco, N. Lo Gullo, et al., “Reservoir engineering using quantum optimal control for qubit reset”, *New Journal of Physics* **21**:9, 093054 (2019) (cit. on p. 51).
- [10] T. Baumgratz, M. Cramer, and M. B. Plenio, “Quantifying coherence”, *Phys. Rev. Lett.* **113**, 140401 (2014) (cit. on p. 2).
- [11] A. J. Beekman, L. Rademaker, and J. van Wezel, “An introduction to spontaneous symmetry breaking”, *SciPost Phys. Lect. Notes*, 11 (2019) (cit. on pp. 87, 88).
- [12] N. K. Bernardes, A. Cuevas, A. Orioux, et al., “Experimental observation of weak non-markovianity”, *Scientific reports* **5**:1, 17520 (2015) (cit. on p. 2).
- [13] H. Bernien, S. Schwartz, A. Keesling, et al., “Probing many-body dynamics on a 51-atom quantum simulator”, *Nature* **551**, 579 (2017) (cit. on pp. 2, 52, 61, 77, 81).

- [14] D. Biswas, S. Utagi, and P. Mandayam, *Noise-adapted quantum error correction for non-markovian noise*, 2024 (cit. on p. 1).
- [15] A. Blais, A. L. Grimsmo, S. M. Girvin, and A. Wallraff, “Circuit quantum electrodynamics”, *Rev. Mod. Phys.* **93**, 025005 (2021) (cit. on p. 20).
- [16] I. Bloch, J. Dalibard, and S. Nascimbene, “Programmable quantum simulations of spin systems with trapped ions”, *Nature Physics* **8**, 267 (2012) (cit. on pp. 51, 67).
- [17] Q. Bouton, J. Nettersheim, D. Adam, et al., “Single-atom quantum probes for ultracold gases boosted by nonequilibrium spin dynamics”, *Phys. Rev. X* **10**, 011018 (2020) (cit. on p. 77).
- [18] S. Boyd and L. Vandenberghe, *Convex optimization*, Berichte über verteilte messsysteme Teil 1 (Cambridge University Press, 2004) (cit. on p. 118).
- [19] S. L. Braunstein and C. M. Caves, “Statistical distance and the geometry of quantum states”, *Phys. Rev. Lett.* **72**, 3439–3443 (1994) (cit. on p. 79).
- [20] H. Breuer and F. Petruccione, *The theory of open quantum systems* (Oxford University Press, 2002) (cit. on pp. 1, 8, 9, 11, 12, 25, 26).
- [21] H.-P. Breuer, B. Kappler, and F. Petruccione, “Stochastic wave-function method for non-markovian quantum master equations”, *Phys. Rev. A* **59**, 1633–1643 (1999) (cit. on pp. 2, 12).
- [22] H.-P. Breuer, E.-M. Laine, and J. Piilo, “Measure for the degree of non-markovian behavior of quantum processes in open systems”, *Phys. Rev. Lett.* **103**, 210401 (2009) (cit. on pp. 1, 8, 39).
- [23] H.-P. Breuer, E.-M. Laine, J. Piilo, and B. Vacchini, “Colloquium: non-markovian dynamics in open quantum systems”, *Rev. Mod. Phys.* **88**, 021002 (2016) (cit. on pp. 8, 9, 39, 62).
- [24] A. Browaeys, D. Barredo, and T. Lahaye, “Experimental investigations of dipole–dipole interactions between a few Rydberg atoms”, *J. Phys. B* **49**:15, 152001 (2016) (cit. on pp. 2, 52, 61, 77, 81).
- [25] M. Bruderer and D. Jaksch, “Probing bec phase fluctuations with atomic quantum dots”, *New Journal of Physics* **8**:6, 87 (2006) (cit. on p. 77).
- [26] G. Burkard, T. D. Ladd, A. Pan, J. M. Nichol, and J. R. Petta, “Semiconductor spin qubits”, *Rev. Mod. Phys.* **95**, 025003 (2023) (cit. on p. 51).
- [27] J. Calsamiglia, L. Hartmann, W. Dür, and H.-J. Briegel, “Spin gases: quantum entanglement driven by classical kinematics”, *Phys. Rev. Lett.* **95**, 180502 (2005) (cit. on pp. 52, 62).
- [28] S. Campbell, M. G. Genoni, and S. Deffner, “Precision thermometry and the quantum speed limit”, *Quantum Science and Technology* **3**:2, 025002 (2018) (cit. on p. 77).
- [29] C. Cao and X. Wang, “Noise-assisted quantum autoencoder”, *Phys. Rev. Appl.* **15**, 054012 (2021) (cit. on p. 1).

- [30] F. Caruso, V. Giovannetti, C. Lupo, and S. Mancini, “Quantum channels and memory effects”, *Rev. Mod. Phys.* **86**, 1203–1259 (2014) (cit. on p. 39).
- [31] D. Cavalcanti and P. Skrzypczyk, “Quantum steering: a review with focus on semidefinite programming”, *Reports on Progress in Physics* **80**:2, 024001 (2016) (cit. on p. 43).
- [32] V. Cavina, L. Mancino, A. De Pasquale, et al., “Bridging thermodynamics and metrology in nonequilibrium quantum thermometry”, *Phys. Rev. A* **98**, 050101 (2018) (cit. on p. 77).
- [33] M. Cetina, M. Jag, R. S. Lous, et al., “Decoherence of impurities in a fermi sea of ultracold atoms”, *Phys. Rev. Lett.* **115**, 135302 (2015) (cit. on pp. 77, 81).
- [34] M. Cetina, M. Jag, R. S. Lous, et al., “Ultrafast many-body interferometry of impurities coupled to a fermi sea”, *Science* **354**:6308, 96–99 (2016) (cit. on pp. 77, 81).
- [35] S. Chaturvedi and F. Shibata, “Time-convolutionless projection operator formalism for elimination of fast variables. applications to brownian motion”, *Zeitschrift für Physik B Condensed Matter* **35**:3, 297–308 (1979) (cit. on pp. 2, 11).
- [36] Z.-H. Chen, Y. Wang, X. Zheng, R.-X. Xu, and Y. Yan, “Universal time-domain prony fitting decomposition for optimized hierarchical quantum master equations”, *The Journal of Chemical Physics* **156**:22, 221102 (2022) (cit. on p. 29).
- [37] H.-B. Chen, N. Lambert, Y.-C. Cheng, Y.-N. Chen, and F. Nori, “Using non-markovian measures to evaluate quantum master equations for photosynthesis”, *Scientific reports* **5**:1, 12753 (2015) (cit. on p. 2).
- [38] A. W. Chin, J. Prior, R. Rosenbach, et al., “The role of non-equilibrium vibrational structures in electronic coherence and recoherence in pigment–protein complexes”, *Nature Physics* **9**:2, 113–118 (2013) (cit. on p. 2).
- [39] G. Chiribella, G. M. D’Ariano, and P. Perinotti, “Theoretical framework for quantum networks”, *Phys. Rev. A* **80**, 022339 (2009) (cit. on pp. 43, 125).
- [40] E. Chitambar and G. Gour, “Quantum resource theories”, *Rev. Mod. Phys.* **91**, 025001 (2019) (cit. on p. 42).
- [41] A. Chiuri, C. Greganti, L. Mazzola, M. Paternostro, and P. Mataloni, “Linear optics simulation of quantum non-markovian dynamics”, *Scientific reports* **2**:1, 968 (2012) (cit. on p. 2).
- [42] M.-D. Choi, “Positive linear maps on c^* -algebras”, *Canadian Journal of Mathematics* **24**:3, 520–529 (1972) (cit. on p. 43).
- [43] I. L. Chuang, R. Laflamme, P. W. Shor, and W. H. Zurek, “Quantum computers, factoring, and decoherence”, *Science* **270**:5242, 1633–1635 (1995) (cit. on p. 61).
- [44] F. Ciccarello, G. M. Palma, and V. Giovannetti, “Collision-model-based approach to non-markovian quantum dynamics”, *Phys. Rev. A* **87**, 040103 (2013) (cit. on p. 2).

- [45] F. Ciccarello, S. Lorenzo, V. Giovannetti, and G. M. Palma, “Quantum collision models: open system dynamics from repeated interactions”, *Physics Reports* **954**, Quantum collision models: Open system dynamics from repeated interactions, 1–70 (2022) (cit. on pp. 2, 65).
- [46] F. Ciccarello, S. Lorenzo, V. Giovannetti, and G. M. Palma, “Quantum collision models: open system dynamics from repeated interactions”, *Phys. Rep.* **954**, 1–70 (2022) (cit. on p. 64).
- [47] L. A. Correa, M. Mehboudi, G. Adesso, and A. Sanpera, “Individual quantum probes for optimal thermometry”, *Phys. Rev. Lett.* **114**, 220405 (2015) (cit. on pp. 77, 82).
- [48] L. A. Correa, M. Perarnau-Llobet, K. V. Hovhannisyan, et al., “Enhancement of low-temperature thermometry by strong coupling”, *Phys. Rev. A* **96**, 062103 (2017) (cit. on p. 82).
- [49] H. Cramér, *Mathematical methods of statistics (pms-9)* (Princeton University Press, 1999) (cit. on p. 79).
- [50] L. Cui, H.-D. Zhang, X. Zheng, R.-X. Xu, and Y. Yan, “Highly efficient and accurate sum-over-poles expansion of fermi and bose functions at near zero temperatures: fano spectrum decomposition scheme”, *The Journal of Chemical Physics* **151**:2, 024110 (2019) (cit. on p. 29).
- [51] G. M. D’Ariano, P. Perinotti, and M. Sedlák, “Extremal quantum protocols”, *Journal of Mathematical Physics* **52**:8, 082202 (2011) (cit. on p. 123).
- [52] E. B. Davies and J. T. Lewis, “An operational approach to quantum probability”, *Communications in Mathematical Physics* **17**:3, 239–260 (1970) (cit. on p. 41).
- [53] A. De Pasquale, D. Rossini, R. Fazio, and V. Giovannetti, “Local quantum thermal susceptibility”, *Nature communications* **7**:1, 12782 (2016) (cit. on pp. 77, 82).
- [54] A. De Pasquale and T. M. Stace, “Quantum thermometry”, *Thermodynamics in the Quantum Regime: Fundamental Aspects and New Directions*, 503–527 (2018) (cit. on p. 76).
- [55] A. De Pasquale and T. M. Stace, “Quantum thermometry”, in *Thermodynamics in the quantum regime: fundamental aspects and new directions*, edited by F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso (Springer International Publishing, Cham, 2018), pp. 503–527 (cit. on pp. 2, 76, 77).
- [56] C. L. Degen, F. Reinhard, and P. Cappellaro, “Quantum sensing”, *Rev. Mod. Phys.* **89**, 035002 (2017) (cit. on p. 1).
- [57] M. J. Degen, S. J. H. Loenen, H. P. Bartling, et al., “Entanglement of dark electron-nuclear spin defects in diamond”, *Nat. Commun.* **12**, 3470 (2021) (cit. on pp. 2, 52, 77, 81).
- [58] D. DeMille, “Quantum computation with trapped polar molecules”, *Phys. Rev. Lett.* **88**, 067901 (2002) (cit. on p. 61).

- [59] R. H. Dicke, “Coherence in spontaneous radiation processes”, *Phys. Rev.* **93**, 99–110 (1954) (cit. on p. 38).
- [60] H. Ding, N. H. Amini, J. E. Gough, and G. Zhang, *On the non-markovian quantum control dynamics*, 2024 (cit. on p. 2).
- [61] J.-J. Ding, R.-X. Xu, and Y. Yan, “Optimizing hierarchical equations of motion for quantum dissipation and quantifying quantum bath effects on quantum transfer mechanisms”, *The Journal of Chemical Physics* **136**:22, 224103 (2012) (cit. on p. 29).
- [62] L. Diósi, N. Gisin, and W. T. Strunz, “Non-markovian quantum state diffusion”, *Phys. Rev. A* **58**, 1699–1712 (1998) (cit. on pp. 2, 15).
- [63] L. Diósi and W. T. Strunz, “The non-markovian stochastic schrödinger equation for open systems”, *Physics Letters A* **235**:6, 569–573 (1997) (cit. on p. 15).
- [64] I. B. Djordjevic, *Quantum communication, quantum networks, and quantum sensing* (Academic Press, 2022) (cit. on p. 1).
- [65] V. V. Dobrovitski, A. E. Feiguin, D. D. Awschalom, and R. Hanson, “Decoherence dynamics of a single spin versus spin ensemble”, *Phys. Rev. B* **77**, 245212 (2008) (cit. on p. 52).
- [66] L. Du, L. Guo, and Y. Li, “Complex decoherence-free interactions between giant atoms”, *Phys. Rev. A* **107**, 023705 (2023) (cit. on p. 19).
- [67] L. Du, Y. Zhang, J.-H. Wu, A. F. Kockum, and Y. Li, “Giant atoms in a synthetic frequency dimension”, *Phys. Rev. Lett.* **128**, 223602 (2022) (cit. on p. 19).
- [68] L.-M. Duan, M. D. Lukin, J. I. Cirac, and P. Zoller, “Long-distance quantum communication with atomic ensembles and linear optics”, *Nature* **414**:6862, 413–418 (2001) (cit. on p. 1).
- [69] R. Dubertrand, A. Cesa, and J. Martin, “Analytical results for the quantum non-markovianity of spin ensembles undergoing pure dephasing dynamics”, *Phys. Rev. A* **97**, 062126 (2018) (cit. on p. 52).
- [70] M. J. Duer, *Solid state nmr spectroscopy: principles and applications* (John Wiley & Sons, 2008) (cit. on p. 52).
- [71] M. J. Duer, “The basics of solid-state NMR”, in *Solid-state NMR spectroscopy principles and applications* (John Wiley & Sons, Ltd, 2001) Chap. 1, pp. 1–72 (cit. on p. 69).
- [72] J. Eckhoff, *Helly, Radon, and Carathéodory type theorems* (Elsevier, 1993), pp. 389–448 (cit. on p. 123).
- [73] M. Esposito, M. A. Ochoa, and M. Galperin, “Quantum thermodynamics: a nonequilibrium green’s function approach”, *Phys. Rev. Lett.* **114**, 080602 (2015) (cit. on p. 2).
- [74] G. Ferrari, “Collisional relaxation in a fermionic gas”, *Phys. Rev. A* **59**, R4125–R4128 (1999) (cit. on p. 77).

