Quantum Quench and Coherent-Incoherent Dynamics of Ising Chains Interacting with Dissipative Baths

Reshmi Dani[1] and Nancy Makri[1,2,3,*]

[1]*Department of Chemistry, University of Illinois, Urbana, Illinois 61801*
[2]*Department of Physics, University of Illinois, Urbana, Illinois 61801*
[3]*Illinois Quantum Information Science and Technology Center*

[*]*Corresponding Author. Email: nmakri@illinois.edu*

Abstract

The modular path integral (MPI) methodology is used to extend the well-known spin-boson dynamics to finite-length quantum Ising chains where each spin is coupled to a dissipative harmonic bath. The chain is initially prepared in the ferromagnetic phase where all spins are aligned, and the magnetization is calculated with spin-spin coupling parameters corresponding to the paramagnetic phase, mimicking a quantum quench experiment. The observed dynamics is found to depend significantly on the location of the tagged spin. In the absence of a dissipative bath the time evolution displays irregular patterns that arise from multiple frequencies associated with the eigenvalues of the chain Hamiltonian. Coupling of each spin to a harmonic bath leads to smoother dynamics, with damping effects that are stronger compared to those observed in the spin-boson model and more prominent in interior spins, a consequence of additional damping from the spin environment. Interior spins exhibit a transition from underdamped oscillatory to overdamped monotonic dynamics as the temperature, spin-bath or spin-spin coupling is increased. In addition to these behaviors, a new dynamical pattern emerges in the evolution of edge spins with strong spin-spin coupling at low and intermediate temperatures, where the magnetization oscillates either above or below the equilibrium value.

I. Introduction

The model of a two-level system (TLS) coupled to a harmonic bath continues to serve as the simplest paradigm of quantum dissipative dynamics, where the interaction with an environment quenches the coherent tunneling oscillations of the isolated TLS. The degree of quenching depends on the strength of TLS-bath coupling, the temperature, as well as the spectral characteristics of the bath, giving rise to very rich behaviors.[1] In addition to its purely theoretical value for understanding the interplay between coherent tunneling and dissipation, the physics of the dissipative TLS is relevant to many chemical processes, such as charge transfer or spin dynamics, and is fundamental to nonadiabatic dynamical phenomena, which are ubiquitous in molecular systems.

It is natural to expect even more complex dynamics in the case where two or more interacting TLSs are coupled to dissipative environments. Such collections of coupled TLSs are common in magnetic materials, where dissipative interactions arise from coupling of the spins to phonons or molecular vibrations. A variety of crystals and metal-organic frameworks with interesting spin topologies have been identified, synthesized, and studied (for example, see [2-7]). The order/disorder behavior, coherence, relaxation and entanglement properties of the spins in such systems are of interest from the perspective of quantum information transfer. In the absence of dissipative bath effects, arrays of interacting TLSs are known as generalized Heisenberg models,[8] and their ground state properties, in various dimensions and topologies, have been intensely investigated. Molecular wires[9] and excitation energy transfer[10] are often described in terms of the Hückel or tight-binding model, which is a special case of the Heisenberg Hamiltonian with a restricted state space. In the special case of a one-dimensional arrangement where the spins are coupled only along the z direction, the model reduces to the famous quantum (or transverse-field) Ising chain. Each of these models displays its own characteristic behaviors, and the diversity of phenomena that can arise from coupled spin Hamiltonians is intriguing.

The quantum Ising model was introduced by de Gennes[11] to describe hydrogen bonding in ferroelectrics. Experimental realizations in ferromagnetic quasi-one-dimensional cobalt niobate in transverse magnetic fields[12] and in systems of cold rubidium atoms confined in an optical lattice[13] have been reported. The infinite quantum Ising chain of identical spins has been solved analytically[14,15] by transforming the interacting spin operators to non-interacting spinless fermions using the Jordan-Wigner transformation and then diagonalizing the transformed Hamiltonian with the aid of the Bogoliubov technique.[16] These and many other analytical tools, primarily renormalization group techniques, have led to valuable insights and a good understanding of important aspects surrounding the intriguing physics that characterizes the quantum phase transition of the isolated Ising chain.[17] More recently, similar studies have been reported on spin chains that include coupling to dissipative baths.[18,19] Numerical investigations of finite-length spin chains have been carried out[20] with methods based on the density matrix renormalization group (DMRG) formulation.[21,22] Imaginary-time path integral calculations have been employed to investigate instanton tunneling paths that connect the two states of aligned spins[23] and to identify critical exponents in Ising chains coupled to dissipative baths.[24]

The two parameters that characterize the quantum Ising model are the tunneling frequency Ω of individual spins (determined by the magnitude of the transverse field) and the spin-spin interaction strength J. These two parameters act against each other, giving rise to an ordered (ferromagnetic) phase with two degenerate ground states and a disordered (paramagnetic) phase with a single ground state, which (in an infinite chain) are separated by a phase transition at zero temperature.[25] This behavior is of much interest in quantum statistical physics and also from the perspective of quantum quench dynamics.[26-29] The quantum Ising chain is also of interest in the design of quantum computers, which rely on the entanglement properties of qubits. For example, adiabatic passage through the quantum phase transition can generate a maximally entangled spin state.[30] The coherence-quenching effects of interacting qubits constitute an important guiding principle in the design of materials for quantum information science (QIS).[6] Dissipative effects are critical in that regard, as they can easily destroy the coherence and entanglement of coupled spins.

