

Fermionic versus spin baths in noninteracting transport models

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We investigate how fermionic anticommutation shapes transport in a noninteracting resonant-level model where a single central site is coupled to an environment. To this end, we compare a fermionic reservoir with a bath of spin- $\frac{1}{2}$ modes using exact diagonalization and a perturbative expansion of the master equation to identify the differences. Notably, we find different reduced dynamics for the spin and fermionic baths even though both models restrict each local mode to at most one excitation; unlike the fermionic bath, however, the spin bath consists of commuting two-level modes and therefore lacks the global exchange antisymmetry of true fermions. These differences originate from higher-order terms in the system-bath coupling, where fermionic anticommutation introduces exchange signs in higher-order correlations. In contrast, all second-order contributions, set solely by two-point correlators, coincide. Deviations are largest for small to intermediate bath sizes, fading in the effectively Markovian regime where higher-order corrections are negligible. These results identify when spin baths can be a substitute for fermionic reservoirs and vice versa.

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I. INTRODUCTION

Transport through discrete quantum systems is a fundamental problem in quantum physics. Intriguing phenomena such as the Kondo effect arise in quantum transport due to many-body interactions, whose study has yielded fundamental advances in theoretical methods [1–5], and which also finds applications in experimental techniques, such as probes for the presence of local spins [6]. Beyond the Kondo effect, quantum transport is central for nanojunctions [7–13] with possible applications as single-electron transistors [14–18]. There, many-body Coulomb interactions are mainly responsible for reducing the active state space in a central site due to the Coulomb blockade effect [19,20], while many-body correlations in the fermionic bath that describes the metallic contacts can be largely ignored. A challenge in modeling nanojunctions is the fact that real-world systems are typically coupled to additional bosonic environments, such as vibrations described by phonons, where different methods are considered depending on whether the coupling to the vibrational environment dominates over the coupling to the fermionic leads or vice versa [21–27].

Commonly, the effects of vibrational environments are treated within the framework of open quantum systems, where the environment is traced out. For bosonic degrees of freedom, open quantum systems theory is very well established with

many techniques available under conditions of strong system-environment coupling, where the environment constitutes a complex, non-Markovian memory [28–33]. In contrast, a central site coupled to a bath of electrons is typically analyzed with nonequilibrium Green's functions, making use of Wick's theorem [34–36]. For the noninteracting resonant-level model, the same quadratic fermionic structure also admits an exact single-body diagonalization, summarized for completeness in Appendix C; this exact noninteracting reduction is absent for the spin bath considered here. As a step toward a unified treatment of a quantum system coupled to fermionic and bosonic environments, particularly when anharmonicities render the environments non-Gaussian and Wick's theorem invalid, it is instructive to also consider the coupling of a central site to a fermionic bath within the framework of open quantum systems [37].

However, fermionic anticommutation poses subtle questions for an open quantum system formulation, e.g., when defining fermionic reduced density matrices [38]. A modern framework where the fermionic reduced density matrix is composed of two parts corresponding to even and odd particle numbers [39] enables the formulation of fermionic influence superoperators, hierarchical equations of motion, including recent extensions to lower temperatures and more general reservoir structures [40,41], and generalized Lindblad master equations for fermionic open quantum systems. Numerical methods to simulate the dynamics of quantum systems coupled to fermionic baths may be derived using the Jordan-Wigner transformation, such as in the fermionic time-evolving density operator with orthogonal polynomials algorithm (TEDOPA) [42] or making use of Grassmann algebra, as in the fermionic version [43] of process tensors [32,33], where the Feynman-Vernon influence functional is efficiently represented using temporal tensor networks. Notably, the fermionic process tensors can also be obtained using the

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Jordan-Wigner mapping instead of Grassmann algebra (see Appendix B of Ref. [44]). The challenge in working with Grassmann numbers is their noncommutativity. However, the Jordan-Wigner transformation maps a fermionic system onto one composed of spin- $\frac{1}{2}$ and can thus also be used to simulate fermionic systems on gate-based quantum computers, but at the cost of introducing nonlocal string operators. It is important to note, however, that the Jordan-Wigner transformation yields an exact fermion-spin equivalence only when the associated nonlocal string operators are retained, and is therefore tied to a one-dimensional ordering of the modes [45,46]. A bath of independent spin- $\frac{1}{2}$ modes in which operators on different sites commute may thus be viewed, in the site basis, as a bath of hard-core-boson modes, i.e., commuting two-level modes with a local occupancy constraint. It shares the local single-occupancy constraint of fermions, but not the basis-independent exclusion principle and exchange-sign structure that follow from global fermionic antisymmetry [47].