- [75] D. A. S. Fraser, “On local unbiased estimation”, *Journal of the Royal Statistical Society: Series B (Methodological)* **26**:1, 46–51 (1964) (cit. on p. 79).
- [76] S. Friedli and Y. Velenik, *Statistical mechanics of lattice systems: a concrete mathematical introduction* (Cambridge University Press, 2017) (cit. on pp. 57, 58, 77, 81, 82).
- [77] A. Frisk Kockum, P. Delsing, and G. Johansson, “Designing frequency-dependent relaxation rates and lamb shifts for a giant artificial atom”, *Phys. Rev. A* **90**, 013837 (2014) (cit. on p. 19).
- [78] F. M. Gambetta, W. Li, F. Schmidt-Kaler, and I. Lesanovsky, “Engineering nonbinary Rydberg interactions via phonons in an optical lattice”, *Phys. Rev. Lett.* **124**, 043402 (2020) (cit. on p. 67).
- [79] F. M. Gambetta, C. Zhang, M. Hennrich, I. Lesanovsky, and W. Li, “Long-range multibody interactions and three-body antiblockade in a trapped Rydberg ion chain”, *Phys. Rev. Lett.* **125**, 133602 (2020) (cit. on pp. 51, 67).
- [80] A. L. Gaunt, T. F. Schmidutz, I. Gotlibovych, R. P. Smith, and Z. Hadzibabic, “Bose-einstein condensation of atoms in a uniform potential”, *Phys. Rev. Lett.* **110**, 200406 (2013) (cit. on p. 76).
- [81] C. Giarmatzi and F. Costa, “Witnessing quantum memory in non-Markovian processes”, *Quantum* **5**, 440 (2021) (cit. on pp. 2, 40).
- [82] N. Gisin and R. Thew, “Quantum communication”, *Nature photonics* **1**:3, 165–171 (2007) (cit. on p. 1).
- [83] N. Goldenfeld, *Lectures on phase transitions and the renormalization group* (CRC Press, 2018) (cit. on pp. 83, 87).
- [84] T. Graham, Y. Song, J. Scott, et al., “Multi-qubit entanglement and algorithms on a neutral-atom quantum computer”, *Nature* **604**:7906, 457–462 (2022) (cit. on p. 61).
- [85] S. Groeblacher, A. Trubarov, N. Prigge, et al., “Observation of non-markovian micromechanical brownian motion”, *Nature communications* **6**:1, 7606 (2015) (cit. on p. 2).
- [86] C. Gross and I. Bloch, “Quantum simulations with ultracold atoms in optical lattices”, *Science* **357**:6355, 995–1001 (2017) (cit. on pp. 2, 52, 61, 77, 81).
- [87] C. Gross and I. Bloch, “Quantum simulations with ultracold atoms in optical lattices”, *Science* **357**:6355, 995–1001 (2017) (cit. on p. 61).
- [88] N. Grzesiak, R. Blümel, K. Wright, et al., “Efficient arbitrary simultaneously entangling gates on a trapped-ion quantum computer”, *Nature communications* **11**:1, 2963 (2020) (cit. on p. 61).
- [89] M. Gulka, D. Wirtitsch, V. Ivády, et al., “Room-temperature control and electrical readout of individual nitrogen-vacancy nuclear spins”, *Nat. Commun.* **12**, 4421 (2021) (cit. on pp. 2, 52, 77, 81).

- [90] L. Guo, A. Grimsmo, A. F. Kockum, M. Pletyukhov, and G. Johansson, “Giant acoustic atom: a single quantum system with a deterministic time delay”, *Phys. Rev. A* **95**, 053821 (2017) (cit. on pp. 20, 31).
- [91] L. Guo, A. F. Kockum, F. Marquardt, and G. Johansson, “Oscillating bound states for a giant atom”, *Phys. Rev. Res.* **2**, 043014 (2020) (cit. on p. 19).
- [92] S. Guo, Y. Wang, T. Purdy, and J. Taylor, “Beyond spontaneous emission: giant atom bounded in the continuum”, *Phys. Rev. A* **102**, 033706 (2020) (cit. on p. 19).
- [93] L. Gurvits, “Classical complexity and quantum entanglement”, *Journal of Computer and System Sciences* **69**:3, Special Issue on STOC 2003, 448–484 (2004) (cit. on p. 127).
- [94] M. V. Gustafsson, T. Aref, A. F. Kockum, et al., “Propagating phonons coupled to an artificial atom”, *Science* **346**:6206, 207–211 (2014) (cit. on pp. 2, 21, 22, 51).
- [95] M. V. Gustafsson, T. Aref, A. F. Kockum, et al., “Propagating phonons coupled to an artificial atom”, *Science* **346**:6206, 207–211 (2014) (cit. on p. 21).
- [96] D. Hangleiter, M. T. Mitchison, T. H. Johnson, et al., “Nondestructive selective probing of phononic excitations in a cold bose gas using impurities”, *Phys. Rev. A* **91**, 013611 (2015) (cit. on pp. 77, 82).
- [97] R. Hanson, V. Dobrovitski, A. Feiguin, O. Gywat, and D. Awschalom, “Coherent dynamics of a single spin interacting with an adjustable spin bath”, *Science* **320**:5874, 352–355 (2008) (cit. on p. 52).
- [98] L. Hartmann, J. Calsamiglia, W. Dür, and H. J. Briegel, “Weighted graph states and applications to spin chains, lattices and gases”, *J. Phys. B* **40**:9, S1–S44 (2007) (cit. on p. 54).
- [99] L. Hartmann, J. Calsamiglia, W. Dür, and H.-J. Briegel, “Spin gases as microscopic models for non-markovian decoherence”, *Phys. Rev. A* **72**, 052107 (2005) (cit. on pp. 52, 62).
- [100] L. Hartmann, W. Dür, and H.-J. Briegel, “Steady-state entanglement in open and noisy quantum systems”, *Phys. Rev. A* **74**, 052304 (2006) (cit. on pp. 66, 67).
- [101] R. Hartmann, M. Werther, F. Grossmann, and W. T. Strunz, “Exact open quantum system dynamics: optimal frequency vs time representation of bath correlations”, *The Journal of Chemical Physics* **150**:23, 234105 (2019) (cit. on p. 29).
- [102] K. Head-Marsden, S. Krastanov, D. A. Mazziotti, and P. Narang, “Capturing non-markovian dynamics on near-term quantum computers”, *Phys. Rev. Res.* **3**, 013182 (2021) (cit. on p. 9).
- [103] M. Hein, J. Eisert, and H. J. Briegel, “Multiparty entanglement in graph states”, *Phys. Rev. A* **69**, 062311 (2004) (cit. on p. 54).
- [104] P. P. Hofer, J. B. Brask, M. Perarnau-Llobet, and N. Brunner, “Quantum thermal machine as a thermometer”, *Phys. Rev. Lett.* **119**, 090603 (2017) (cit. on pp. 77, 82).

- [105] M. Hohmann, F. Kindermann, T. Lausch, et al., “Single-atom thermometer for ultracold gases”, *Phys. Rev. A* **93**, 043607 (2016) (cit. on p. 77).
- [106] K. V. Hovhannisyan and L. A. Correa, “Measuring the temperature of cold many-body quantum systems”, *Phys. Rev. B* **98**, 045101 (2018) (cit. on p. 77).
- [107] J. Hu, M. Luo, F. Jiang, R.-X. Xu, and Y. Yan, “Padé spectrum decompositions of quantum distribution functions and optimal hierarchical equations of motion construction for quantum open systems”, *The Journal of Chemical Physics* **134**:24, 244106 (2011) (cit. on p. 29).
- [108] J. Hu, R.-X. Xu, and Y. Yan, “Communication: padé spectrum decomposition of fermi function and bose function”, *The Journal of Chemical Physics* **133**:10, 101106 (2010) (cit. on p. 29).
- [109] K. Hueck, N. Luick, L. Sobirey, et al., “Two-dimensional homogeneous fermi gases”, *Phys. Rev. Lett.* **120**, 060402 (2018) (cit. on p. 76).
- [110] M. Hughes, M. D. Frye, R. Sawant, et al., “Robust entangling gate for polar molecules using magnetic and microwave fields”, *Phys. Rev. A* **101**, 062308 (2020) (cit. on p. 61).
- [111] A. Ishizaki and Y. Tanimura, “Quantum dynamics of system strongly coupled to low-temperature colored noise bath: reduced hierarchy equations approach”, *Journal of the Physical Society of Japan* **74**:12, 3131–3134 (2005) (cit. on p. 29).
- [112] F. Jelezko, T. Gaebel, I. Popa, A. Gruber, and J. Wrachtrup, “Observation of coherent oscillations in a single electron spin”, *Phys. Rev. Lett.* **92**, 076401 (2004) (cit. on pp. 2, 51, 77, 81).
- [113] F. Jelezko, T. Gaebel, I. Popa, et al., “Observation of coherent oscillation of a single nuclear spin and realization of a two-qubit conditional quantum gate”, *Phys. Rev. Lett.* **93**, 130501 (2004) (cit. on pp. 2, 77, 81).
- [114] S. Jevtic, D. Newman, T. Rudolph, and T. M. Stace, “Single-qubit thermometry”, *Phys. Rev. A* **91**, 012331 (2015) (cit. on pp. 77, 82).
- [115] M. Jiang, S. Luo, and S. Fu, “Channel-state duality”, *Phys. Rev. A* **87**, 022310 (2013) (cit. on p. 7).
- [116] J. Jing and T. Yu, “Non-markovian relaxation of a three-level system: quantum trajectory approach”, *Phys. Rev. Lett.* **105**, 240403 (2010) (cit. on p. 2).
- [117] T. H. Johnson, F. Cosco, M. T. Mitchison, D. Jaksch, and S. R. Clark, “Thermometry of ultracold atoms via nonequilibrium work distributions”, *Phys. Rev. A* **93**, 053619 (2016) (cit. on p. 77).
- [118] M. R. Jørgensen, P. P. Potts, M. G. A. Paris, and J. B. Brask, “Tight bound on finite-resolution quantum thermometry at low temperatures”, *Phys. Rev. Res.* **2**, 033394 (2020) (cit. on p. 77).
- [119] B. Kannan, M. J. Ruckriegel, D. L. Campbell, et al., “Waveguide quantum electrodynamics with superconducting artificial giant atoms”, *Nature* **583**:7818, 775–779 (2020) (cit. on p. 19).

- [120] Y. Kim, A. Lanuza, and D. Schneble, “Super-and subradiant dynamics of quantum emitters mediated by atomic matter waves”, *Nature Physics*, 1–7 (2024) (cit. on p. 38).
- [121] J. Kitzman, J. Lane, C. Undershute, et al., “Phononic bath engineering of a superconducting qubit”, *Nature Communications* **14**:1, 3910 (2023) (cit. on pp. 2, 51).
- [122] J. Koch, T. M. Yu, J. Gambetta, et al., “Charge-insensitive qubit design derived from the cooper pair box”, *Phys. Rev. A* **76**, 042319 (2007) (cit. on p. 20).
- [123] A. F. Kockum, G. Johansson, and F. Nori, “Decoherence-free interaction between giant atoms in waveguide quantum electrodynamics”, *Phys. Rev. Lett.* **120**, 140404 (2018) (cit. on p. 19).
- [124] K. Kraus, “Lecture notes in physics”, *States, Effects and Operations. Fundamental Notions of Quantum Theory* **190** (1983) (cit. on p. 6).
- [125] M. G. Krein and D. P. Milman, “On extreme points of regular convex sets”, *Studia Mathematica* **9**, 133–138 (1940) (cit. on p. 123).
- [126] S. Kretschmer, K. Luoma, and W. T. Strunz, “Collision model for non-markovian quantum dynamics”, *Phys. Rev. A* **94**, 012106 (2016) (cit. on p. 2).
- [127] R. Kühne and P. Reineker, “Nakajima-zwanzig’s generalized master equation: evaluation of the kernel of the integro-differential equation”, *Zeitschrift für Physik B Condensed Matter* **31**:1, 105–110 (1978) (cit. on p. 2).
- [128] T. D. Ladd, F. Jelezko, R. Laflamme, et al., “Quantum computers”, *nature* **464**:7285, 45–53 (2010) (cit. on pp. 1, 76).
- [129] N. Lambert, T. Raheja, S. Cross, et al., “Qutip-bofin: a bosonic and fermionic numerical hierarchical-equations-of-motion library with applications in light-harvesting, quantum control, and single-molecule electronics”, *Phys. Rev. Res.* **5**, 013181 (2023) (cit. on pp. 15, 17).
- [130] A. J. Leggett, S. Chakravarty, A. T. Dorsey, et al., “Dynamics of the dissipative two-state system”, *Rev. Mod. Phys.* **59**, 1–85 (1987) (cit. on p. 31).
- [131] M. Levitt, *Spin dynamics: basics of nuclear magnetic resonance* (Wiley, 2013) (cit. on p. 70).
- [132] C.-F. Li, J.-S. Tang, Y.-L. Li, and G.-C. Guo, “Experimentally witnessing the initial correlation between an open quantum system and its environment”, *Phys. Rev. A* **83**, 064102 (2011) (cit. on p. 2).
- [133] V. Link, H.-H. Tu, and W. T. Strunz, “Open quantum system dynamics from infinite tensor network contraction”, *Phys. Rev. Lett.* **132**, 200403 (2024) (cit. on pp. 2, 15).
- [134] Y.-G. Liu and S. Chen, “Lindbladian dynamics with loss of quantum jumps”, *Phys. Rev. B* **111**, 024303 (2025) (cit. on p. 8).

- [135] B.-H. Liu, L. Li, Y.-F. Huang, et al., “Experimental control of the transition from markovian to non-markovian dynamics of open quantum systems”, *Nature Physics* **7**:12, 931–934 (2011) (cit. on p. 2).
- [136] L. R. Liu, J. D. Hood, Y. Yu, et al., “Molecular assembly of ground-state cooled single atoms”, *Phys. Rev. X* **9**, 021039 (2019) (cit. on p. 69).
- [137] Z.-D. Liu, H. Lyyra, Y.-N. Sun, et al., “Experimental implementation of fully controlled dephasing dynamics and synthetic spectral densities”, *Nature Communications* **9**:1, 3453 (2018) (cit. on p. 2).
- [138] R. S. Lous, I. Fritsche, M. Jag, B. Huang, and R. Grimm, “Thermometry of a deeply degenerate fermi gas with a bose-einstein condensate”, *Phys. Rev. A* **95**, 053627 (2017) (cit. on p. 77).
- [139] Y.-N. Lu, Y.-R. Zhang, G.-Q. Liu, et al., “Observing information backflow from controllable non-markovian multichannels in diamond”, *Phys. Rev. Lett.* **124**, 210502 (2020) (cit. on p. 9).
- [140] I. A. Luchnikov, E. O. Kiktenko, M. A. Gavreev, et al., “Probing non-markovian quantum dynamics with data-driven analysis: beyond “black-box” machine-learning models”, *Phys. Rev. Res.* **4**, 043002 (2022) (cit. on p. 9).
- [141] I. A. Luchnikov, S. V. Vintskevich, D. A. Grigoriev, and S. N. Filippov, “Machine learning non-markovian quantum dynamics”, *Phys. Rev. Lett.* **124**, 140502 (2020) (cit. on p. 9).
- [142] J. Ma, Z. Sun, X. Wang, and F. Nori, “Entanglement dynamics of two qubits in a common bath”, *Phys. Rev. A* **85**, 062323 (2012) (cit. on p. 15).
- [143] D. Maile and J. Ankerhold, “Performance of quantum registers in diamond in the presence of spin impurities”, *Phys. Rev. B* **110**, 035407 (2024) (cit. on p. 75).
- [144] W. A. Majewski and T. I. Tylec, “Comment on “channel-state duality””, *Phys. Rev. A* **88**, 026301 (2013) (cit. on p. 7).
- [145] Z.-X. Man, Y.-J. Xia, and R. Lo Franco, “Harnessing non-markovian quantum memory by environmental coupling”, *Phys. Rev. A* **92**, 012315 (2015) (cit. on p. 39).
- [146] L. Mancino, M. Sbroscia, I. Gianani, E. Roccia, and M. Barbieri, “Quantum simulation of single-qubit thermometry using linear optics”, *Phys. Rev. Lett.* **118**, 130502 (2017) (cit. on pp. 77, 82).
- [147] R. Manenti, A. F. Kockum, A. Patterson, et al., “Circuit quantum acoustodynamics with surface acoustic waves”, *Nature communications* **8**:1, 975 (2017) (cit. on p. 19).
- [148] D. Manzano, “A short introduction to the lindblad master equation”, *AIP Advances* **10**:2, 025106 (2020) (cit. on p. 8).
- [149] D. McKay and B. DeMarco, “Thermometry with spin-dependent lattices”, *New Journal of Physics* **12**:5, 055013 (2010) (cit. on p. 77).