In this paper we investigate the dynamics of the spin magnetization in relatively short quantum Ising chains in the presence of dissipative harmonic baths attached to the spins. In contrast to previous studies, we simulate the *real-time evolution* of individual spins in various parameter regimes. We use our simulation results to characterize the behavior of the quantum Ising chain in comparison to that of the simpler, single TLS coupled to a bath. Our emphasis is on the coherence properties of the spin dynamics and on edge effects during a quantum quench, where the system evolves under the Hamiltonian that corresponds to the paramagnetic (disordered) phase following preparation in the ordered, ferromagnetic phase (aligned spins). To maintain the relevance of the model to molecular aggregates, we couple each spin to its own vibrational bath.

Starting from the state of fully aligned spins, we investigate the time evolution under a Hamiltonian that describes the paramagnetic Ising chain. The average value of the z-projection of a particular spin, which is proportional to the magnetization, is obtained from the population of the "up" state (the diagonal element of the reduced density matrix), which we calculate using numerically exact, fully quantum mechanical real-time path integral methods. We choose a bath model characterized by the commonly used Ohmic spectral density.[31] We find that the magnetization dynamics of edge spins is considerably different from that of spins located in the interior of the Ising chain.

Even in the absence of a dissipative bath, coupling to the spin chain leads to population damping on the tagged TLS.[27] However, the spin dynamics is quite distinct from that resulting from typical harmonic environments. This is a consequence of the spectral properties of the quantum Ising chain environment, which are rather different from those of a harmonic bath.

Coupling to harmonic baths introduces decoherence through thermal effects as well as zero-point fluctuations, which alter the dynamics, leading to smoother behaviors. Generally, we find that the observed spin transitions from "coherent" (underdamped oscillatory) dynamics at weak system-bath coupling to "incoherent" (monotonic) decay at stronger coupling, and that this transition is dependent on temperature, spin-spin interaction strength, and the position of the particular spin in the chain. In contrast to the typical behavior of a single TLS coupled to a harmonic bath, the characteristics of the coherent-incoherent transition in an Ising chain are considerably more complex. With sufficiently large spin-spin coupling, once the damping effects are strong enough to prevent the magnetization of interior spins from oscillating about its equilibrium value $\langle \sigma_z(\infty) \rangle = 0$, the evolution slows down considerably before eventually decaying, while edge spins may exhibit unusual oscillatory dynamics where the population oscillates above or below the equilibrium line.

The Hilbert space of an Ising chain containing n spins consists of 2^n states, thus there are over 10^3 states even for a rather short chain of $n \simeq 10$. While direct diagonalization of the Hamiltonian with such numbers of states is routinely feasible, the inclusion of harmonic baths to such a large system would result in an extremely challenging problem. Our calculations are based on the modular decomposition of the real-time path integral[32,33] (MPI), which links the TLS units sequentially, while allowing the full inclusion of bath degrees of freedom that couple to each spin. Throughout this paper we restrict attention to the paramagnetic phase.

In section II we describe the quantum Ising chain Hamiltonian and the coupling of each spin to a finite-temperature dissipative bath. A short overview of the MPI algorithm is given in section III. In section IV we present numerically exact, fully quantum mechanical results for the magnetization dynamics of each spin in a chain of length $n=10$ for various values of the spin-spin coupling parameter, the spin-bath coupling strength, and the temperature. Through MPI calculations with $n=20$, we find that the results are invariant to an increase in the length of the chain in the presence of dissipation. In section V we explore in more detail the evolution in the vicinity of the transition from coherent to overdamped dynamics. We also summarize these results through coherent-incoherent diagrams that display the parameter ranges where these behaviors are observed. Last, in section VI we give some concluding remarks.

II. Quantum Ising chain with spin-bath coupling

The isolated quantum Ising spin chain is described by the Hamiltonian:

$$\hat{H}_{\text{Ising}} = -\hbar\Omega\sum_{\alpha=1}^{n}\hat{\sigma}_x^{\alpha} - J\sum_{\alpha=1}^{n-1}\hat{\sigma}_z^{\alpha}\hat{\sigma}_z^{\alpha+1} \tag{2.1}$$

where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the Pauli spin operators. This Hamiltonian describes a chain of n identical, symmetric TLSs connected through nearest-neighbor interactions. Each TLS has two localized states $|\uparrow\rangle$ and $|\downarrow\rangle$, which are eigenstates of $\hat{\sigma}_z$ with eigenvalues ± 1. The Hamiltonian is characterized by two parameters, the tunneling parameter $\hbar\Omega$ (which is equal to half of the tunneling splitting of an individual TLS) and the nearest-neighbor coupling strength J. In the context of magnetic materials, $\hbar\Omega$ is proportional to the magnitude of the transverse magnetic field, which flips the sign of the spin on which it operates, while J is the spin-spin magnetic interaction, which favors parallel (ferromagnetic, $J>0$) or anti-parallel (anti-ferromagnetic, $J<0$) alignment. The competition between the two terms governs the equilibrium structure and the dynamics. The Ω terms favor eigenstates where each spin is in a superposition of the "up" and "down" states, while the spin-spin coupling term J tries to align the spins. As a result, depending on the relation of these two parameters in the Hamiltonian, the infinite Ising chain undergoes a quantum phase transition at $J=\hbar\Omega$. Variations are expected in chains of finite length, where edge spins which couple to only one neighboring spin are less strongly aligned with those in the interior and the phase transition is broadened.