This naturally raises the question of whether it is really necessary to account for the proper fermionic anticommutation relation in quantum transport, and under which circumstances it is a good approximation to replace a fermionic environment by a bath of two-level (spin- $\frac{1}{2}$) systems while simply ignoring any possible sign change due to the fermionic anticommutation. Then, conventional open quantum system methods for bosonic or other commuting environments could be directly transferred to systems coupled to fermionic baths. Noting that the most prominent phenomena arising from the fermionic anticommutation are a basis-independent exclusion principle and exchange-sign structure, one may ask whether, in the absence of additional many-body interactions, a bath of commuting two-level modes, which shares the same local single-occupancy constraint in the site basis, can reproduce similar environment effects as a fermionic bath.

Here, to test this hypothesis, we consider a noninteracting transport model that is small enough to be solved by exact diagonalization for both the fermionic bath and the corresponding spin bath. Surprisingly, we find that both systems only show the same dynamics up to second order in the system-bath coupling, while for small to moderately sized baths near half filling, sizable discrepancies are identified.

The remainder of the paper is organized as follows. In Sec. II, we define the resonant-level model in fermionic and spin formulations and summarize the perturbative master-equation approach, highlighting where algebra-dependent terms arise. Section III presents and discusses exact-diagonalization results across different bath sizes and compares them to the second-order master-equation prediction. We conclude in Sec. IV by summarizing the regimes of agreement and difference and discussing implications for simulations of open quantum systems.

II. THEORY

A. Model

We consider an open quantum system described by the total Hamiltonian:

$$H = H_S + H_E, \quad (1)$$

where H_S represents the system Hamiltonian and H_E describes the environment and its interaction with the system. Explicitly, these are defined as (throughout this work, we adopt natural units, i.e., $\hbar = 1$)

$$H_S = \omega_0 O_0^\dagger O_0, \quad (2)$$

$$H_E = \sum_{k=1}^{N_E} [\omega_k O_k^\dagger O_k + V_k (O_0^\dagger O_k + O_k^\dagger O_0)]. \quad (3)$$

Here, the system is represented by a single mode at frequency ω_0 , coupled to an environment composed of N_E modes with frequencies ω_k . The coupling strength between the system mode and the k th bath mode is given by V_k . The operator O_j is a generic two-level lowering operator associated with mode j , and we study two distinct physical realizations:

(1) *Fermionic model*. Here, we set $O_j \equiv c_j$, where c_j are fermionic annihilation operators satisfying the canonical anticommutation relations:

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i, c_j\} = 0. \quad (4)$$

(2) *Spin model*. Alternatively, we choose spin (two-level) lowering operators $O_j \equiv \sigma_j^-$. The corresponding algebra is

$$\{\sigma_j^-, \sigma_j^+\} = 1, \quad [\sigma_i^-, \sigma_j^\pm] = 0 \quad \text{for } i \neq j. \quad (5)$$

In the site basis, this algebra can be viewed as a hard-core-boson description, i.e., as bosonic modes subject to an infinite on-site repulsion that restricts each mode to at most one excitation [47]. The exact fermion-spin equivalence, however, requires the nonlocal string operators of the Jordan-Wigner mapping, which encode the fermionic exchange signs [45,46]. It is also important to note that the total Hamiltonian conserves the total particle number. Throughout this work, the exact-diagonalization calculations are therefore carried out at fixed total occupation, so the closed-system dynamics remain at fixed total parity from the outset.

The *resonant-level model* [48] serves as a minimal yet powerful framework for exploring open quantum dynamics, transport, and many-body effects in nonequilibrium settings. While the fermionic and spin variants differ in their algebraic structure, both capture the essential dynamics of impurity-bath coupling. Figure 1 illustrates the system-bath coupling common to both fermionic and spin realizations of the resonant-level model.

It is worth noting that in the fermionic model the total Hamiltonian is quadratic in creation and annihilation operators and thus admits an exact single-particle (one-body) diagonalization. In contrast, in the local spin or hard-core-boson representation used here, the same hopping structure corresponds to a constrained many-body problem; equivalently, in canonical-boson language it carries an infinite on-site repulsion, so the efficient single-particle diagonalization available for fermions does not carry over to spins. For completeness, we outlined this briefly in Appendix C.