- [150] J. Medford, Ł. Cywiński, C. Barthel, et al., “Scaling of dynamical decoupling for spin qubits”, *Phys. Rev. Lett.* **108**, 086802 (2012) (cit. on p. 51).
- [151] M. Mehboudi, A. Lampo, C. Charalambous, et al., “Using polarons for sub-nk quantum nondemolition thermometry in a bose-einstein condensate”, *Phys. Rev. Lett.* **122**, 030403 (2019) (cit. on pp. 77, 82).
- [152] M. Mehboudi, A. Sanpera, and L. A. Correa, “Thermometry in the quantum regime: recent theoretical progress”, *Journal of Physics A: Mathematical and Theoretical* **52**:30, 303001 (2019) (cit. on pp. 2, 76, 77, 79, 82).
- [153] M. Miller, K.-D. Wu, M. Scalici, et al., “Optimally preserving quantum correlations and coherence with eternally non-markovian dynamics”, *New Journal of Physics* **24**:5, 053022 (2022) (cit. on p. 9).
- [154] S. Milz, D. Egloff, P. Taranto, et al., “When is a non-markovian quantum process classical?”, *Phys. Rev. X* **10**, 041049 (2020) (cit. on pp. 2, 40).
- [155] W.-K. Mok, K. Bharti, L.-C. Kwek, and A. Bayat, “Optimal probes for global quantum thermometry”, *Commun. Phys.* **4**, 1–8 (2021) (cit. on p. 82).
- [156] C. Monroe, W. C. Campbell, L.-M. Duan, et al., “Programmable quantum simulations of spin systems with trapped ions”, *Rev. Mod. Phys.* **93**, 025001 (2021) (cit. on p. 67).
- [157] B. Mukherjee, P. B. Patel, Z. Yan, et al., “Spectral response and contact of the unitary fermi gas”, *Phys. Rev. Lett.* **122**, 203402 (2019) (cit. on p. 76).
- [158] B. Mukherjee, Z. Yan, P. B. Patel, et al., “Homogeneous atomic fermi gases”, *Phys. Rev. Lett.* **118**, 123401 (2017) (cit. on p. 76).
- [159] S. Nakajima, “On quantum theory of transport phenomena: steady diffusion”, *Progress of Theoretical Physics* **20**:6, 948–959 (1958) (cit. on p. 9).
- [160] S. Nascimbène, N. Navon, K. Jiang, F. Chevy, and C. Salomon, “Exploring the thermodynamics of a universal fermi gas”, *Nature* **463**:7284, 1057–1060 (2010) (cit. on p. 77).
- [161] N. Navon, A. L. Gaunt, R. P. Smith, and Z. Hadzibabic, “Critical dynamics of spontaneous symmetry breaking in a homogeneous bose gas”, *Science* **347**:6218, 167–170 (2015) (cit. on p. 76).
- [162] M. Nery, M. T. Quintino, P. A. Guérin, T. O. Maciel, and R. O. Vianna, “Simple and maximally robust processes with no classical common-cause or direct-cause explanation”, *Quantum* **5**, 538 (2021) (cit. on pp. 2, 40).
- [163] D. Newman, F. Mintert, and A. Nazir, “Performance of a quantum heat engine at strong reservoir coupling”, *Phys. Rev. E* **95**, 032139 (2017) (cit. on p. 2).
- [164] M. A. Nielsen and I. L. Chuang, *Quantum computation and quantum information: 10th anniversary edition* (Cambridge University Press, 2010) (cit. on pp. 1, 7, 76).

- [165] M. Niknam, L. F. Santos, and D. G. Cory, “Experimental detection of the correlation rényi entropy in the central spin model”, *Phys. Rev. Lett.* **127**, 080401 (2021) (cit. on pp. 2, 61, 69).
- [166] R. Olf, F. Fang, G. E. Marti, A. MacRae, and D. M. Stamper-Kurn, “Thermometry and cooling of a bose gas to 0.02 times the condensation temperature”, *Nature Physics* **11**:9, 720–723 (2015) (cit. on p. 77).
- [167] M. Onizhuk, K. C. Miao, J. P. Blanton, et al., “Probing the coherence of solid-state qubits at avoided crossings”, *PRX Quantum* **2**, 010311 (2021) (cit. on p. 2).
- [168] L. Onsager, “Crystal statistics. i. a two-dimensional model with an order-disorder transition”, *Phys. Rev.* **65**, 117–149 (1944) (cit. on p. 87).
- [169] O. Oreshkov and T. A. Brun, “Continuous quantum error correction for non-markovian decoherence”, *Phys. Rev. A* **76**, 022318 (2007) (cit. on p. 39).
- [170] M. G. A. Paris, “Achieving the landau bound to precision of quantum thermometry in systems with vanishing gap”, *Journal of Physics A: Mathematical and Theoretical* **49**:3, 03LT02 (2015) (cit. on p. 77).
- [171] M. G. A. Paris, “Quantum estimation for quantum technology”, *International Journal of Quantum Information* **07**:supp01, 125–137 (2009) (cit. on pp. 79, 80).
- [172] J.-P. Pellonpää, “Quantum instruments: ii. measurement theory”, *Journal of Physics A: Mathematical and Theoretical* **46**:2, 025303 (2012) (cit. on p. 123).
- [173] M. B. Plenio, “Logarithmic negativity: a full entanglement monotone that is not convex”, *Phys. Rev. Lett.* **95**, 090503 (2005) (cit. on p. 63).
- [174] P. P. Potts, J. B. Brask, and N. Brunner, “Fundamental limits on low-temperature quantum thermometry with finite resolution”, *Quantum* **3**, 161 (2019) (cit. on p. 77).
- [175] M. Puviani, S. Borah, R. Zen, J. Olle, and F. Marquardt, “Non-markovian feedback for optimized quantum error correction”, *Phys. Rev. Lett.* **134**, 020601 (2025) (cit. on pp. 2, 9, 40, 51).
- [176] S. Razavian, C. Benedetti, M. Bina, Y. Akbari-Kourbolagh, and M. G. Paris, “Quantum thermometry by single-qubit dephasing”, *The European Physical Journal Plus* **134**:6, 284 (2019) (cit. on p. 77).
- [177] A. G. Redfield, “On the theory of relaxation processes”, *IBM Journal of Research and Development* **1**:1, 19–31 (1957) (cit. on p. 12).
- [178] C. Regal and D. S. Jin, *Experimental realization of bcs-bec crossover physics with a fermi gas of atoms*, 2006 (cit. on p. 77).
- [179] Á. Rivas and S. Huelga, *Open quantum systems: an introduction*, SpringerBriefs in Physics (Springer Berlin Heidelberg, 2011) (cit. on pp. 7, 8, 39).

- [180] Á. Rivas, S. F. Huelga, and M. B. Plenio, “Entanglement and non-markovianity of quantum evolutions”, *Phys. Rev. Lett.* **105**, 050403 (2010) (cit. on pp. 1, 8, 39, 43, 45, 62).
- [181] L. Robledo, L. Childress, H. Bernien, et al., “High-fidelity projective read-out of a solid-state spin quantum register”, *Nature* **477**, 574 (2011) (cit. on pp. 2, 51, 77, 81).
- [182] R. Roy and T. Kailath, “Esprit-estimation of signal parameters via rotational invariance techniques”, *IEEE Transactions on Acoustics, Speech, and Signal Processing* **37**:7, 984–995 (1989) (cit. on p. 29).
- [183] C. Sabín, A. White, L. Hackermuller, and I. Fuentes, “Impurities as a quantum thermometer for a bose-einstein condensate”, *Scientific reports* **4**:1, 6436 (2014) (cit. on p. 77).
- [184] M. Saffman, T. G. Walker, and K. Mølmer, “Quantum information with Rydberg atoms”, *Rev. Mod. Phys.* **82**, 2313–2363 (2010) (cit. on pp. 61, 63, 67).
- [185] A. C. Santos and R. Bachelard, “Generation of maximally entangled long-lived states with giant atoms in a waveguide”, *Phys. Rev. Lett.* **130**, 053601 (2023) (cit. on p. 19).
- [186] D. Schaubert, “Application of prony’s method to time-domain reflectometer data and equivalent circuit synthesis”, *IEEE Transactions on Antennas and Propagation* **27**:2, 180–184 (1979) (cit. on p. 29).
- [187] M. Schlosshauer, “Decoherence, the measurement problem, and interpretations of quantum mechanics”, *Rev. Mod. Phys.* **76**, 1267–1305 (2005) (cit. on p. 1).
- [188] M. Schlosshauer, “Quantum decoherence”, *Physics Reports* **831**, Quantum decoherence, 1–57 (2019) (cit. on pp. 51, 61).
- [189] T. F. Schmidutz, I. Gotlibovych, A. L. Gaunt, et al., “Quantum joule-thomson effect in a saturated homogeneous bose gas”, *Phys. Rev. Lett.* **112**, 040403 (2014) (cit. on p. 76).
- [190] M. Scully and M. Zubairy, *Quantum optics*, Quantum Optics (Cambridge University Press, 1997) (cit. on p. 31).
- [191] F. Shibata, Y. Takahashi, and N. Hashitsume, “A generalized stochastic liouville equation. non-markovian versus memoryless master equations”, *Journal of Statistical Physics* **17**, 171–187 (1977) (cit. on p. 11).
- [192] A. Smirne, D. Brivio, S. Cialdi, B. Vacchini, and M. G. A. Paris, “Experimental investigation of initial system-environment correlations via trace-distance evolution”, *Phys. Rev. A* **84**, 032112 (2011) (cit. on p. 2).
- [193] J. A. Smolin, F. Verstraete, and A. Winter, “Entanglement of assistance and multipartite state distillation”, *Phys. Rev. A* **72**, 052317 (2005) (cit. on p. 40).
- [194] F. M. Spiegelhalder, A. Trenkwalder, D. Naik, et al., “Collisional stability of ^{40}K immersed in a strongly interacting fermi gas of ^6Li ”, *Phys. Rev. Lett.* **103**, 223203 (2009) (cit. on p. 77).

- [195] T. M. Stace, “Quantum limits of thermometry”, *Phys. Rev. A* **82**, 011611 (2010) (cit. on p. 82).
- [196] H. Stanley, *Introduction to phase transitions and critical phenomena*, International series of monographs on physics (Oxford University Press, 1987) (cit. on pp. 88, 89, 136).
- [197] A. Steane, “Quantum computing”, *Reports on Progress in Physics* **61**:2, 117 (1998) (cit. on p. 1).
- [198] M. Steiner, “Generalized robustness of entanglement”, *Phys. Rev. A* **67**, 054305 (2003) (cit. on p. 42).
- [199] A. Strathearn, P. Kirton, D. Kilda, J. Keeling, and B. W. Lovett, “Efficient non-markovian quantum dynamics using time-evolving matrix product operators”, *Nature communications* **9**:1, 3322 (2018) (cit. on pp. 2, 15).
- [200] A. Streltsov, G. Adesso, and M. B. Plenio, “Colloquium: quantum coherence as a resource”, *Rev. Mod. Phys.* **89**, 041003 (2017) (cit. on p. 2).
- [201] D. Suess, A. Eisfeld, and W. T. Strunz, “Hierarchy of stochastic pure states for open quantum system dynamics”, *Phys. Rev. Lett.* **113**, 150403 (2014) (cit. on p. 2).
- [202] D. Suess, W. T. Strunz, and A. Eisfeld, “Hierarchical equations for open system dynamics in fermionic and bosonic environments”, *Journal of Statistical Physics* **159**, 1408–1423 (2015) (cit. on p. 38).
- [203] H. Takahashi, S. Rudge, C. Kaspar, M. Thoss, and R. Borrelli, “High accuracy exponential decomposition of bath correlation functions for arbitrary and structured spectral densities: emerging methodologies and new approaches”, *The Journal of Chemical Physics* **160**:20, 204105 (2024) (cit. on p. 29).
- [204] J. Tan, T. H. Kyaw, and Y. Yeo, “Non-markovian environments and entanglement preservation”, *Phys. Rev. A* **81**, 062119 (2010) (cit. on p. 9).
- [205] Y. Tanimura, “Nonperturbative expansion method for a quantum system coupled to a harmonic-oscillator bath”, *Phys. Rev. A* **41**, 6676–6687 (1990) (cit. on pp. 2, 15, 26, 29).
- [206] Y. Tanimura, “Numerically “exact” approach to open quantum dynamics: The hierarchical equations of motion (HEOM)”, *The Journal of Chemical Physics* **153**:2, 020901 (2020) (cit. on p. 2).
- [207] Y. Tanimura and R. Kubo, “Time evolution of a quantum system in contact with a nearly gaussian-markoffian noise bath”, *Journal of the Physical Society of Japan* **58**:1, 101–114 (1989) (cit. on pp. 15, 26).
- [208] P. Taranto, M. T. Quintino, M. Murao, and S. Milz, “Characterising the Hierarchy of Multi-time Quantum Processes with Classical Memory”, *Quantum* **8**, 1328 (2024) (cit. on pp. 2, 40).
- [209] Q.-J. Tong, J.-H. An, H.-G. Luo, and C. H. Oh, “Mechanism of entanglement preservation”, *Phys. Rev. A* **81**, 052330 (2010) (cit. on p. 9).

- [210] R. Uola, T. Kraft, J. Shang, X.-D. Yu, and O. Gühne, “Quantifying quantum resources with conic programming”, *Phys. Rev. Lett.* **122**, 130404 (2019) (cit. on p. 42).
- [211] A. M. Vadiraj, A. Ask, T. G. McConkey, et al., “Engineering the level structure of a giant artificial atom in waveguide quantum electrodynamics”, *Phys. Rev. A* **103**, 023710 (2021) (cit. on p. 19).
- [212] L. Vandenberghe and S. Boyd, “Semidefinite programming”, *SIAM Review* **38**:1, 49–95 (1996) (cit. on p. 43).
- [213] S. Vanhuffel, H. Chen, C. Decanniere, and P. Vanhecke, “Algorithm for time-domain nmr data fitting based on total least squares”, *Journal of Magnetic Resonance, Series A* **110**:2, 228–237 (1994) (cit. on p. 29).
- [214] I. de Vega and D. Alonso, “Dynamics of non-markovian open quantum systems”, *Rev. Mod. Phys.* **89**, 015001 (2017) (cit. on p. 39).
- [215] S. Veroni, M. Müller, and G. Giudice, “Optimized measurement-free and fault-tolerant quantum error correction for neutral atoms”, *Phys. Rev. Res.* **6**, 043253 (2024) (cit. on pp. 2, 9, 51).
- [216] S. Viciani, M. Lima, M. Bellini, and F. Caruso, “Observation of noise-assisted transport in an all-optical cavity-based network”, *Phys. Rev. Lett.* **115**, 083601 (2015) (cit. on p. 1).
- [217] G. Vidal and R. F. Werner, “Computable measure of entanglement”, *Phys. Rev. A* **65**, 032314 (2002) (cit. on p. 63).
- [218] G. Vidal and R. Tarrach, “Robustness of entanglement”, *Phys. Rev. A* **59**, 141–155 (1999) (cit. on p. 42).
- [219] Z. Wang, A. V. Lim, and I. M. Mirza, “Non-markovianity in photosynthetic reaction centers: a noise-induced quantum coherence perspective”, *Opt. Continuum* **1**:8, 1848–1858 (2022) (cit. on p. 2).
- [220] K. X. Wei, E. Pritchett, D. M. Zajac, D. C. McKay, and S. Merkel, “Characterizing non-markovian off-resonant errors in quantum gates”, *Phys. Rev. Appl.* **21**, 024018 (2024) (cit. on p. 39).
- [221] Q. Wei, Y. Cao, S. Kais, B. Friedrich, and D. Herschbach, “Quantum computation using arrays of n polar molecules in pendular states”, *ChemPhysChem* **17**:22, 3714–3722 (2016) (cit. on p. 61).
- [222] U. Weiss, *Quantum dissipative systems*, Series in modern condensed matter physics (World Scientific, 2008) (cit. on pp. 1, 12, 26).
- [223] G. White, “Characterization and control of non-markovian quantum noise”, *Nature Reviews Physics* **4**:5, 287–287 (2022) (cit. on p. 40).
- [224] G. A. White, C. D. Hill, F. A. Pollock, L. C. Hollenberg, and K. Modi, “Demonstration of non-markovian process characterisation and control on a quantum processor”, *Nature Communications* **11**:1, 6301 (2020) (cit. on p. 40).