Qubit coherence is critically important in the design of materials for quantum information science. The coherence-quenching effects from qubit-qubit interactions are a serious consideration in the placement of qubits. Interaction of the spins with intramolecular vibrations and phonon modes introduces additional damping effects to the spin dynamics." In the case of a single spin, the interplay between tunneling and dissipative bath degrees of freedom leads to the intricate behaviors of the famous spin-boson model,[1] which have been thoroughly investigated. The main observable in that case is the average position $\langle\sigma_z(t)\rangle$ of the spin along the *z* direction, which is obtained from the population $P_\uparrow$ of the "up" state, and this observable is examined during the tunneling dynamics that follows the non-equilibrium initial condition $P_\uparrow(0)=1$. This observable is proportional to the spin magnetization. In the case of the Ising chain, the same initial preparation, where all spins are placed in the "up" state, corresponds to one of the two eigenstates of the ordered phase (which are degenerate in the limit $n \to \infty$). Since the isolated chain is in the disordered (paramagnetic) phase for $J < \hbar\Omega$, where at equilibrium $\left\langle \sigma_z^\alpha \right\rangle = 0$ for all spins, the spin chain will undergo a quantum quench across the phase transition.

In this work we explore the role of model dissipative environments on the spin dynamics of the quantum Ising model by adding to H_{Ising} a harmonic bath to each spin. The total Ising + harmonic bath Hamiltonian is

$$\hat{H} = \hat{H}_{\text{Ising}} + \sum_j \frac{\left(\hat{p}_j^\alpha\right)^2}{2m_j} + \frac{1}{2} m_j^\alpha \omega_j^2 \left(\hat{x}_j^\alpha - \frac{c_j \hat{\sigma}_z^\alpha}{m_j \omega_j} \right)^2 . \tag{2.2}$$

In the present work we use identical parameters for all TLSs in order to investigate the rich dynamics of the traditional quantum Ising chain. (However, we note that the MPI methodology allows considerable flexibility, and future work will explore more complex systems.) The parameters of the baths are collectively defined by the spectral density function[31]

$$J\left(\omega\right) = \tfrac{1}{2}\pi \sum_j \frac{c_j^2}{m_j \omega_j} \delta\left(\omega - \omega_j\right). \tag{2.3}$$

We choose the common Ohmic spectral density model, $J\left(\omega\right) = \frac{1}{2}\pi\hbar\xi\omega e^{-\omega/\omega_c}$, which has an exponential cutoff frequency ω_c and where the overall strength of TLS-bath coupling is characterized by the dimensionless Kondo parameter ξ. We emphasize that the MPI methodology may be used with any type of spectral density, and discrete normal mode vibrations may also be treated exactly.

Initially all spins of the chain are placed in the $\left|\uparrow\right\rangle$ state, such that the initial density operator is

$$\hat{\rho}(0) = \prod_{\alpha=1}^{n} \left|\uparrow^\alpha\right\rangle\left\langle\uparrow^\alpha\right| \prod_j \frac{e^{-\beta \hat{h}_j^\alpha}}{\operatorname{Tr} e^{-\beta \hat{h}_j^\alpha}} \tag{2.4}$$

where

$$\hat{h}_j^\alpha = \frac{\left(\hat{p}_j^\alpha\right)^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left(\hat{x}_j^\alpha\right)^2 \tag{2.5}$$

is the Hamiltonian for the harmonic bath degrees of freedom that couple to spin α. The population of the "up" state of a particular spin is given by

$$P^\alpha(t) = \operatorname{Tr}\left\langle \uparrow^\alpha \right| e^{-i\hat{H}N\Delta t/\hbar} \hat{\rho}(0) e^{i\hat{H}N\Delta t/\hbar} \left| \uparrow^\alpha \right\rangle \tag{2.6}$$

where the trace is with respect to all bath degrees of freedom and both states of all spins besides α, and the magnetization is proportional to $\left\langle \sigma_z^\alpha(t) \right\rangle = 2P_\uparrow^\alpha(t) - 1$. Within the paramagnetic phase ($J < \hbar\Omega$), we refer to spin-spin coupling values as weak, intermediate or strong.