B. Perturbative master equations

Master equations provide a standard yet powerful analytical framework for studying the dynamics of open quantum

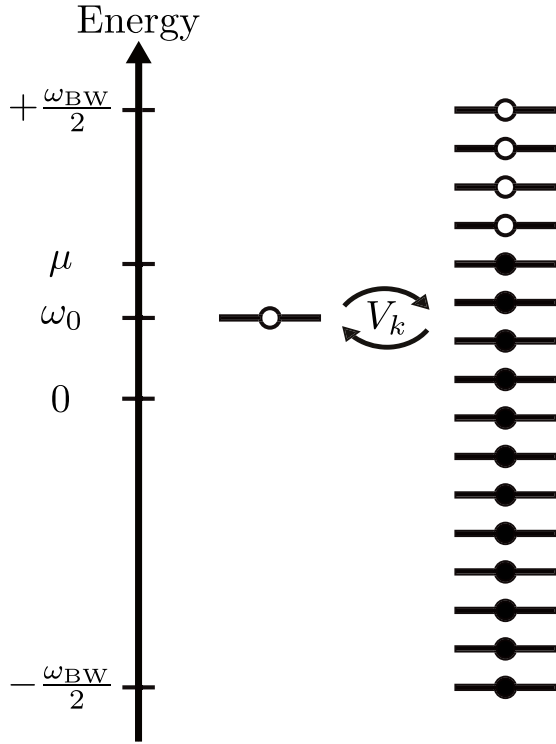


FIG. 1. Schematic representation of the resonant-level model: A system mode at energy ω_0 is coupled (with coupling strengths V_k) to an environment consisting of discrete modes within a bandwidth ω_{BW} , partially filled up to the chemical potential μ .

systems [28]. By tracing out the environment degrees of freedom and expanding perturbatively in the system-bath coupling strengths, one obtains an effective dynamical equation governing the reduced density matrix of the system. In this section, we examine the perturbative expansion, beginning with the second-order master equation (ME2), where the dynamics remain unaffected despite the distinct operator algebra of the spin and fermionic models. At fourth order, this correspondence need not hold in general; to explore this, we analyze a representative term that naturally arises in the expansion.

1. Second-order master equation

At second order in the coupling strength, the master equation governing the reduced density matrix $\rho_S(t)$ can be obtained. A detailed derivation is provided in Appendix A. The resulting equation reads

$$\begin{aligned} \frac{d\rho_S(t)}{dt} = & - \int_0^t dt' [C_1(\tau)[O_0, O_0^\dagger \rho_S(t')] \\ & + C_2(\tau)[\rho_S(t') O_0^\dagger, O_0] + \text{H.c.}], \end{aligned} \quad (6)$$

where H.c. is the Hermitian conjugate and $\tau = t - t'$, and the bath correlation functions are

$$\begin{aligned} C_1(\tau) &= \sum_k |V_k|^2 e^{-i(\omega_0 - \omega_k)\tau} \langle O_k^\dagger O_k \rangle \\ &= \sum_k |V_k|^2 e^{-i(\omega_0 - \omega_k)\tau} f(\omega_k), \end{aligned} \quad (7)$$

$$\begin{aligned} C_2(\tau) &= \sum_k |V_k|^2 e^{-i(\omega_0 - \omega_k)\tau} \langle O_k O_k^\dagger \rangle \\ &= \sum_k |V_k|^2 e^{-i(\omega_0 - \omega_k)\tau} [1 - f(\omega_k)]. \end{aligned} \quad (8)$$

The operators appearing in Eq. (6) are kept deliberately generic and may correspond to either fermionic or spin operators. Crucially, at second order, the master equation we derive is identical for both the fermionic and spin models in the present single-mode, number-conserving excitation setting. Although a general fermionic reduced-state formalism distinguishes even- and odd-parity blocks [39], no coherences between them are generated here, so Eq. (6) is sufficient for the reduced dynamics relevant to the observables studied below. This equivalence arises because the bath correlation functions depend only on the occupation of bath modes, such as $\langle O_k^\dagger O_k \rangle = f(\omega_k)$, which reflect the local single-occupancy constraint obeyed by each bath mode in both models. These expectation values capture only the population of each mode and are insensitive to the underlying commutation or anticommutation relations.

Consequently, at second order, the dynamics account only for direct, single-excitation exchange events between the system and the bath. Interference pathways—such as those arising from higher-order processes involving multiple bath excitations or exchange loops—are entirely absent. As a result, the evolution is insensitive to operator ordering, and the reduced dynamics of the system are indistinguishable between the two models. This agreement, however, is limited to second order; as we will see, differences between the fermionic and spin formulations begin to emerge at higher orders.