- [225] W. K. Wootters, “Entanglement of formation of an arbitrary state of two qubits”, *Phys. Rev. Lett.* **80**, 2245–2248 (1998) (cit. on p. 40).
- [226] Z.-J. Xu and J.-H. An, “Noise mitigation in quantum teleportation”, *Phys. Rev. A* **110**, 012442 (2024) (cit. on p. 40).
- [227] Z. Yan, P. B. Patel, B. Mukherjee, et al., “Boiling a unitary fermi liquid”, *Phys. Rev. Lett.* **122**, 093401 (2019) (cit. on p. 76).
- [228] S. F. Yelin, K. Kirby, and R. Côté, “Schemes for robust quantum computation with polar molecules”, *Phys. Rev. A* **74**, 050301 (2006) (cit. on p. 61).
- [229] X.-L. Yin and J.-Q. Liao, “Generation of two-giant-atom entanglement in waveguide-qed systems”, *Phys. Rev. A* **108**, 023728 (2023) (cit. on p. 19).
- [230] X.-L. Yin, W.-B. Luo, and J.-Q. Liao, “Non-markovian disentanglement dynamics in double-giant-atom waveguide-qed systems”, *Phys. Rev. A* **106**, 063703 (2022) (cit. on p. 19).
- [231] H. Yu, Z. Wang, and J.-H. Wu, “Entanglement preparation and nonreciprocal excitation evolution in giant atoms by controllable dissipation and coupling”, *Phys. Rev. A* **104**, 013720 (2021) (cit. on p. 19).
- [232] M. Yu, O. Gühne, and S. Nimmrichter, “Exact entanglement dynamics of two spins in finite baths”, *Phys. Rev. A* **108**, 022415 (2023) (cit. on p. 9).
- [233] H.-D. Zhang, L. Cui, H. Gong, et al., “Hierarchical equations of motion method based on fano spectrum decomposition for low temperature environments”, *The Journal of Chemical Physics* **152**:6, 064107 (2020) (cit. on pp. 29, 69).
- [234] W. Zhao and Z. Wang, “Single-photon scattering and bound states in an atom-waveguide system with two or multiple coupling points”, *Phys. Rev. A* **101**, 053855 (2020) (cit. on p. 19).
- [235] J. Zhou, X.-L. Yin, and J.-Q. Liao, “Chiral and nonreciprocal single-photon scattering in a chiral-giant-molecule waveguide-qed system”, *Phys. Rev. A* **107**, 063703 (2023) (cit. on p. 19).
- [236] M. Ziman, “Process positive-operator-valued measure: a mathematical framework for the description of process tomography experiments”, *Phys. Rev. A* **77**, 062112 (2008) (cit. on pp. 43, 125).
- [237] W. H. Zurek, “Decoherence, einselection, and the quantum origins of the classical”, *Rev. Mod. Phys.* **75**, 715–775 (2003) (cit. on p. 1).
- [238] R. Zwanzig, “Ensemble method in the theory of irreversibility”, *The Journal of Chemical Physics* **33**:5, 1338–1341 (1960) (cit. on p. 9).

List of Figures

3.1	A giant atom couples to 1D surface acoustic waves via two contacts. . .	21
3.2	(a) Time-dependent decay rate and (b) Lamb shift as function of time. We consider an Ohmic spectral density of SAWs environment, $\gamma(\omega) = \eta\omega e^{-\omega/\omega_c}$ with the coupling strength η and cutoff frequency ω_c . The parameters are selected as $\eta/\omega_0 = 2.74 \times 10^{-3}$ and $\omega_c/\omega_0 = 1.2$ for consistency with following plots 3.3.	25
3.3	Spontaneous decay of an initially excited two-level giant atom in (a) the Markovian regime with zero time delay ($\eta\tau = 0$) and (b) the non-Markovian regime with a time delay ($\eta\tau = 0.6$), calculated using various methods. The parameters are set as $\eta/\omega_0 = 2.74 \times 10^{-3}$, $\omega_c/\omega_0 = 1.2$	28
3.4	(a) Effective bath spectral density of the SAWs field at zero temperature; (b) The corresponding bath correlation function as function of time at zero temperature. The parameters are the same as in Fig. 3.3. The dashed lines represent fits based on the ESPRITE method, with a relative error threshold of $\varepsilon_r = 10^{-3}$	30
3.5	The spontaneous decay of a two-level giant atom in (a) Markovian regime with zero time delay ($\eta\tau = 0$) and (b) the non-Markovian regime with a time delay ($\eta\tau = 0.6$) with respect to different relative coupling strengths. The parameters are set as $\eta/\omega_c = 2.3 \times 10^{-3}$	32
3.6	(a) The real part of thermal BCF for the SAWs field as function of time at various temperatures, along with their corresponding ESPRIT fittings. The parameters are chosen as $\eta/\omega_0 = 2.74 \times 10^{-3}$, $\omega_c/\omega_0 = 1.2$, $\eta\tau = 0.6$ and $\varepsilon_r = 10^{-3}$ for the fitting. (b) The number of exponential functions used in the ESPRIT fitting for the real and imaginary parts of the thermal BCF at different temperatures.	33
3.7	The spontaneous decay of a two-level giant atom at various temperatures. The parameters are set as $\eta/\omega_0 = 2.74 \times 10^{-3}$, $\omega_c/\omega_0 = 1.2$	34

3.8	A Λ -type three-level giant atom coupled to two one-dimensional waveguides. The transition between excited state and ground state, $ e\rangle \leftrightarrow g\rangle$, and the transition between excited state and metastable state, $ e\rangle \leftrightarrow s\rangle$, are coupled to two distinct waveguide modes via two separate contact points, respectively.	36
3.9	Excited-state probability P_e of the Λ -type giant atom as function of time and (a) the time delay ratio τ_2/τ_1 ; (c) the coupling strength ratio η_2/η_1 of two waveguides. The lower panels (b) and (d) correspond to the horizontal dashed lines in (a) and (c), respectively. The parameters are set as $\eta_2 = \eta_1$ in (a, b) and $\tau_2 = \tau_1$ in (c, b), respectively. The remaining parameters are chosen as $\omega_e/\omega_s = 2$, $\omega_c/\omega_s = 6.4$, $\eta_1/\omega_s = 0.016$, and $\eta_1\tau_1 = 0.6$	37
4.1	Sketch of the quantum memory robustness of a channel $\mathcal{E}(t_2)$ that lies outside of the classical future $\mathcal{F}(\mathcal{E}(t_1))$ of a channel $\mathcal{E}(t_1)$	42
4.2	Quantum memory robustness of the two-level giant atom versus time γt_1 and $\gamma \Delta t$ with fixed parameters $\omega_0\tau = 40\pi$, $\gamma\tau = 12$	46
4.3	Quantum memory robustness of the three-level giant atom dynamics with fixed parameters $\omega_s\tau = 20\pi$, $\omega_e\tau = 40\pi$, $\gamma_1\tau = 4$, $\gamma_2\tau = 8$	49
5.1	Sketch of a dynamical spin lattice model for non-Markovian dephasing, with N_A quantum spins (green, $N_A = 2$) surrounded by N_B environmental spins (blue) on a periodic lattice. The configuration can be static or dynamic, with phase exchange via Ising-type interactions. Intrasystem and system-environment couplings are represented by g_{AA} and g_{AB} , respectively. A three-body phase interaction of strength h is also considered between neighboring spins.	53
5.2	Curie-Weiss spin bath: Every spin interacts uniformly with all others, represented by a complete graph. In this graph, vertices correspond to spins, and edges between vertices i and j denote the coupling term $-(J/N_B)\hat{\sigma}_z^i \otimes \hat{\sigma}_z^j$ in the total interaction energy, where J is the coupling rate and N_B is the total number of bath spins.	57
5.3	The decoherence factor (5.22) as a function of time at various temperatures for two scenarios: (a) in the absence of a magnetic field ($h = 0$) and (b) in the presence of a magnetic field. Different colors correspond to different temperature values.	60

- 5.4 Entanglement negativity between system spins as a function of normalized time g_{AB}/π and system-environment coupling g_{AB}/g_{AA} . become entangled through their phase interaction, with $g_{AA}\Delta t = 0.05$, while experiencing (a) nearly Markovian and (b) non-Markovian dephasing induced by an infinite-temperature spin environment. The hopping rate of environmental spins is $\eta_B = 1/5$. In (a), undergo random jumps between lattice sites at each time step Δt . Entanglement negativity is computed for ensemble-averaged states over 2×10^5 trajectories. . . . 63
- 5.5 Entanglement negativity as a function of time at $g_{AB}\Delta t = 0.05$ and $g_{AB}/g_{AA} = 0.5$. We compare the almost Markovian (red circles) and the non-Markovian case (green dots) from Fig. 5.4 against the strictly Markovian collision model based Eq. 5.29 with $n_B = 8$ (solid line). . . 65
- 5.6 Entanglement negativity versus time in the presence of dephasing and random simulation reset operations on the two system spins. The solid and dashed lines represent the almost Markovian and the non-Markovian case, respectively; the colors represent different combinations of intrasystem coupling and reset rate. (b) Steady-state negativity versus reset rate κ and intrasystem coupling g_{AA} , as evaluated at $t = 15\Delta t$. The dots show the maximum negativity with respect to $\kappa/g_{AA} = 7$. We fix $g_{AB}\Delta t = 0.1$ and average over 2×10^5 trajectories. . 67
- 5.7 Entanglement negativity as function of time with and without three-body coupling effect. We choose the same parameters setting as in Fig. 5.5 (dashed line), with an additional three-body coupling of strength $h = -0.015g_{AB}$ (solid). The comparison is made for (a) the almost Markovian case and (b) the non-Markovian case, with results averaged over 10^5 trajectories. 68
- 5.8 Structure of the 1,2-Bis(dimethylphosphino)ethane (dpme) molecule $C_6H_{16}P_2$ possesses C_2 molecular symmetry, with the two phosphorus atoms (yellow) occupying symmetry-equivalent positions.. The nuclear spins of the two phosphorus atoms (yellow) act as the quantum system subject to non-Markovian dephasing from the 16 surrounding hydrogen spins (light grey) via magnetic dipole interactions. We average over random orientations of the molecule with respect to the external magnetic field axis. 70

5.9	The decay of entanglement negativity over time for two nuclear P-spins, initially in a Bell-entangled state, subjected to dephasing by the surrounding H-spins of the dpme molecule under a magnetic field of (a, c) $B_z = 0.05$ mT and (b, d) 1 mT. The molecule is oriented (a, b) at a fixed configuration with $\theta = \pi/2$ and $\gamma = 0$, and (c, d) averaged over 5000 random orientations relative to the magnetic field axis. The dephasing dynamics are compared for an interacting (solid line) and a non-interacting (dashed line) thermal environment across different temperatures.	72
5.10	(a) Initial rate of entanglement negativity decay $\mathcal{R}$ at $\tau = 10 \mu\text{s}$ as a function of temperature, comparing the correlated (solid line) and uncorrelated (dashed line) spin baths in the Gibbs state. (b) Number of bath spin states occupied by 99% of the Gibbs distribution. The results were obtained for a weak magnetic field of $B_z = 0.05$ mT, averaged over 5×10^3 random orientations of the molecule.	74
6.1	Qubit phase thermometry scheme: A two-level system couples to a sample system in thermal equilibrium with a reservoir at temperature T . The temperature information is encoded in the probe state and can be estimated by measuring the probe state.	78
6.2	Coherence decay time as a function of inverse temperature, as predicted by the Curie-Weiss model in the thermodynamic limit. The parameters are set to $N = 400$ and $h = 0$	83
6.3	The optimal QFI of the phase probe (maximized in Eq. (6.15) with respect to time) and local FI (6.18) for direct lattice spin measurement are shown as functions of the relative temperature deviation ϵ from the critical point. We consider the probe-lattice coupling $\hbar g/J = 0.4$ and lattice coupling $J = 1/4$ in arbitrary energy units.	85
6.4	(a) Optimal QFI of the phase probe (optimized over time) interacting with spin clusters of varying size n in a 20×20 Ising lattice, as a function of inverse temperature relative to the critical point (vertical dashed line). (b) local FI from Eq. (6.20) associated to a direct local measurement of the configuration of the n cluster spins. (c) Ratio of optimal probe QFI and direct local FI close to the critical point. We use the probe-cluster coupling strength $\hbar g/J = 0.4$ and set $J = 1/4$ (in arbitrary reference units).	86

6.5	The scaling of the optimal probe QFI with the size n of the lattice spin cluster, based on the parameters in Fig. 6.4. The rightmost data points represent $n = 21$, with smaller cluster sizes obtained by sequentially removing outer spins. Scaling is compared at the critical point, at 10 % above ($\beta = 0.9\beta_c$), and at 10 % below the critical temperature. Solid lines represent linear fits on a double-logarithmic scale, with slopes of 0.73, 0.71, and 0.49, respectively.	87
6.6	Optimal QFI of the phase probe as a function of inverse temperature relative to the critical point (vertical dashed line), extending the results in Fig. 6.4(a). We separate the four cases corresponding to different cluster sizes n into different diagrams (a)-(d), comparing the exact Monte-Carlo simulation data to the approximate predictions of the mean-field theory (solid lines) and the high-temperature expansion (dashed).	90
6.7	Construction of pair bond doublets in the Ising lattice. The cluster C of spins interacting with the probe (dark blue) are contained in a circle. Exemplary red lines symbolize pair bonds due to the Ising interaction between any two neighbouring lattice spins. From left to right, each marked doublet of pair bonds represents one possible contribution that is counted by the numbers K_{22} , K_{23} , K_{24} , respectively. In the depicted configuration there are $n = 13$ cluster spins, $K_{12} = 16$ intra-cluster bonds, and one obtains $(K_{22}, K_{23}, K_{24}) = (8, 34, 86)$	91
A.1	Geometric construction in the proof of the classical description of the qubit dephasing dynamics. The complex numbers $\alpha(t_1)$ and $\alpha(t_2)$ are confined to the unit disk. For every complex number z on the unit disk, there exists at least one number w such that $ w = \frac{1}{2}$ as well as $ z - w = \frac{1}{2}$. The number w is an intersection point of the circle with radius $\frac{1}{2}$ around 0 and the circle with radius $\frac{1}{2}$ around z . For $\alpha(t_1)$ we call this number γ and for $\alpha(t_2)$ we call it δ	120
B.1	Magnetization in Curie-Weiss model in the absence of magnetic field. .	134

List of Tables

3.1	Number of exponential terms in the ESPRIT fit to the BCF for various time delays, given a relative error threshold $\varepsilon_r = 10^{-3}$	31
-----	--	----

Appendix to Chapter 4

In this appendix, we provide proofs for the technical results from Chapter 4.