III. Summary of MPI methodology

Feynman's path integral formulation of time-dependent quantum mechanics[34,35] offers an attractive alternative to the Schrödinger equation when wavefunction storage is not practical. In its original form, however, evaluation of the path integral hinges on one's ability to compute highly multidimensional integrals with respect to auxiliary variables for each degree of freedom. This poses a severe problem in real time, as Monte Carlo-based methods fail to converge when the integrand is highly oscillatory. Optimal representations of the real-time path integral, combined with tensor decompositions in time, circumvent issues associated with the oscillatory character of the quantum mechanical amplitude and have led to efficient, fully quantum mechanical propagation algorithms for system-bath Hamiltonians[36,37] and also to a rigorous and consistent quantum-classical methodology.[38]

The MPI algorithm is a decomposition of the real-time path integral for extended systems with a primarily one-dimensional topology, such as the Ising spin chain considered in this work or molecular aggregates with interactions of the Frenkel exciton type. By connecting the discretized paths of each unit to those of the adjacent unit prior to discarding them, the MPI decomposition leads to linear scaling with respect to the number of units in the system of interest.[32,33] Typically, each unit comprises a small number of quantum (spin or electronic) states which are coupled to a large number of harmonic degrees of freedom that may be the normal mode coordinates of molecular vibrations or may represent a generic dissipative bath. Any number of quadratic degrees of freedom may be treated exactly in the MPI algorithm, through the influence functional[39] approach, which leads to analytical expressions for the relevant coefficients.[40] The MPI decomposition attains a particularly simple form in the case of the Ising spin chain, but also has been generalized to Hamiltonians with non-diagonal couplings between units.[41] In both cases an additional factorization[42] leads to highly efficient evaluation.

The sequential treatment of units in the MPI algorithm can also be viewed as an efficient, fully quantum mechanical construction of the influence functional from all preceding units. For example, once the kth unit is reached, the path amplitudes contain all the dynamical effects from units $1,2,\ldots,k$. Thus, each such amplitude is precisely the influence functional (with all spin-spin and spin-bath interactions summed exactly) from these units, which augments the path amplitudes of unit $k+1$ upon linking. The influence functional from the Ising chain segments is different from that of a harmonic bath, giving rise to distinct dynamical behaviors.

Last, motivated by the small decomposition of the path integral for system-bath Hamiltonians,[43,44] a small matrix decomposition of the modular path integral (SMatMPI) has recently been introduced,[45] which is based on the small matrix decomposition of path amplitudes.[46] The SMatMPI algorithm allows the sequential linking of units when path storage is not practical and leads to an iterative algorithm in time as well, thereby allowing calculations in situations of long memory and extending calculations to long times.

The calculations presented in the next two sections used a combination of these methods. Calculations with small-to-intermediate spin-spin and spin-bath coupling converged well with the original MPI algorithm. The regime of large spin-spin coupling and strong dissipation is more challenging, in particular at low temperatures. Calculations in that regime were performed with the SMatMPI method.

IV. Dynamics of the quantum Ising chain

As is well known, the magnetization of a single, isolated, symmetric spin exhibits fully coherent tunneling oscillations where the spin projection $\langle \sigma_z(t) \rangle$ oscillates between ± 1, while coupling to a harmonic bath introduces damping. By contrast, the same observable for a tagged spin in a quantum Ising chain of infinite length displays damping effects even in the absence of coupled baths. This is so because the neighboring spins act as an environment of 2^{n-1} states to the particular spin that is being observed, introducing phase randomization which resembles that induced by a dissipative environment. The coherence quenching effect qubit-qubit interactions is well appreciated and constitutes an important design principle in framework design for quantum information science.[6] In the case of a chain with n units, one generally expects to observe recurrences which should be pushed to longer time as n increases. Coupling to a harmonic bath leads to quenched oscillations even in the case of a single TLS, thus all spins in the quantum Ising chain exhibit dissipative dynamics regardless of the number of units.

As discussed in the introduction, earlier work focused primarily on chains of infinite size. Finite-size effects are known to impact phenomena in interesting ways, causing edge or surface properties to be different from those in the bulk. Our focus in this paper is on the dynamical behaviors of finite-length quantum Ising chains. Apart from pure phenomemological interest in the edge vs. bulk dynamics of these important model systems, finite-length Ising chains can serve as the simplest paradigm for spin dynamics in molecular structures of various geometries,[2-5,7] where edge effects are expected to play a significant role in the behavior of the tagged spin, depending on its location within the chain. We explore the effect of the two Ising parameters, $\hbar\Omega$ and J (whose ratio determines the location of the quantum phase transition) on the resulting evolution and the particular patterns of the spin population curves, with particular emphasis on the transition from underdamped to overdamped dynamics for edge and interior spins. Further, we investigate how coupling to harmonic baths affects this transition, as a function of dissipation strength and temperature. Calculations on isolated quantum Ising chains are performed using basis set methods. All results on chains where the spins are coupled to harmonic dissipative baths are obtained with the MPI and SMatMPI algorithms.

In this work we use a chain of $n = 10$ spins, each of which is coupled to an Ohmic bath characterized by the Kondo parameter ξ and cutoff frequency $\omega_c = 5\Omega$. The isolated Ising chain has 1024 eigenstates. The lowest eigenvalues of the isolated Ising chain are shown in Figure 1 for weak, intermediate and strong spin-spin coupling (within the paramagnetic parameter space). As one expects based on simple perturbation theory, with small J the ground state is well separated from the cluster of singly excited states, and a cluster of doubly-excited states can be identified. The clusters merge and the eigenvalue spectrum becomes rather complex as the spin-spin coupling is increased, approaching the quantum phase transition parameter $J = \hbar\Omega$. (We note that the eigenvalue spectrum simplifies again as J is increased beyond the critical point, but we do not present behaviors in the ferromagnetic phase in this paper.)