A.1 Quantum memory detection

A.1.1 Basic concepts

To characterize and detect quantum memory in dynamical processes, we make use of the concept of the classical future of a channel and its corresponding dual cone. Before we discuss the details about these mathematical objects, it might be helpful to briefly review the concept of convex cones. We are especially interested in cones which are subsets of the real Hilbert space $\mathcal{L}^h(\mathbb{C}^d)$ of complex hermitian $d \times d$ – matrices equipped with the Hilbert-Schmidt inner product $(A, B) := \text{tr}(AB)$. A subset $K \in \mathcal{L}^h(\mathbb{C}^d)$ is called a convex cone if $c_1 k_1 + c_2 k_2 \in K$ for all $k_1, k_2 \in K$ and $c_1, c_2 \in \mathbb{R}_+$.

For an arbitrary (not necessarily convex) subset $C \in \mathcal{L}^h(\mathbb{C}^d)$, the dual cone denoted by C^* is defined as

$$C^* = \{X \in \mathcal{L}^h(\mathbb{C}^d) : \text{tr}(XY) \geq 0 \text{ for all } Y \in C\}. \quad (\text{A.1})$$

One important example for a convex cone are the positive semidefinite matrices $\mathcal{P}_d \subset \mathcal{L}^h(\mathbb{C}^d)$ defined by hermitian matrices whose eigenvalues are all nonnegative. It is a well known fact, see for instance Ref. [18], that the cone $\mathcal{P}_d$ is self-dual, i.e. $\mathcal{P}_d^* = \mathcal{P}_d$.

The term quantum channel refers to maps $\mathcal{C} : \mathcal{L}^h(\mathbb{C}^d) \rightarrow \mathcal{L}^h(\mathbb{C}^{d'})$ that are completely positive and trace-preserving. Via the Choi isomorphism $\mathcal{C} \mapsto C^{AB} = \frac{1}{d^2} \sum_{i,j=0}^{d-1} |i\rangle\langle j| \otimes \mathcal{C}[|i\rangle\langle j|]$, there is a correspondence between quantum channels $\mathcal{C}$ and bipartite quantum states C^{AB} that fulfill $\text{tr}_B(C^{AB}) = \frac{\mathbb{1}^A}{d}$. We denote the set of quantum channels $\mathcal{C} : \mathcal{L}^h(\mathbb{C}^d) \rightarrow \mathcal{L}^h(\mathbb{C}^d)$ as $\mathcal{C}_d$.

A.1.2 The classical future and its properties

An important set for the characterisation of quantum memory is the classical future of a quantum channel.

Definition 1 Let $\mathcal{E} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ be a quantum channel. Then the **classical future** $\mathcal{F}[\mathcal{E}]$ is defined as the set of channels $\mathcal{R} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ that can be decomposed as

$$\mathcal{R} = \sum_{i=1}^L \mathcal{K}^i \mathcal{I}^i \quad (\text{A.2})$$

where $L \in \mathbb{N}$, $\mathcal{K}^i : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ are quantum channels for $i \in \{1, \dots, L\}$ and $\mathcal{I}^i : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ is an instrument decomposition of $\mathcal{E}$.

The classical future possesses an invariance property under specific unitary transformations and Markovian evolutions. This will be demonstrated step by step in what follows.

Proposition 1 Let $\mathcal{E}, \mathcal{R} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ be two quantum channels and let $\mathcal{R}$ be in the classical future of $\mathcal{E}$, i.e. $\mathcal{R} \in \mathcal{F}[\mathcal{E}]$. Furthermore, let $\mathcal{M}, \mathcal{N} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ be some channels and let $\mathcal{U} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ be a unitary channel. Then, it holds that $\mathcal{M}\mathcal{R}\mathcal{N}$ is in the classical future of $\mathcal{U}\mathcal{E}\mathcal{N}$, i.e. $\mathcal{M}\mathcal{R}\mathcal{N} \in \mathcal{F}[\mathcal{U}\mathcal{E}\mathcal{N}]$. Especially, in the case that $\mathcal{M}$ and $\mathcal{N}$ are unitary, this property expresses a certain unitary equivalence of the classical future of quantum channels.

Proof 1 We assume that $\mathcal{R} \in \mathcal{F}[\mathcal{E}]$. Then by definition of the classical future, there exists an $L \in \mathbb{N}$, quantum channels $\{\mathcal{K}^i\}_{i=1}^L$ and an instrument decomposition $\{\mathcal{I}^i\}_{i=1}^L$ of $\mathcal{E}$ such that

$$\mathcal{R} = \sum_{i=1}^L \mathcal{K}^i \mathcal{I}^i.$$

For the channel $\mathcal{M}\mathcal{R}\mathcal{N}$, one obtains

$$\begin{aligned} \mathcal{M}\mathcal{R}\mathcal{N} &= \sum_{i=1}^L \mathcal{M}\mathcal{K}^i \mathcal{I}^i \mathcal{N} \\ &= \sum_{i=1}^L \underbrace{\mathcal{M}\mathcal{K}^i \mathcal{U}^{-1}}_{=: \tilde{\mathcal{K}}^i} \circ \underbrace{\mathcal{U} \mathcal{I}^i \mathcal{N}}_{=: \tilde{\mathcal{I}}^i} \\ &= \sum_{i=1}^L \tilde{\mathcal{K}}^i \tilde{\mathcal{I}}^i \end{aligned}$$

where $\{\tilde{\mathcal{I}}^i\}_{i=1}^L$ is easily seen to be an instrument decomposition of $\mathcal{U}\mathcal{E}\mathcal{N}$ and $\tilde{\mathcal{K}}^i$ are channels.

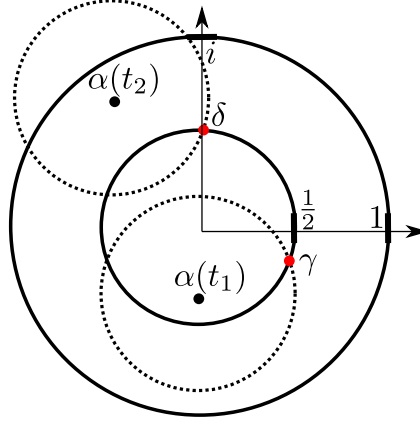


Fig. A.1.: Geometric construction in the proof of the classical description of the qubit dephasing dynamics. The complex numbers $\alpha(t_1)$ and $\alpha(t_2)$ are confined to the unit disk. For every complex number z on the unit disk, there exists at least one number w such that $|w| = \frac{1}{2}$ as well as $|z - w| = \frac{1}{2}$. The number w is an intersection point of the circle with radius $\frac{1}{2}$ around 0 and the circle with radius $\frac{1}{2}$ around z . For $\alpha(t_1)$ we call this number γ and for $\alpha(t_2)$ we call it δ .

We use an example to illustrate the concept of classical memory and classical futures as a proper generalisation of Markovian dynamics is given by the dephasing qubit dynamics $\mathcal{D}_\alpha(t)$ defined by

$$\mathcal{D}_\alpha(t)[|0\rangle\langle 0|] = |0\rangle\langle 0| \quad (\text{A.3})$$

$$\mathcal{D}_\alpha(t)[|1\rangle\langle 1|] = |1\rangle\langle 1| \quad (\text{A.4})$$

$$\mathcal{D}_\alpha(t)[|0\rangle\langle 1|] = \alpha(t)|0\rangle\langle 0| \quad (\text{A.5})$$

$$\mathcal{D}_\alpha(t)[|1\rangle\langle 0|] = \alpha(t)^*|1\rangle\langle 0| \quad (\text{A.6})$$

where $\alpha(t)$ is any function such that $|\alpha(t)| \leq 1$ for all t so that $\mathcal{D}_\alpha(t)$ is completely positive for all times.

Proposition 2 *The two point qubit dephasing dynamics $(\mathcal{D}_\alpha(t_1), \mathcal{D}_\alpha(t_2))$ with $t_1 \leq t_2$ is Markovian if and only if*

$$|\alpha(t_2)| \leq |\alpha(t_1)|. \quad (\text{A.7})$$

Otherwise, the dynamics exhibits a non-monotonic decay, indicating non-Markovianity. This dynamics can be implemented with classical memory in the sense that $\mathcal{D}_\alpha(t_2) \in \mathcal{F}[\mathcal{D}_\alpha(t_1)]$ for all functions $\alpha(t)$ such that $|\alpha(t)| \leq 1$ and for all time points t_1 and t_2 . In particular, the size L of the instrument can be chosen as $L = 2$.

Proof 2 For the Markovianity, consider the map $\mathcal{K}_\alpha(t_2, t_1)$ that satisfies $\mathcal{D}_\alpha(t_2) = \mathcal{K}_\alpha(t_2, t_1)\mathcal{D}_\alpha(t_1)$. It is straightforward to see that $\mathcal{K}_\alpha(t_2, t_1)$ must be given by the action

$$\mathcal{K}_\alpha(t_2, t_1)[|0\rangle\langle 0|] = |0\rangle\langle 0| \quad (\text{A.8})$$

$$\mathcal{K}_\alpha(t_2, t_1)[|1\rangle\langle 1|] = |1\rangle\langle 1| \quad (\text{A.9})$$

$$\mathcal{K}_\alpha(t_2, t_1)[|0\rangle\langle 1|] = \frac{\alpha(t_2)}{\alpha(t_1)}|0\rangle\langle 1| \quad (\text{A.10})$$

$$\mathcal{K}_\alpha(t_2, t_1)[|1\rangle\langle 0|] = \frac{\alpha(t_2)^*}{\alpha(t_1)^*}|1\rangle\langle 0| \quad (\text{A.11})$$

such that $\mathcal{K}_\alpha(t_2, t_1)$ is completely positive if and only if $|\alpha(t_2)| \leq |\alpha(t_1)|$. otherwise, we will show that it is always possible to decompose $\mathcal{D}_\alpha(t_2)$ as

$$\mathcal{D}_\alpha(t_2) = \sum_{i=1}^2 \mathcal{K}_\alpha^i(t_2, t_1)\mathcal{I}_\alpha^i(t_1) \quad (\text{A.12})$$

with channels $\mathcal{K}_\alpha^i(t_2, t_1)$ and completely positive maps $\mathcal{I}_\alpha^i(t_1)$ such that $\mathcal{D}_\alpha(t_1) = \mathcal{I}_\alpha^1(t_1) + \mathcal{I}_\alpha^2(t_1)$. The Choi matrices of the channels and instrument elements are on their support, that is spanned by $|00\rangle$ and $|11\rangle$, explicitly given by

$$I_\alpha^1(t_2) = \begin{pmatrix} \frac{1}{2} & \gamma \\ \gamma^* & \frac{1}{2} \end{pmatrix} \quad I_\alpha^1(t_2) = \begin{pmatrix} \frac{1}{2} & \alpha(t_1) - \gamma \\ \alpha(t_1)^* - \gamma^* & \frac{1}{2} \end{pmatrix} \quad (\text{A.13})$$

and

$$K_\alpha^1(t_2, t_1) = \begin{pmatrix} 1 & \frac{\delta}{\gamma} \\ \frac{\delta^*}{\gamma^*} & 1 \end{pmatrix} \quad K_\alpha^2(t_2, t_1) = \begin{pmatrix} 1 & \frac{\alpha(t_2) - \delta}{\alpha(t_1) - \gamma} \\ \frac{\alpha(t_2)^* - \delta^*}{\alpha(t_1)^* - \gamma^*} & 1 \end{pmatrix} \quad (\text{A.14})$$

and all 2×2 matrices are with respect to the subspace with basis elements $|00\rangle$ and $|11\rangle$. It can be straightforwardly checked that the instrument and the channels satisfy Eq. (A.12). The complex numbers γ and δ are chosen to obey $|\gamma| = |\delta| = 1$ and $|\alpha(t_1) - \gamma| = |\alpha(t_2) - \delta| = 1$. A simple geometric argument reveals that such numbers γ and δ always exists for $\alpha(t_1)$ and $\alpha(t_2)$ on the complex unit disk, see Figure A.1. In this way, the maps are all completely positive which shows that $\mathcal{D}_\alpha(t_2) \in \mathcal{F}[\mathcal{D}_\alpha(t_1)]$.

Therefore, the dephasing dynamics $\mathcal{D}_\alpha(t)$ is an example for a process that shows non-Markovianity that solely arises from classical memory effects.

The following theorem gives characterizes the classical future of a channel. Especially, if the Hilbert space dimension d is finite, there is a fixed bound dependent on d

on the amount of classical memory that is needed to implement a channel in the classical future.

Theorem 1 *The classical future $\mathcal{F}[\mathcal{E}]$ of a quantum channel $\mathcal{E} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ is a compact and convex set. Furthermore, if for a channel $\mathcal{R}$ it holds that $\mathcal{R} \in \mathcal{F}[\mathcal{E}]$, then one has*

$$\mathcal{R} = \sum_{i=1}^L \mathcal{K}^i \mathcal{I}^i \quad (\text{A.15})$$

with $L \leq d^4(d^4 + 1)$ for some set of channels $\{\mathcal{K}^i\}_{i=1}^L$ and an instrument $\{\mathcal{I}^i\}_{i=1}^L$ such that $\sum_{i=1}^L \mathcal{I}^i = \mathcal{E}$.

Proof 3 *We start by proving convexity. Let $\mathcal{R}_1$ and $\mathcal{R}_2$ be quantum channels that are in the classical future $\mathcal{F}[\mathcal{E}]$ of the channel $\mathcal{E}$. Then, these channels admit decompositions of the form*

$$\mathcal{R}_1 = \sum_{i=1}^{L_1} \mathcal{K}_1^i \mathcal{I}_1^i \quad (\text{A.16})$$

$$\mathcal{R}_2 = \sum_{j=1}^{L_2} \mathcal{K}_2^j \mathcal{I}_2^j \quad (\text{A.17})$$

where $\mathcal{K}_l^j$ are quantum channels for all l, j and $\mathcal{I}_l^j$ are completely positive maps such that $\sum_{i=1}^{L_1} \mathcal{I}_1^i = \mathcal{E}_1$ as well as $\sum_{j=1}^{L_2} \mathcal{I}_2^j = \mathcal{E}_2$ and $L_1, L_2 \in \mathbb{N}$. Let now $\mathcal{R}$ be a convex combination, i.e., $\mathcal{R} = \lambda \mathcal{R}_1 + (1 - \lambda) \mathcal{R}_2$ for some $\lambda \in [0, 1]$. Then we get

$$\mathcal{R} = \sum_{i=1}^{L_1} \mathcal{K}_1^i \circ \lambda \mathcal{I}_1^i + \sum_{j=1}^{L_2} \mathcal{K}_2^j \circ (1 - \lambda) \mathcal{I}_2^j \quad (\text{A.18})$$

which shows that $\mathcal{R}$ is in the classical future of $\mathcal{E}$ since $\{\lambda \mathcal{I}_1^i\}_{i=1}^{L_1} \cup \{(1 - \lambda) \mathcal{I}_2^j\}_{j=1}^{L_2}$ is an instrument decomposition of $\mathcal{E}$. Hence, $\mathcal{F}[\mathcal{E}]$ is a convex set.