As discussed earlier, we simulate a quantum quench, thus restrict attention to spin-spin coupling values $J < \hbar\Omega$. We thus characterize the values $J = 0.2\,\hbar\Omega$, $J = 0.5\,\hbar\Omega$, $J = 0.8\,\hbar\Omega$ as weak, intermediate and strong spin-spin coupling, respectively. We track the magnetization of all spins ($\alpha = 1,\ldots,5$) through the time evolution of the z projections, $\langle \sigma_z^\alpha \rangle$. When the spins are coupled to harmonic baths, the spin populations either decay to equilibrium or settle into a slow, monotonic decay within a relatively short time, such that the dynamics of interior spins becomes indistinguishable after $\alpha = 5$. By performing calculations with $n = 20$, we show at the end of this section that the magnetization does not change upon increasing the length of the Ising chain in the presence of dissipative baths. Thus, the dynamics of the $\alpha = 5$ spin that we present is characteristic of "interior" spins in long Ising chains when the spins are coupled to dissipative baths.

For a given value of J, the dynamics is oscillatory at lower ξ and transitions to monotonic decay as ξ increases. As J increases, the ξ value at which this transition occurs decreases. We also observe an intermediate behavior, where the magnetization oscillates *above or below* zero before reaching equilibrium.

A. Weak spin-spin coupling

With $J << \hbar\Omega$ the spins interact only weakly. In this case the effects of the isolated Ising chain environment on the dynamics of interior spins are somewhat similar to those from a dissipative bath. However, significant edge effects are observed.

Figure 2 shows the magnetization of the five spins in the isolated Ising chain. All spins exhibit underdamped dynamics over the time interval shown. The oscillation amplitude of the edge spin is slightly larger, reflecting the weaker damping environment of this spin, which is coupled to the chain only on one side. The dynamics of the second spin initially follows the interior spins, but its behavior changes during the second oscillation cycle. Interestingly, the amplitude does not vary monotonically with the location of a spin in the chain; the oscillation of the second spin is more damped than that of the third and other interior spins.

Further, the dynamics of the edge spin is considerably more complex. While the first two oscillations are synchronized with those of the other spins, a jitter develops around the third peak, after which the edge spin oscillates out of phase. A similar but somewhat weaker effect is observed in the dynamics of the second spin, which overall remains synchronized with the edge spin. Interior spins are synchronized with each other and exhibit smoother dynamics which resembles that of a single underdamped oscillator, with nearly identical populations. In this regime the effective damping on a spin induced by the other spins is reminiscent of that from a harmonic bath, which has been found to synchronize the oscillations of different *bath* degrees of freedom.[47]

In order to compare the damping effects of Ising and harmonic environments, we have performed calculations for a single spin coupled to a harmonic bath at zero temperature and $\omega_c = 5\Omega$ with various spin-bath coupling parameters. We find that a harmonic bath with $\xi = 0.1$ produces spin population dynamics that resembles that of interior spins in the Ising chain with $J = 0.2\,\hbar\Omega$. The single spin results are also shown in Fig. 2. While the damping effect of the spin environment on interior spins is overall similar to that of a harmonic dissipative bath with these parameters, Fig. 2 shows that the harmonic bath is more effective at decreasing the oscillation amplitude at short times.

In Figure 3 we show the magnetization for the Ising chain in the presence of dissipative harmonic baths attached to each spin with moderate strength, $\xi = 0.3$, at low ($\hbar\Omega\beta = 5$), intermediate ($\hbar\Omega\beta = 1$) and high ($\hbar\Omega\beta = 0.1$) temperatures. For comparison, the magnetization of the isolated chain is shown in this figure as well, on the same scale. The dissipative bath is seen to have a very pronounced effect on spin coherence. At the low and intermediate temperature all $\langle \sigma_z^\alpha \rangle$ oscillate below zero only once, and evolve to the equilibrium value after a very minor recurrence. Further, the harmonic bath synchronizes the dynamics of almost all spins; only the edge spin deviates somewhat from the common behavior, displaying a slightly larger amplitude. The bath also slows down the oscillations of all spins; this effect is more pronounced in the populations of interior spins. In the high-temperature case all spins exhibit indistinguishable overdamped dynamics.

For this small value of J, moderately strong interaction of the spins with dissipative baths dominates the dynamics in comparison to the effects of coupling to the other spins. Fig. 3 shows that the magnetization dynamics of a single spin coupled to a harmonic bath is not drastically different from that of a spin within the Ising chain, which is coupled to the other spins as well as the harmonic bath, while the oscillations are strongly damped when compared to the magnetization of a spin in the isolated chain.

B. Moderate and strong spin-spin coupling

The dynamics undergoes several noteworthy changes as the strength of spin-spin coupling increases. In the absence of dissipative baths, the major recurrence time of the $n = 10$ chain shifts to earlier times, and with sufficiently large J moves within the time window displayed in the figures. Figure 4 shows the magnetization of all spins for $J = 0.5\hbar\Omega$ and $J = 0.8\hbar\Omega$. The coherence-quenching effects of the Ising chain on the short-time dynamics are now much more pronounced. The first oscillation minimum of the edge spin is deeper than that of interior spins, reflecting again the weaker damping effects on the spin coupled to the Ising chain only on one side. With the larger coupling value $J = 0.8\hbar\Omega$ the dynamics of the second spin is differentiated from that of interior spins even during the first half-oscillation. Unlike in the weak coupling case, the short-time amplitude variation is now monotonically dependent on spin position. In addition to the observed stronger quenching effects, it is seen that the magnetization minima of the second and third spins are shifted to later times, indicating lowered characteristic frequencies. Interestingly, more complex evolution is observed at longer times, which is characterized by multiple frequencies that generate unique beating patterns.

Again, coupling to dissipative harmonic baths simplifies the dynamics and causes a gradual damping of the oscillatory behavior. However, the effect of a weakly or moderately dissipative bath does not dominate the dynamics observed with larger J values, and stronger dissipation is needed to wipe out the patterns created by the strongly interacting spins. Figure 5 shows the magnetization for all spins in a chain with the moderate spin-spin coupling value $J = 0.5\hbar\Omega$, which is coupled to a bath with $\xi = 0.3$ at three temperatures. Overall, the oscillatory behavior is more effectively suppressed here compared to the $J = 0.2\hbar\Omega$ case. This damping effect is the combined result of the Ising chain environment and the harmonic bath. Further, the harmonic bath does not succeed at synchronizing the dynamics, and the first four spins are seen to oscillate with different frequencies and amplitudes. The shallow oscillations of interior spins, and eventually of the edge spins as well, disappear rapidly as the temperature is increased.

More complex patterns emerge with stronger spin-spin coupling. Figure 6 shows the magnetization for an Ising chain with $J = 0.8\,\hbar\Omega$ coupled to baths characterized by $\xi = 0.1$, 0.3 and 0.5, at an intermediate temperature $\hbar\Omega\beta = 1$. The dissipative bath again introduces damping effects, but its overall effect on the magnetization dynamics exhibits some unusual features in this regime, which depend on the magnitude of spin-bath coupling strength and spin location. As seen in Fig. 6 (and seen more clearly in Figure 8d), the magnetization of the edge spin exhibits early-time oscillations below the $\langle \sigma_z \rangle = 0$ line before reaching equilibrium. This behavior, which we term “biased oscillatory” dynamics, is the remnant of the pattern observed in the isolated Ising chain (Fig. 4 and 8a) and is the consequence of strong interaction between nearest neighbor spins.

An analogous biased oscillatory behavior, with oscillations above the $\langle \sigma_z \rangle = 0$ line, emerges as the spin-bath coupling increases to intermediate values. This can be identified in Fig. 6c, where the magnetization of the edge spin displays a very shallow minimum before it settles into its decay toward equilibrium. A larger oscillation amplitude results with $\xi = 0.2$ (see Fig. 8d). As discussed in the next section, the biased oscillatory behavior (either below or above the equilibrium value) is even more prominent at lower temperatures (Fig. 8), where it can persist over a wider range of spin-bath coupling.

At longer times, the main effect of strongly coupled dissipative baths at intermediate and low temperatures is a substantial slowing of the dynamics. The magnetization of interior spins settles into this regime of slow decay following a short transient behavior, while edge spins follow with a short delay.

Last, we show that (within the parameter range we consider) when the spins are coupled to harmonic baths, the magnetization dynamics of interior spins does not change in any noticeable way compared to the $\alpha = 5$ spin of the $n = 10$ Ising chains for which we presented results. Figure 7 compares results for the magnetization of the edge spin with $\hbar\Omega\beta = 1$, $\xi = 0.3$ and $J = 0.2$ and 0.8, in chains with 10 and 20 spins. This is easily feasible with the MPI methodology, because the effort scales linearly with the number of units in the chain. It is seen that the results are practically indistinguishable. We conclude that, as long as the spin-bath coupling is not very weak, our results characterize the behaviors of edge and interior spins (located at least 5 spins away from chain edges) in chains of any length.

V. Coherent, incoherent and biased oscillatory dynamics

As discussed in the previous section, for small values of J the magnetization dynamics of the edge spin is oscillatory with small ξ at low temperatures and eventually transitions to a monotonic decay as ξ and/or the temperature increases. With larger values of J, the range of ξ values over which ordinary underdamped or monotonic oscillatory behavior is observed shrinks. With strong spin-spin and intermediate spin-bath coupling the magnetization of the edge spin oscillates above or below the $\langle \sigma_z \rangle = 0$ value while decaying, giving rise to biased oscillatory dynamics at short times that resemble sigmoidal curves. This pattern is observed over a wider range of ξ values at low temperatures when the spin-spin coupling is stronger. At large ξ values the eventual decay of the magnetization becomes very slow for all spins. In this section we present more detailed magnetization graphs in the parameter range where these interesting behaviors are observed and summarize the dynamics through coherent-incoherent diagrams that characterize the transition from "coherent" (common underdamped oscillatory) to "incoherent" (monotonically decaying), which in some cases involves an intermediate "biased oscillatory" regime.