To show compactness and the bound on the number of instrument elements, notice first that $\mathcal{F}[\mathcal{E}]$ is a subset of the set C_d of all channels $\mathcal{C} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ which is compact and hence bounded. As $\mathcal{F}[\mathcal{E}]$ is a subset of a bounded set, it is certainly bounded and hence it suffices to prove that $\mathcal{F}[\mathcal{E}]$ is closed. The first step for showing this, is to notice that the classical future can be equivalently defined via

$$\mathcal{F}[\mathcal{E}] = \bigcup_{n \in \mathbb{N}} \mathcal{F}_n[\mathcal{E}] \quad (\text{A.19})$$

where the sets $\mathcal{F}_n[\mathcal{E}]$ describe subsets of the classical future that are defined as

$$\mathcal{F}_n[\mathcal{E}] := \left\{ \mathcal{R} : \mathcal{R} = \sum_{i=1}^n \mathcal{K}^i \mathcal{I}^i, \mathcal{K}^i \text{ are channels, } \{\mathcal{I}^i\}_{i=1}^n \text{ is instrument decomposition of } \mathcal{E} \right\}. \quad (\text{A.20})$$

In other words, the sets $\mathcal{F}_n[\mathcal{E}]$ contain elements in the classical future that can be obtained by instruments of size n . In the following, we will show that $\mathcal{F}_n[\mathcal{E}] = \mathcal{F}_{n+1}[\mathcal{E}]$ if $n \geq d^4(d^4 + 1)$. First, $\mathcal{F}_n[\mathcal{E}]$ is compact for each n as it is closed and bounded. $\mathcal{F}_n[\mathcal{E}]$ is closed as it is the image of the continuous map $F_n : \underbrace{C_d \times \cdots \times C_d}_{n \text{ times}} \times I_{d,n}(\mathcal{E}) \rightarrow C_d$ that is defined as

$$F_n(\mathcal{K}^1, \dots, \mathcal{K}^n, \{\mathcal{I}^i\}_{i=1}^n) := \sum_{i=1}^n \mathcal{K}^i \mathcal{I}^i. \quad (\text{A.21})$$

Since the domain $C_d \times \cdots \times C_d \times I_{d,n}(\mathcal{E})$ is closed and continuous maps map closed sets to closed sets, also $\mathcal{F}_n[\mathcal{E}]$ is closed and hence compact. Since $\mathcal{F}_n[\mathcal{E}]$ is a compact set embedded in a finite-dimensional space, its convex hull $\text{conv}(\mathcal{F}_n[\mathcal{E}])$ is a compact convex set, which can be proven by Carathéodory's theorem [72]. By the Krein-Milman theorem [125], $\text{conv}(\mathcal{F}_n[\mathcal{E}])$ is the convex hull of its extreme points which comprise a subset of $\mathcal{F}_n[\mathcal{E}]$. Furthermore, by Carathéodory's theorem [72], every element of $\text{conv}(\mathcal{F}_n[\mathcal{E}])$, and thus every element of $\mathcal{F}_n[\mathcal{E}]$, is a convex combination of at most $d^4 + 1$ extreme points. Now, the question is how the extreme points within $\mathcal{F}_n[\mathcal{E}]$ can be characterised. First, it is easy to see that a necessary condition for $\mathcal{R} \in \mathcal{F}_n(\mathcal{E})$ being extremal is the condition that the corresponding channels $\mathcal{K}^i$ for $i = 1, \dots, n$ as well as the instrument $\{\mathcal{I}^i\}_{i=1}^n$ in the decomposition (A.2) of $\mathcal{R}$ have to be extremal, too. To unravel this requirement further, we have to discuss the extremality of instruments discussed in Refs. [51, 172].

Extremality of an instrument $\{\mathcal{I}^i\}_{i=1}^n$ with $\sum_{i=1}^n \mathcal{I}^i = \mathcal{E}$ means that for all decompositions $\mathcal{I}^i = p\mathcal{I}_1^i + (1-p)\mathcal{I}_2^i$, where $\{\mathcal{I}_1^i\}_{i=1}^n$ and $\{\mathcal{I}_2^i\}_{i=1}^n$ are instruments such that $\sum_{i=1}^n \mathcal{I}_1^i = \sum_{i=1}^n \mathcal{I}_2^i = \mathcal{E}$ and where $p \in (0, 1)$, it holds that $\mathcal{I}_1^i = \mathcal{I}_2^i$ for all i . In the following, we will show that the non-zero elements of an extremal instrument have to form a linearly independent set. Let us assume the opposite statement, that there exists an instrument $\{\mathcal{I}^i\}_{i=1}^n$ with a subset of non-zero instrument elements $\{\mathcal{I}^i\}_{i=1}^{n'}$ such that there exists a non-zero vector $\alpha \in \mathbb{R}^{n'}$ such that $\sum_{i=1}^{n'} \alpha_i \mathcal{I}^i = 0$. This equality would also hold in the Choi picture in the sense that $\sum_{i=1}^{n'} \alpha_i I^i = 0$ where I^i are the

positive semidefinite operators given by the Choi operators of $\mathcal{I}^i$. We can now define the operators

$$I_1^i = (1 + \epsilon \alpha_i) I^i \quad (\text{A.22})$$

$$I_2^i = (1 - \epsilon \alpha_i) I^i \quad (\text{A.23})$$

for some $\epsilon > 0$ such that I_1^i and I_2^i are positive semidefinite for all $i = 1, \dots, n'$. Such an ϵ exists and can for instance be chosen as

$$\epsilon = \max\{r : 1 - |r \alpha_i| \geq 0 \text{ for all } i\}. \quad (\text{A.24})$$

One can see that $\{\mathcal{I}_1^i\}_{i=1}^{n'}$ and $\{\mathcal{I}_2^i\}_{i=1}^{n'}$ are distinct instruments that sum up to $\mathcal{E}$ and that the instrument $\{\mathcal{I}^i\}_{i=1}^{n'}$ can be decomposed as via $\mathcal{I}^i = \frac{1}{2}(\mathcal{I}_1^i + \mathcal{I}_2^i)$ for all $i = 1, \dots, n'$. But this means that $\{\mathcal{I}_1^i\}_{i=1}^{n'}$ is not extremal implying a contradiction. Therefore, we have that the non-zero elements of an extremal instrument are linearly independent.

It follows that extremal instruments $\{\mathcal{I}^i\}_{i=1}^n$ can be represented with at most d^4 elements and together with Carathéodory's theorem, every channel $\mathcal{R} \in \mathcal{F}_n[\mathcal{E}]$ for all $n \in \mathbb{N}$ can be decomposed as

$$\mathcal{R} = \sum_{j=1}^{d^4+1} p_j \mathcal{R}_j = \sum_{j=1}^{d^4+1} \sum_{i=1}^{d^4} p_j \mathcal{K}_j^i \mathcal{I}_j^i = \sum_{i=1}^{d^4(d^4+1)} \mathcal{K}^i \mathcal{I}^i. \quad (\text{A.25})$$

where $\{\mathcal{K}^i\}_i = \bigcup_{j=1, \dots, d^4+1} \{\mathcal{K}_j^l\}_{l=1}^{d^4}$, $\{\mathcal{I}^i\}_i = \bigcup_{j=1, \dots, d^4+1} \{p_j \mathcal{I}_j^l\}_{l=1}^4$ and $\{p_j\}_{j=1}^{d^4+1}$ is a probability distribution. The maps $\mathcal{K}_j^i$ are all extremal channels and $\{\mathcal{I}_j^i\}_{i=1}^{d^2}$ are extremal instruments for all $j \in \{1, \dots, d^4 + 1\}$. It follows that $\mathcal{F}_n[\mathcal{E}] = \mathcal{F}_{n+1}[\mathcal{E}]$ if $n \geq d^4(d^4 + 1)$ so that

$$\mathcal{F}[\mathcal{E}] = \bigcup_{n=1, \dots, d^4(d^4+1)} \mathcal{F}_n[\mathcal{E}] = \mathcal{F}_{d^4(d^4+1)}[\mathcal{E}] \quad (\text{A.26})$$

such that $\mathcal{F}[\mathcal{E}]$ is compact which completes the proof.

A.1.3 SDP relaxations of the classical future

By studying classical futures of quantum channels, quantitative statements about the presence of quantum memory effects in a dynamical process may be deduced. Consider an evolution of quantum mechanical system given by a family $\mathcal{E}(t)$ of quantum channels, parametrised by the time $t \in \mathbb{R}_+$, and pick two time points t_1 and t_2 such that $t_1 < t_2$. If it holds that $\mathcal{E}(t_2) \in F[\mathcal{E}(t_1)]$, the two point dynamics $(\mathcal{E}(t_1), \mathcal{E}(t_2))$, is in accordance with a classical description of potentially emerging

memory effects. Otherwise if $\mathcal{E}(t_2) \notin F[\mathcal{E}(t_1)]$, the dynamics shows the presence of quantum memory.

An important insight for the characterisation of the classical future $\mathcal{F}[\mathcal{E}]$ of a channel $\mathcal{E}$ can be derived from the Choi representation. Technically, the characterisation is based on the form of Choi operators of compositions of quantum maps that is well known, see e.g. Ref. [39, 236], and is described by the following Proposition. For the sake of completeness, a proof of this well known result is added below.

Proposition 3 *Let $\mathcal{C} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^{d'})$ and $\mathcal{E} : \mathcal{L}(\mathbb{C}^{d'}) \rightarrow \mathcal{L}(\mathbb{C}^{d''})$ be maps with Choi operators $C^{\text{AD}} = \mathcal{J}[\mathcal{C}]$ and $E^{\text{D'B}} = \mathcal{J}[\mathcal{E}]$, respectively. Then, the Choi operator $\mathcal{J}[\mathcal{EC}]$ of the composition $\mathcal{EC} : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^{d''})$ is computed as*

$$\mathcal{J}[\mathcal{EC}] = {}^{\text{DD}'} \langle \phi^+ | C^{\text{AD}} \otimes E^{\text{D'B}} | \phi^+ \rangle^{\text{DD}'} \quad (\text{A.27})$$

where $|\phi^+\rangle^{\text{DD}'} = \frac{1}{\sqrt{d'}} \sum_{i=0}^{d'-1} |ii\rangle$ is a maximally entangled state.

Proof 4 *The maps $\mathcal{C}$ and $\mathcal{E}$ can be described via their action on operators $|i\rangle\langle j|$ as*

$$\mathcal{C}[|i\rangle\langle j|] = \sum_{k,j=0}^{d'-1} C_{ij,kl} |k\rangle\langle l| \quad (\text{A.28})$$

$$\mathcal{E}[|i\rangle\langle j|] = \sum_{k,j=0}^{d''-1} E_{ij,kl} |k\rangle\langle l| \quad (\text{A.29})$$

Based on those decompositions, the Choi operator $\mathcal{J}[\mathcal{EC}]$ of the composition $\mathcal{EC}$ reads

$$\mathcal{J}[\mathcal{EC}] = \frac{1}{d} \sum_{i,j=0}^{d-1} |i\rangle\langle j| \otimes \mathcal{E}[\mathcal{C}[|i\rangle\langle j|]] \quad (\text{A.30})$$

$$= \frac{1}{d} \sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d'-1} \sum_{m,n=0}^{d''-1} C_{ij,kl} E_{kl,mn} |i\rangle\langle j| \otimes |m\rangle\langle n| \quad (\text{A.31})$$

$$= \sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d'-1} \sum_{r,s=0}^{d'-1} \sum_{m,n=0}^{d''-1} C_{ij,kl} E_{rs,mn} \langle \phi^+ | kr \rangle \langle rs | \phi^+ \rangle \times (|i\rangle\langle j| \otimes |m\rangle\langle n|) \quad (\text{A.32})$$

$$= {}^{\text{DD}'} \langle \phi^+ | \left(\sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d'-1} C_{ij,kl} |i\rangle\langle j|^{\text{A}} \otimes |k\rangle\langle l|^{\text{D}} \right) \quad (\text{A.33})$$

$$\otimes \left(\sum_{r,s=0}^{d'-1} \sum_{m,n=0}^{d''-1} E_{rs,mn} |r\rangle\langle s|^{\text{D}'} \otimes |m\rangle\langle n|^{\text{B}} \right) | \phi^+ \rangle^{\text{DD}'} \quad (\text{A.34})$$

$$= {}^{\text{DD}'} \langle \phi^+ | C^{\text{AD}} \otimes E^{\text{D'B}} | \phi^+ \rangle^{\text{DD}'} \quad (\text{A.35})$$

where the identity $\langle \phi^+ | ij \rangle = \frac{1}{\sqrt{d}} \delta_{ij}$ has been used for the third equality.

Using Proposition 3, the following criterion for membership in the classical future may be formulated.

Proposition 4 Let $\mathcal{E}, \mathcal{R}$ be channels on a d -dimensional quantum system such that $\mathcal{R} \in \mathcal{F}[\mathcal{E}]$. Then there exists an operator $X^{\text{ADD}'\text{B}} \in \mathcal{L}(\mathbb{C}^d \otimes \mathbb{C}^d \otimes \mathbb{C}^d \otimes \mathbb{C}^d)$ of the form

$$X = \sum_{i=1}^L I_i^{\text{AD}} \otimes K_i^{\text{D}'\text{B}} \quad (\text{A.36})$$

such that $R = {}^{\text{DD}'} \langle \phi^+ | X^{\text{ADD}'\text{B}} | \phi^+ \rangle^{\text{DD}'}$ where R is the Choi matrix of $\mathcal{R}$ and where $|\phi^+\rangle^{\text{DD}'} = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |ii\rangle$. The matrices I_i^{AD} are bipartite positive semidefinite operators satisfying $\sum_{i=1}^L I_i^{\text{AD}} = E$ and $K_i^{\text{D}'\text{B}}$ are bipartite positive semidefinite operators such that $\text{tr}_B(K_i^{\text{D}'\text{B}}) = \frac{\mathbb{1}_d}{d}$ for all $i \in \{1, \dots, L\}$.