Figure 8 shows the magnetization of edge spins in the vicinity of the coherent-incoherent boundary at high, intermediate and low temperatures, with moderate and large spin-spin coupling for which the most interesting dynamics are observed. The biased oscillatory behavior, primarily above but also below the equilibrium value, is seen very distinctly at low and intermediate temperatures. The overdamped oscillatory regime shrinks as the temperature is increased, and eventually the magnetization dynamics changes directly from coherent to incoherent at high temperatures. In the high-temperature regime the sigmoidal shapes and the very slow decay observed at low temperatures disappear as well, giving rise to simpler dynamics similar to that of a single spin coupled to a dissipative bath.

These behaviors are summarized in Figure 9, which shows the three regimes on the J, ξ plane for edge and interior spins at low, intermediate and high temperatures. These hand-drawn diagrams are primarily suggestive and the boundaries are not sharp, as the crossover from one regime to another is continuous and the classification is to some extent subjective. In the case of edge spins, the biased oscillatory behavior is seen to occupy a large fraction of parameter space at low temperatures, but this region becomes narrower as the temperature is raised and eventually disappears. Interior spins located far from edges transition directly from underdamped oscillatory to overdamped dynamics at all temperatures.

The shape of the low-temperature crossover boundary for interior spins resembles that of the ordered-disordered phase boundary identified through imaginary-time path integral calculations,[24] but only qualitatively, because these two boundaries describe different physical phenomena. For example, in the $J \to 0$ limit the ordered-disordered phase boundary was found[24] to be at $\xi = 1$, i.e. the Ising chain is in the disordered phase for any $\alpha < 1$. However, for $J = 0$ the Ising chain reduces to uncoupled spins, whose coherent-incoherent boundary at zero temperature is known[1] to be $\xi = \frac{1}{2}$. The coherent-incoherent boundary seen in Fig. 9 is $\xi \simeq 0.42$ at $J = 0.2\,\hbar\Omega$, which extrapolates to about 0.5 in the $J = 0$ limit, in agreement with the expected value.

VI. Concluding Remarks

In this paper we have used fully quantum mechanical path integral methods to investigate the magnetization dynamics of individual spins in quantum Ising chains where each spin is coupled to a harmonic bath. This study extends the well-studied spin-boson tunneling dynamics to multiple spins in a one-dimensional arrangement. The spins were initially prepared in the fully aligned configuration, which characterizes the ordered, ferromagnetic phase. As the system evolves under the Ising Hamiltonian with $J < \hbar\Omega$, which corresponds to the paramagnetic phase, the calculated magnetization describes the dynamics of a quantum quench. We focused on the time evolution of the magnetization and the coherent-incoherent transition at various temperatures, spin-spin coupling values and spin-bath dissipation parameters, with particular emphasis on the variation of these properties with spin location.

In the absence of coupling to dissipative baths, the spin environment produces damping effects. This is so because the observed spin couples to the 2^n eigenstates of the chain, which for large n act as a large environment. However, because the eigenstates of the Ising chain are not the same as those of a dissipative harmonic bath, dynamical observables exhibit irregularities and some characteristics that are not found in spin-boson dynamics. Further, spin state populations do not completely die out and major recurrences are observed at long times. The recurrence time increases with n and becomes shorter upon increasing the spin-spin coupling parameter.

We emphasize that the Ising spin bath differs fundamentally from a bath of noninteracting TLSs, each coupled to the observed spin. If the coupling parameters are scaled appropriately such that observables remain well-behaved in the thermodynamic limit,[48] such a spin bath displays a Gaussian response[49] and thus can be mapped on a harmonic bath with an effective spectral density. This equivalence has been verified by numerical calculations.[50-52] On the other hand, the Ising bath of coupled spins affects the dynamics of the tagged spin in different ways that do not appear compatible with those from a harmonic environment.

Regardless of the presence or absence of dissipative baths, the spin magnetization dynamics shows a significant dependence on the location of the tracked spin within the chain. Damping effects are more pronounced in interior spins. The dynamics of the edge spin, which interacts with a single neighbor, remains oscillatory over a wider range of temperature and spin-bath coupling strength compared to spins located in the interior of the chain. Spins near the edge exhibit behaviors that tend to be intermediate, although a nonmonotonic variation of amplitude with spin location was observed in dissipationless Ising chains.

Coupling of the spins to dissipative harmonic baths leads to irreversible dynamics where the magnetization eventually approaches zero. In contrast to the dynamics of isolated spin chains, the magnetization of all spins saturates at $n \simeq 10$ over the range of parameters examined, such that the behaviors of the central spins presented in the previous two sections are representative of interior spin dynamics in long Ising chains.

Just as in the case of a single spin coupled to a harmonic bath, the spin magnetization in Ising chains exhibits coherent (underdamped oscillatory) and incoherent (monotonically decaying) regimes, which depend on the dissipation strength and the temperature. Because of the additional damping effects from the spin environment, the coherent regime spans a smaller portion of parameter space in comparison to the spin-boson case. Edge spins exhibit more complex behaviors than spins located in the interior of the chain. With weak spin-spin coupling, and also for any value of J at high temperatures, edge-spin magnetization curves have underdamped oscillatory shapes or exhibit monotonic decay. However, with intermediate-to-strong spin-spin coupling, a third behavior was identified at intermediate and low temperatures, where the magnetization undergoes biased oscillatory evolution above or below the equilibrium value. We have presented diagrams that illustrate these behaviors in the J vs. ξ plane at low, intermediate and high temperatures. We emphasize that the coherent-incoherent crossover is quite distinct from the ordered-disordered phase transition, which has been the subject of many earlier studies.

Even though we have restricted attention to a simple spectral density with parameters typical of interesting spin-boson regimes, MPI calculations can also be performed with structured spectral densities characteristic of specific materials. By exploring the coherence-quenching role of strongly coupled molecular vibrations in relation to the mode frequency, such calculations can contribute to the establishment of important design principles for QIS materials.

The numerical results presented in this paper offer a glimpse of the rich behaviors that characterize the dynamics of quantum Ising chains. Further explorations, along with investigations of other coupled spin models and different topologies, will be the target of future work.

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Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Figure Captions

Fig. 1. Lowest 120-160 eigenvalues of the quantum Ising chain for $n = 10$ within the paramagnetic phase, in units of $\hbar\Omega$. Left: $J = 0.2\,\hbar\Omega$. Middle: $J = 0.5\,\hbar\Omega$. Right: $J = 0.8\,\hbar\Omega$.

Fig. 2. Time evolution of spin magnetization. (a) Isolated quantum Ising chain with $J = 0.2\,\hbar\Omega$. Results for all spins are shown. (b) Single spin coupled to a harmonic bath with $\xi = 0.1$, $\omega_c = 5\Omega$, at zero temperature.

Fig. 3. Magnetization in quantum Ising chains with $J = 0.2\hbar\Omega$ where each spin is coupled to a harmonic bath. The first panel shows results in the absence of spin-bath coupling. The other three panels show results for a moderate spin-bath coupling value, $\xi = 0.3$. (a) Isolated chain. (b) Low temperature, $\hbar\Omega\beta = 5$. (c) Intermediate temperature, $\hbar\Omega\beta = 1$. (d) high temperature, $\hbar\Omega\beta = 0.1$. Also shown with markers are results for a single spin coupled to the same dissipative harmonic bath.

Fig. 4. Magnetization of various spins in an isolated quantum Ising chain with moderately strong spin interactions. (a) $J = 0.5\,\hbar\Omega$. (b) $J = 0.8\,\hbar\Omega$.

Fig. 5. Magnetization of various spins in quantum Ising chains with $J = 0.5\hbar\Omega$ where each spin is coupled to a harmonic bath. The first panel shows results in the absence of spin-bath coupling. The other three panels show results for a moderate spin-bath coupling value, $\xi = 0.3$. (a) Isolated chain. (b) Low temperature, $\hbar\Omega\beta = 5$. (c) Intermediate temperature, $\hbar\Omega\beta = 1$. (d) High temperature, $\hbar\Omega\beta = 0.1$.

Fig 6. Magnetization of various spins in quantum Ising chains with $J = 0.8\hbar\Omega$ where each spin is coupled to a harmonic bath. The top left panel shows results in the absence of spin-bath coupling. The other three panels show results with spin-bath coupling at an intermediate temperature, $\hbar\Omega\beta = 1$. (a) Isolated chain. (b) $\xi = 0.1$. (c) $\xi = 0.3$. (d) $\xi = 0.5$.

Fig. 7. Comparison of edge spin magnetization in quantum Ising chains of different lengths with $\xi = 0.3$, $J = 0.2\hbar\Omega$ (blue) and $J = 0.8\hbar\Omega$ (red), at $\hbar\Omega\beta = 1$. Lines: $n = 10$. Markers: $n = 20$.

Fig. 8. Edge spin population for moderate and strong spin-spin coupling at high, intermediate and low temperatures. (a) $J = 0.5\hbar\Omega$, $\hbar\Omega\beta = 0.1$. (b) $J = 0.8\hbar\Omega$, $\hbar\Omega\beta = 0.1$. (c) $J = 0.5\hbar\Omega$, $\hbar\Omega\beta = 1$. (d) $J = 0.8\hbar\Omega$, $\hbar\Omega\beta = 0.1$. (e) $J = 0.5\hbar\Omega$, $\hbar\Omega\beta = 5$. (f) $J = 0.8\hbar\Omega$, $\hbar\Omega\beta = 5$. Cyan: coherent regime. Purple: biased oscillatory regime. Red: incoherent regime.

Fig 9. Coherent-incoherent diagrams for edge and interior spins at two temperatures. Blue: coherent regime. Yellow: biased oscillatory regime. Red: Incoherent regime. Top: $\hbar\Omega\beta$ = 0.1. Middle: $\hbar\Omega\beta$ = 1. Bottom: $\hbar\Omega\beta$ = 5. Left: edge spin. Right: interior spin.