Especially, the operator $X^{\text{ADD}'\text{B}}$ is positive semidefinite, separable in the decomposition $\text{AD}|\text{D}'\text{B}$ and fulfills

$$\text{tr}_B(X^{\text{ADD}'\text{B}}) = E^{\text{AD}} \otimes \frac{\mathbb{1}_d}{d}. \quad (\text{A.37})$$

Proof 5 Let $\mathcal{R} \in \mathcal{F}[\mathcal{E}]$. This means we can decompose $\mathcal{R}$ as

$$\mathcal{R} = \sum_{i=1}^L \mathcal{K}^i \mathcal{I}^i$$

with channels $\mathcal{K}^i$ and an instrument decomposition $\{\mathcal{I}^i\}_{i=1}^L$ of $\mathcal{E}$. The Choi operator $R = \mathcal{J}[\mathcal{R}]$ can then, by linearity of the Choi isomorphism, be decomposed as

$$R = \sum_{i=1}^L \mathcal{J}[\mathcal{K}^i \mathcal{I}^i] = \sum_{i=1}^L {}^{\text{DD}'} \langle \phi^+ | I_i^{\text{AD}} \otimes K_i^{\text{D}'\text{B}} | \phi^+ \rangle^{\text{DD}'} \quad (\text{A.38})$$

where the second equality follows from Proposition 3. Now for the operator $X^{\text{ADD}'\text{B}}$ given by

$$X^{\text{ADD}'\text{B}} = \sum_{i=1}^L I_i^{\text{AD}} \otimes K_i^{\text{D}'\text{B}}$$

it holds that

$$\text{tr}_B(X^{\text{ADD}'\text{B}}) = \sum_{i=1}^L I_i^{\text{AD}} \otimes \text{tr}_B(K_i^{\text{D}'\text{B}}) = \sum_{i=1}^L I_i^{\text{AD}} \otimes \frac{\mathbb{1}_d}{d} = E^{\text{AD}} \otimes \frac{\mathbb{1}_d}{d}. \quad (\text{A.39})$$

Proposition 4 gives rise to a necessary criterion that a channel $\mathcal{R}$ belongs to the classical future of another channel $\mathcal{E}$, that is formulated in form of a certain separability property. Inverting the logic, a violation of this necessary condition directly certifies the presence of quantum memory within the dynamics. The criterion described by Proposition 4 can thus be used to detect and quantify the presence of quantum memory. However, this detection criterion is equivalent to characterisation of separable quantum states that in general is known to be NP-hard [93].

Definition 2 Let $\mathcal{E}$ be a quantum channel. The PPT-relaxation $\mathcal{F}_{\text{PPT}}[\mathcal{E}]$ of the classical future $\mathcal{F}[\mathcal{E}]$ is defined by the set of channels $\mathcal{G}$ for which there exists a positive semidefinite operator $X^{\text{ADD}'\text{B}}$ such that

$$(X^{\text{ADD}'\text{B}})^{T_{\text{AD}}} \succcurlyeq 0 \quad (\text{A.40})$$

$$R^{\text{AB}} = {}^{\text{DD}'}\langle \phi^+ | X^{\text{ADD}'\text{B}} | \phi^+ \rangle^{\text{DD}'} \quad (\text{A.41})$$

$$\text{tr}_B(X^{\text{ADD}'\text{B}}) = E^{\text{AD}} \otimes \frac{\mathbb{I}_d}{d} \quad (\text{A.42})$$

where R^{AB} and E^{AD} are the Choi operators of $\mathcal{R}$ and $\mathcal{E}$, respectively.

The set $\mathcal{F}_{\text{PPT}}[\mathcal{E}]$ is an outer approximation of the classical future in the sense that $\mathcal{F}[\mathcal{E}] \subset \mathcal{F}_{\text{PPT}}[\mathcal{E}]$.

To still make predictions about the presence of quantum memory, we make use of the PPT criterion which provides an outer approximation of the set of positive semidefinite separable operators.

A.1.4 Witnesses of quantum memory

As a witness of quantum memory, we consider observables whose value can detect the presence of quantum memory. Before, we have argued that quantum memory is present if the channel $\mathcal{E}(t_2)$ does not lie in the classical future of the channel $\mathcal{E}(t_1)$ for an earlier time $t_1 \leq t_2$. Given those time points, information about the process can be extracted by state preparations at $t = 0$, measurements at $t = t_1$ and measurements at $t = t_2$. Using the Choi representation of quantum channels, witnesses of quantum memory can be defined as follows.

Definition 3 A pair of hermitian observables $W_1^{\text{AB}}, W_2^{\text{AD}} \in \mathcal{L}(\mathbb{C}^d \otimes \mathbb{C}^d)$ is a witness of quantum memory if it holds that

$$\text{tr}(W_1^{\text{AB}} E_1^{\text{AB}}) + \text{tr}(W_2^{\text{AD}} E_2^{\text{AD}}) \geq 0 \quad (\text{A.43})$$

for all Choi matrices E_1^{AB} and E_2^{AD} of channels $\mathcal{E}_1, \mathcal{E}_2 : \mathcal{L}(\mathbb{C}^d) \rightarrow \mathcal{L}(\mathbb{C}^d)$ such that $\mathcal{E}_2 \in \mathcal{F}[\mathcal{E}_1]$.

An important subset of quantum memory witnesses, constructed from the PPT relaxation of the classical future, is characterized by the following Theorem.

Theorem 2 Let $W_1^{\text{AB}}, W_2^{\text{AD}} \in \mathcal{L}(\mathbb{C}^d \otimes \mathbb{C}^d)$ be a pair of hermitian observables such that there exists positive operators Q^{ABCD} and F^{ABCD} such that

$$W_1^{\text{AB}} \otimes \mathbb{I}^{\text{CD}} + P_{\text{B} \leftrightarrow \text{DD}'}(W_2^{\text{AD}} \otimes \Phi_+^{\text{BC}})P_{\text{B} \leftrightarrow \text{DD}'}^\dagger = Q^{\text{ADD'B}} + (F^{\text{ADD'B}})^{T_{\text{D'B}}}. \quad (\text{A.44})$$

Then the pair $W_1^{\text{AB}}, W_2^{\text{AD}}$ is a witness of quantum memory.

Proof 6 Let $\mathcal{E}_1$ and $\mathcal{E}_2$ be a pair of channels such that $\mathcal{E}_2 \in \mathcal{F}[\mathcal{E}_1]$. By Proposition 4 there exists a positive operator X^{ABCD} such that $\text{tr}_B(X^{\text{ADD'B}}) = E_1^{\text{AD}} \otimes \frac{\mathbb{I}^{\text{D'}}}{d}$ and $E_2^{\text{AB}} = {}^{\text{DD'}}\langle \phi^+ | X^{\text{ADD'B}} | \phi^+ \rangle^{\text{DD'}}$. Now, a straightforward calculation reveals

$$\text{tr}(W_1^{\text{AD}} E_1^{\text{AD}}) + \text{tr}(W_2^{\text{AB}} E_2^{\text{AB}}) \quad (\text{A.45})$$

$$= \text{tr}(W_1^{\text{AD}} \otimes \mathbb{I}_{\text{D'}} E_1^{\text{AD}} \otimes \frac{\mathbb{I}^{\text{D'}}}{d}) + \text{tr}(W_2^{\text{AB}} {}^{\text{DD'}}\langle \phi^+ | X^{\text{ADD'B}} | \phi^+ \rangle^{\text{DD'}}) \quad (\text{A.46})$$

$$= \text{tr}(W_1^{\text{AD}} \otimes \mathbb{I}_{\text{D'}} \text{tr}_D(X^{\text{ADD'B}})) + \text{tr}(P_{\text{B} \leftrightarrow \text{DD}'}(W_2^{\text{AD}} \otimes \Phi_+^{\text{BC}})P_{\text{B} \leftrightarrow \text{DD}'}^\dagger X^{\text{ADD'B}}) \quad (\text{A.47})$$

$$= \text{tr}((W_1^{\text{AD}} \otimes \mathbb{I}_{\text{D'B}} + P_{\text{B} \leftrightarrow \text{DD}'}(W_2^{\text{AD}} \otimes \Phi_+^{\text{BC}})P_{\text{B} \leftrightarrow \text{DD}'}^\dagger) X^{\text{ADD'B}}) \quad (\text{A.48})$$

$$= \text{tr}((Q^{\text{ADD'B}} + (F^{\text{ADD'B}})^{T_{\text{D'B}}}) X^{\text{ADD'B}}) \quad (\text{A.49})$$

$$= \text{tr}(Q^{\text{ADD'B}} X^{\text{ADD'B}}) + \text{tr}(F^{\text{ADD'B}}(X^{\text{ADD'B}})^{T_{\text{D'B}}}) \geq 0 \quad (\text{A.50})$$

showing that W_1^{AB} and W_2^{AD} are a witness of quantum memory.

The memory witnesses defined above in 3 are associated to the Choi operators E_1 and E_2 of quantum channels $\mathcal{E}_1$ and $\mathcal{E}_2$. One might ask how these witnesses are measured in practice. To answer this question, notice that the observables W_l can be expanded in some local basis via $W_l = \sum_{i,j=0}^{d-1} w_{ij}^l \hat{\sigma}_i \otimes \hat{\sigma}_j$. This leads to the equation

$$\text{tr}(W_l E_l) = \sum_{ij} w_{ij}^l \text{tr}(\mathcal{E}_l(\hat{\sigma}_i^T) \hat{\sigma}_j) \quad (\text{A.51})$$

and allows to measure W_l "on the channel E_l " by preparing suitable states, acting on them with $\mathcal{E}_l$ and finally performing a suitable measurement.

To illustrate, let us consider the example of a qubit system and the observable $W = \hat{\sigma}_x \otimes \hat{\sigma}_z$. To measure W with respect to a Choi matrix E of a qubit channel $\mathcal{E}$, it suffices

to prepare the eigenstates $|+\rangle\langle+|$ and $|-\rangle\langle-|$, let the system evolve and finally measure in the Z -basis. The obtained probabilities can be post-processed to get the expectation value $\text{tr}(WE) = \langle 1|\mathcal{E}[|+\rangle\langle+||1\rangle + \langle 0|\mathcal{E}[|-\rangle\langle-||0\rangle - \langle 0|\mathcal{E}[|+\rangle\langle+||0\rangle - \langle 1|\mathcal{E}[|-\rangle\langle-||1\rangle]$.

A.2 Quantum memory detection in giant atom dynamics

In this part, we will provide the proofs of quantum memory detection criteria in the specific dynamics of two and three-level artificial giant atoms.

A.2.1 Two-level giant atom dynamics

Based on the Choi state of the dynamical map in Eq. (4.12), we can investigate the properties of the dynamical map. The distinction between Markovianity, classical memory and quantum memory for the two-level system can be characterised as follows.

Theorem 3 *The two-point dynamics $(\mathcal{E}(t_1), \mathcal{E}(t_2))$ of the two-level system with $\mathcal{E}(t)$ as given in Eq. (4.7)-(4.10) can be implemented with classical memory if and only if*

$$|G(t_1)| \geq |G(t_2)| \quad (\text{A.52})$$

with $G(t)$ defined in Eq. (4.11). Furthermore, if $(\mathcal{E}(t_1), \mathcal{E}(t_2))$ is classical, it is even Markovian (CP-divisible) in the sense that there exists a channel $\mathcal{K}(t_2, t_1)$ such that

$$\mathcal{E}(t_2) = \mathcal{K}(t_2, t_1)\mathcal{E}(t_1) \quad (\text{A.53})$$

Proof 7 *For the first direction assume that $|G(t_1)| \geq |G(t_2)|$. Then the Choi matrix K of the map $\mathcal{K}(t_2, t_1)$ takes the form*

$$K = \frac{1}{2} \begin{pmatrix} \frac{|G(t_2)|^2}{|G(t_1)|^2} & 0 & 0 & \frac{G^*(t_2)}{G^*(t_1)} \\ 0 & \frac{|G(t_1)|^2 - |G(t_2)|^2}{|G(t_1)|^2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{G(t_2)}{G(t_1)} & 0 & 0 & 1 \end{pmatrix} \quad (\text{A.54})$$

which is the Choi matrix of a quantum channel since $|G(t_1)| \geq |G(t_2)|$. Hence, $(\mathcal{E}(t_1), \mathcal{E}(t_2))$ is CP-divisible which clearly implies that it can be implemented with classical memory.

For the other direction, assume that $(\mathcal{E}(t_1), \mathcal{E}(t_2))$ can be implemented with classical memory, i.e., $\mathcal{E}(t_2) \in \mathcal{F}[\mathcal{E}(t_1)]$. This means that there is a subchannel decomposition $\mathcal{I}^l(t_1)$ of $\mathcal{E}(t_1)$ and channels $\mathcal{K}(t_2, t_1)^l$ such that

$$\mathcal{E}(t_2) = \sum_l \mathcal{K}^l(t_2, t_1) \mathcal{I}^l(t_1) \quad (\text{A.55})$$

Assume now that $\mathcal{I}(t_1)$ is the Choi operator of a subchannel $\mathcal{I}(t_1)$ of $\mathcal{E}(t_1)$, i.e., $0 \leq \mathcal{I}(t_1) \leq E(t_1)$ where $E(t_1)$ is the Choi operator of $\mathcal{E}(t_1)$. Furthermore assume that there is a channel $\mathcal{N}(t_2, t_1)$ such that $\mathcal{R}(t_2) := \mathcal{N}(t_2, t_1) \mathcal{I}(t_1)$ is a subchannel of $\mathcal{E}(t_2)$. From the action (4.7)-(4.10) of $\mathcal{E}(t)$ it is easy to see that the operators $|g\rangle\langle e|$, $|e\rangle\langle g|$ and $|e\rangle\langle e|$ are eigenvectors of $\mathcal{R}(t_2)$ and $\mathcal{I}(t_1)$ which implies that they must also be eigenvectors of the channel $\mathcal{N}(t_2, t_1)$. Furthermore, since the operators $\mathcal{I}(t_1)[|g\rangle\langle g|]$ and $\mathcal{R}(t_2)[|g\rangle\langle g|]$ live on the subspace spanned by $|g\rangle\langle g|$ and $|e\rangle\langle e|$, it has to hold true that $\mathcal{N}(t_2, t_1)[|g\rangle\langle g|]$ is also part of this subspace. Taking the above considerations into account, the Choi operator $N(t_2, t_1)$ of the channel $\mathcal{N}(t_2, t_1)$ must be of the form

$$N(t_2, t_1) = \frac{1}{2} \begin{pmatrix} n_{gg,gg} & 0 & 0 & n_{ge,ge} \\ 0 & n_{gg,ee} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ n_{eg,eg} & 0 & 0 & 1 \end{pmatrix}. \quad (\text{A.56})$$

From this, one obtains the equality

$$\langle e | \mathcal{R}(t_2) [|g\rangle\langle g|] | e \rangle = \langle e | \mathcal{I}(t_1) [|g\rangle\langle g|] | e \rangle + \underbrace{n_{gg,ee} \langle g | \mathcal{I}(t_1) [|g\rangle\langle g|] | g \rangle}_{\geq 0} \quad (\text{A.57})$$

so that

$$\langle e | \mathcal{I}(t_1) [|g\rangle\langle g|] | e \rangle \leq \langle e | \mathcal{R}(t_2) [|g\rangle\langle g|] | e \rangle. \quad (\text{A.58})$$

Together with Eq. (A.55), Eq. (A.58) implies that

$$\langle e | \mathcal{E}(t_1) [|g\rangle\langle g|] | e \rangle \leq \langle e | \mathcal{E}(t_2) [|g\rangle\langle g|] | e \rangle \quad (\text{A.59})$$

which is equivalent to

$$|G(t_1)| \geq |G(t_2)|. \quad (\text{A.60})$$

A.2.2 Three-level giant atom dynamics

The quantum dynamical map governing the three-level giant atom dynamics is obtained from Eqs. (4.14)-(4.22), and its Choi state is given in (4.23). The presence of quantum memory for such a quantum process can then be characterised as follows.

Theorem 4 *The two-point dynamics $(\mathcal{E}(t_1), \mathcal{E}(t_2))$ with $\mathcal{E}(t)$ as given in Eq. (4.14)-(4.22) can be implemented with classical memory if and only if*

$$S(t_2) \geq S(t_1) \quad (\text{A.61})$$

$$S(t_1) + |G(t_1)|^2 \geq S(t_2) + |G(t_2)|^2. \quad (\text{A.62})$$

For the proof of Theorem 4 we need the following technical proposition.

Proposition 5 *Let $\mathcal{E}, \mathcal{R} : \mathcal{L}(\mathbb{C}^3) \rightarrow \mathcal{L}(\mathbb{C}^3)$ be completely positive maps with corresponding Choi operators $E = \mathcal{J}(\mathcal{E})$ and $G = \mathcal{J}(\mathcal{R})$ that are both elements of the subspace of matrices M parametrised as*

$$M = \begin{pmatrix} a & 0 & 0 & 0 & b & 0 & c & d & e \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b^* & 0 & 0 & 0 & f & 0 & g & h & j \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c^* & 0 & 0 & 0 & g^* & 0 & k & l & m \\ d^* & 0 & 0 & 0 & h^* & 0 & l^* & n & p \\ e^* & 0 & 0 & 0 & j^* & 0 & m^* & p^* & r \end{pmatrix}. \quad (\text{A.63})$$

If there exists a completely positive and trace-preserving map $\mathcal{K} : \mathcal{L}(\mathbb{C}^3) \rightarrow \mathcal{L}(\mathbb{C}^3)$ such that

$$\mathcal{R} = \mathcal{K}\mathcal{E}, \quad (\text{A.64})$$

then the inequalities

$$k_R \geq k_E \quad (\text{A.65})$$

$$n_R \geq n_E \quad (\text{A.66})$$

hold where k_R is the k -component of the Choi matrix R according to the parametrisation (A.63).

Proof 8 We first show that the Choi operator $K = \mathcal{J}(\mathcal{K})$ is also parametrised as in Eq. (A.63). To see this, notice that from Eq. (A.63) one can read off that the operators $|g\rangle\langle g|$, $|s\rangle\langle s|$, $|g\rangle\langle s|$ and $|s\rangle\langle g|$ are all eigenvectors of the maps $\mathcal{E}$ and $\mathcal{G}$ with eigenvalues $a_{E/G}$, $f_{E/G}$, $b_{E/G}$ and $b_{E/G}^*$, respectively. Consequently these operators are also eigenvectors of $\mathcal{K}$, already giving rise to the correct parametrisation of the four upper left 3×3 matrix blocks of K . Next, consider $\mathcal{R}[|g\rangle\langle e|]$ that via Eq. (A.63) and (A.64) is computed as

$$\mathcal{R}[|g\rangle\langle e|] = \mathcal{K}\mathcal{E}[|g\rangle\langle e|] = c_E \mathcal{K}[|g\rangle\langle s|] + d_E \mathcal{K}[|g\rangle\langle g|] + e_E \mathcal{K}[|g\rangle\langle e|] \quad (\text{A.67})$$

$$= c_E a_K |g\rangle\langle g| + d_E b_K |g\rangle\langle s| + e_E \mathcal{K}[|g\rangle\langle e|] \quad (\text{A.68})$$

$$= c_R |g\rangle\langle g| + d_R |g\rangle\langle s| + e_R |g\rangle\langle e| \quad (\text{A.69})$$

which shows that there exists numbers c_K , d_K and e_K such that

$$\mathcal{K}[|g\rangle\langle e|] = c_K |g\rangle\langle g| + d_K |g\rangle\langle s| + e_K |g\rangle\langle e|. \quad (\text{A.70})$$

Hence, K has also correct the parametrisation for the upper right and lower left 3×3 blocks. By analogous reasoning for the decomposition of $\mathcal{K}[|g\rangle\langle s|]$, one can conclude that K is of the form (A.63).

Furthermore, $\mathcal{K}$ is assumed to be trace-preserving which implies that $a_K = f_K = 1$ and $c_K = h_K = 0$. From that and Eq. (A.64), k_E and k_R are related via

$$k_R = k_E + r_E k_K. \quad (\text{A.71})$$

If $r_E = 0$, we get that $k_R = k_E$. Otherwise if $r_E > 0$, we have that

$$k_K = \frac{k_R - k_E}{r_E} \quad (\text{A.72})$$

and since $\mathcal{K}$ is completely positive, we have $k_K \geq 0$ and hence $k_R \geq k_E$. By similar reasoning, one also obtains the inequality $h_R \geq h_E$.

Appendix to Chapter 5 and 6

This appendix presents the magnetization plot for the Curie-Weiss model along with its interpretation, which aids in understanding Chapter 5 and Chapter 6. Additionally, it provides detailed derivations of key quantities related to the probe QFI, which quantifies the precision of temperature estimation using a phase probe, as well as the decoherence function in the HTE of the Ising model discussed in Chapter 6.

B.1 Magnetization in Curie-Weiss model

In the Curie-Weiss model, described by the Hamiltonian (5.14), the system undergoes a phase transition between a disordered paramagnetic phase and an ordered ferromagnetic phase as the temperature varies, as shown in Fig. B.1. At high temperatures ($J\beta < J\beta_c$), thermal fluctuations dominate over spin-spin interactions, preventing long-range order and causing the spins to orient randomly. In this regime, the system remains in the paramagnetic phase, with the magnetization m_0 approaching zero. At the critical temperature ($J\beta_c = 1$), the system reaches a phase transition point characterized by strong spin correlations and critical fluctuations. Here, the magnetization undergoes a rapid but continuous change, indicating the emergence of ordering, though it remains relatively small. Below the critical temperature ($J\beta > J\beta_c$), spin-spin interactions become dominant, leading to spontaneous alignment of spins and the onset of ferromagnetic order. In this phase, the system exhibits a nonzero magnetization even in the absence of an external field, a phenomenon known as spontaneous magnetization.

B.2 QFI derivation for Curie-Weiss model

To derive the expression (6.15) for the QFI of the phase probe in the Curie-Weiss model, we start from the approximate decoherence factor $D_t(\beta)$ in the thermodynamic limit, as given in (6.14). To obtain the QFI using (6.10), we need to compute the derivative of $D_t(\beta)$ with respect to β ,

$$\partial_\beta D_t(\beta) = e^{-i\tilde{g}tm_0 - \tilde{g}^2 t^2 / [2N f''(m_0)]} \left(-i\tilde{g}t \frac{\partial m_0}{\partial \beta} + \frac{\tilde{g}^2 t^2}{2N f''(m_0)^2} \frac{\partial f''(m_0)}{\partial \beta} \right). \quad (\text{B.1})$$

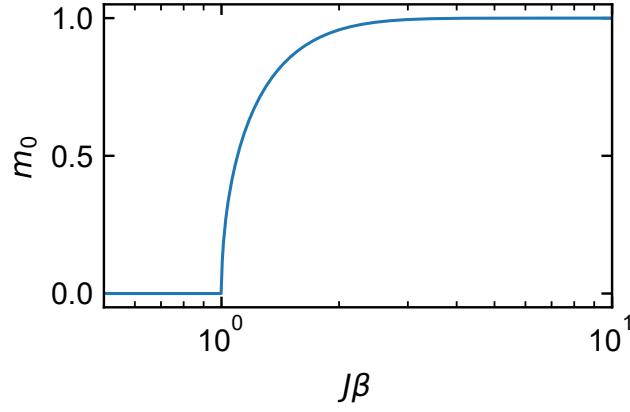


Fig. B.1.: Magnetization in Curie-Weiss model in the absence of magnetic field.

From this we obtain the terms

$$\begin{aligned}
 |\partial_\beta D_t(\beta)|^2 &= e^{-\tilde{g}^2 t^2 / [N f''(m_0)]} \left(\tilde{g}^2 t^2 \left(\frac{\partial m_0}{\partial \beta} \right)^2 + \frac{\tilde{g}^4 t^4}{4 N^2 f''(m_0)^4} \left(\frac{\partial f''(m_0)}{\partial \beta} \right)^2 \right), \\
 D_t(\beta)^* \partial_\beta D &= e^{-\tilde{g}^2 t^2 / [N f''(m_0)]} \left(-i \tilde{g} t \frac{\partial m_0}{\partial \beta} + \frac{\tilde{g}^2 t^2}{2 N f''(m_0)} \frac{\partial f''(m_0)}{\partial \beta} \right), \\
 D_t(\beta) \partial_\beta D^* &= e^{-\tilde{g}^2 t^2 / [N f''(m_0)]} \left(i \tilde{g} t \frac{\partial m_0}{\partial \beta} + \frac{\tilde{g}^2 t^2}{2 N f''(m_0)} \frac{\partial f''(m_0)}{\partial \beta} \right), \\
 |D_t(\beta)|^2 &= e^{-\tilde{g}^2 t^2 / [N f''(m_0)]}.
 \end{aligned} \tag{B.2}$$

Now, making use of the fact that $f''(m_0) = 1/(1 - m_0^2) - J\beta$, we can take the derivative of the magnetization m_0 with respect to β in the self-consistency equation (5.19) at $h = 0$ and get

$$\begin{aligned}
 \frac{\partial m_0}{\partial \beta} &= \underbrace{\left[1 - \tanh^2(J\beta m_0) \right]}_{=1-m_0^2} \left(J m_0 + J\beta \frac{\partial m_0}{\partial \beta} \right) \\
 \Rightarrow \frac{\partial m_0}{\partial \beta} &= \frac{J m_0 (1 - m_0^2)}{1 - J\beta (1 - m_0^2)} = \frac{J m_0}{f''(m_0)}.
 \end{aligned} \tag{B.3}$$

Plugging all these expressions into Eq. (6.10) yields

$$\begin{aligned}
\mathcal{F}_\beta^Q(t) &= e^{-\tilde{g}^2 t^2 / [N f''(m_0)]} \tilde{g}^2 t^2 \left(\frac{\partial m_0}{\partial \beta} \right)^2 + \frac{e^{-\tilde{g}^2 t^2 / [N f''(m_0)]}}{1 - e^{-\tilde{g}^2 t^2 / [N f''(m_0)]}} \frac{\tilde{g}^4 t^4}{4 N^2 f''(m_0)^4} \\
&\times \left(\frac{\partial f''(m_0)}{\partial \beta} \right)^2 \\
&= e^{-\tilde{g}^2 t^2 / [N f''(m_0)]} \frac{J^2 m_0^2 \tilde{g}^2 t^2}{f''(m_0)^2} + \frac{e^{-\tilde{g}^2 t^2 / [N f''(m_0)]}}{1 - e^{-\tilde{g}^2 t^2 / [N f''(m_0)]}} \\
&\times \frac{J^2 \tilde{g}^4 t^4 [(1 - m_0^2)^2 f''(m_0) - 2 m_0^2]^2}{4 N^2 (1 - m_0^2)^4 f''(m_0)^6} \\
&= \frac{J^2}{4} \frac{[(1 - m_0^2)^2 f''(m_0) - 2 m_0^2]^2}{(1 - m_0^2)^4 [f''(m_0)]^4} \frac{t^4 / \tau^4(\beta)}{e^{t^2 / \tau^2(\beta)} - 1} \\
&+ N J^2 \frac{m_0^2}{f''(m_0)} \frac{t^2}{\tau^2(\beta)} e^{-t^2 / \tau^2(\beta)}, \tag{B.4}
\end{aligned}$$

where $\tau(\beta) = \sqrt{N f''(m_0)} / \tilde{g}$ sets the coherence decay time scale. The last equation is stated in (6.15).

B.3 Derivation in high temperature expansion

At high temperature, we can expand the partition function to the second order in $\tanh(\beta J)$ as

$$\begin{aligned}
\mathcal{Z} &= \text{tr} \left\{ e^{\beta \sum_{\langle ij \rangle} J \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j} \right\} \tag{B.5} \\
&= \text{tr} \left\{ \prod_{\langle ij \rangle} \left[\cosh(\beta J) + \sinh(\beta J) \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j \right] \right\} \\
&\approx \text{tr} \left\{ \cosh^K(\beta J) \left[1 + \tanh(\beta J) \sum_{\langle ij \rangle} \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j \right. \right. \\
&\quad \left. \left. + \tanh^2(\beta J) \sum_{\langle ij \rangle < \langle kl \rangle} (\hat{\sigma}_z^i \otimes \hat{\sigma}_z^j)(\hat{\sigma}_z^k \otimes \hat{\sigma}_z^l) \right] \right\} \\
&= 2^N \cosh^K(\beta J),
\end{aligned}$$

where the K is the total number of pair bonds (i.e., interacting spin pairs) in the lattice. The double sum over pair bonds in the fourth line counts each pair only once. To obtain the final form, notice that the first- and second-order terms in $\tanh(\beta J)$ in the third and fourth line vanish when taking the trace, since there are always at least two distinct spins contributing a factor $\text{tr}\{\hat{\sigma}_z^i\} = 0$. Here, the first non-vanishing contribution would come from the fourth-order summation over

products of four pair bonds forming a closed loop between four adjacent spins [196]: $\langle ij \rangle, \langle jk \rangle, \langle kl \rangle, \langle li \rangle$.

The phase probe's decoherence function (6.19) expands as

$$\begin{aligned} D_t(\beta) &= \frac{1}{Z} \text{tr} \left\{ e^{\beta \sum_{\langle ij \rangle} J \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j} e^{-igt \hat{Z}_n} \right\} \\ &\approx \frac{1}{Z} \cosh^K(\beta J) \left[\text{tr} \left\{ e^{-igt \hat{Z}_n} \right\} + \tanh(\beta J) \sum_{\langle ij \rangle} \text{tr} \left\{ (\hat{\sigma}_z^i \otimes \hat{\sigma}_z^j) e^{-igt \hat{Z}_n} \right\} \right. \\ &\quad \left. + \tanh^2(\beta J) \sum_{\langle ij \rangle < \langle kl \rangle} \text{tr} \left\{ (\hat{\sigma}_z^i \otimes \hat{\sigma}_z^j) (\hat{\sigma}_z^k \otimes \hat{\sigma}_z^l) e^{-igt \hat{Z}_n} \right\} \right], \end{aligned} \quad (\text{B.6})$$

with the moments of the n -site cluster's magnetization $\hat{Z} = \sum_{i=1}^n \hat{\sigma}_z^i$. Here, the first- and second-order terms in $\tanh(\beta J)$ no longer vanish due to the additional unitary generated by the cluster magnetization $\hat{Z}_n$. Writing

$$e^{-igt \hat{Z}_n} = \cos^n(gt) \prod_{m=1}^n [1 - i \tan(gt) \hat{\sigma}_z^m], \quad (\text{B.7})$$

we see that the first-order term in the third line of (B.6) adds a term $\propto \tan^2(gt)$ for every pair bond $\langle ij \rangle$ whose both spins are contained in the cluster. Let K_{12} denote the number of such intra-cluster pair bonds. For the second-order term in the fourth line of (B.6), non-vanishing contributions can come from doublets of pair bonds with at least two spins inside the cluster, as illustrated in Fig. 6.7: K_{22} counts the number of pair bond doublets with two spins inside and one mutual spin outside the cluster, K_{23} counts doublets of intra-cluster pair bonds with one mutual spin, and $K_{24} = K_{12}(K_{12} - 1)/2 - K_{23}$ counts doublets of intra-cluster pair bonds with no mutual spin. We arrive at

$$\begin{aligned} D_t(\beta) &= \cos^n(gt) \left\{ 1 - \tanh(\beta J) \tan^2(gt) \right. \\ &\quad \left. \times \left[K_{12} - \tanh(\beta J) (K_{22} + K_{23} - \tan^2(gt) K_{24}) \right] \right\}. \end{aligned}$$