2. Fourth-order master equation

At higher orders in the perturbative expansion, the structure of the reduced dynamics becomes qualitatively richer because the system and bath can exchange excitations repeatedly before the bath is traced out. At fourth order, two such system-bath exchange events are involved, giving rise to four-time bath correlation functions involving multiple bath operators. In such cases, the ordering of operators becomes relevant—particularly when comparing fermionic and spin environments, whose operator algebras differ fundamentally.

A complete fourth-order master equation contains many contributions. Rather than printing the full raw expansion, Appendix B classifies the six bath-operator orderings with two creation and two annihilation operators that can survive the bath trace for the number-diagonal product state considered here. We focus below on a minimal exchange-sensitive correlator, denoted by $\mathcal{K}_{\text{fermion}}$ and $\mathcal{K}_{\text{spin}}$ for the two baths, because for this ordering the nonzero distinct-mode contributions reduce to a direct index structure and an exchange index structure whose relative sign already exposes the fermion-spin difference. In this sense, the term is used as an explicit demonstration of the recurring bath-algebra distinction rather than as a stand-alone derivation of the full fourth-order kernel. The mode frequencies enter only through the phase factors in Appendix B and do not alter this structure. In the standard nonequilibrium language, these four-time bath correlators may equivalently be viewed as branch-resolved

components of contour-ordered correlators on the Keldysh contour [36,49]. The nested real-time integrals used here simply pick out the corresponding contour ordering in the perturbative expansion.

For the fermionic bath, the relevant correlation function is

$$\begin{aligned} \mathcal{C}_{\text{fermion}} &= \text{Tr}_B[c_{k_1}^\dagger c_{k_2} c_{k_3} c_{k_4}^\dagger \rho_B] \\ &= \delta_{k_1,k_2} \delta_{k_3,k_4} (1 - \delta_{k_1,k_3}) f_{k_1} (1 - f_{k_3}) \\ &\quad - \delta_{k_1,k_3} \delta_{k_2,k_4} (1 - \delta_{k_1,k_2}) f_{k_1} (1 - f_{k_2}). \end{aligned} \quad (9)$$

For this ordering, the only nonzero cases are $k_1 = k_2$, $k_3 = k_4$, $k_1 \neq k_3$ and $k_1 = k_3$, $k_2 = k_4$, $k_1 \neq k_2$. The case $k_1 = k_4$, $k_2 = k_3$, $k_1 \neq k_2$ and the fully equal case $k_1 = k_2 = k_3 = k_4$ both vanish. Because we assume a Gaussian fermionic bath, Wick's theorem [34] applies, and the same two contributions follow from the corresponding pairings of two-point functions. The crucial minus sign in the second term originates entirely from fermionic anticommutation.

For a spin bath, the corresponding correlation function reads

$$\begin{aligned} \mathcal{C}_{\text{spin}} &= \text{Tr}_B[\sigma_{k_1}^\dagger \sigma_{k_2} \sigma_{k_3} \sigma_{k_4}^\dagger \rho_B] \\ &= \delta_{k_1,k_2} \delta_{k_3,k_4} (1 - \delta_{k_1,k_3}) f_{k_1} (1 - f_{k_3}) \\ &\quad + \delta_{k_1,k_3} \delta_{k_2,k_4} (1 - \delta_{k_1,k_2}) f_{k_1} (1 - f_{k_2}). \end{aligned} \quad (10)$$

Unlike the fermionic case, spin operators commute on different sites, so the exchange contribution enters with a plus sign. For this ordering, the same two cases contribute, while the case $k_1 = k_4$, $k_2 = k_3$, $k_1 \neq k_2$ and the fully equal case again vanish. More generally, as summarized in Appendix B, other balanced fourth-order operator orderings can contain non-vanishing terms when indices coincide in the non-Gaussian spin bath.

The resulting representative fourth-order terms, $\mathcal{K}_{\text{fermion}}$ and $\mathcal{K}_{\text{spin}}$, derived explicitly in Appendix B, thus differ in a fundamental way: For the exchange-sensitive case displayed above, fermionic anticommutation introduces a relative minus sign in the exchange contribution that has no analog in the spin case. This sign reflects the exchange statistics of indistinguishable fermions, a feature absent in the spin bath, and gives different fourth-order contributions to the reduced dynamics.

Consequently, although the second-order master equations for the two baths are identical, their fourth-order dynamics diverge significantly. The fermionic bath encodes antisymmetric exchange correlations through its operator algebra, whereas spin baths treat operators on different sites as commuting. This distinction becomes important when multiexcitation processes are relevant—particularly in strongly coupled or small baths—and motivates the use of exact diagonalization methods discussed in the next subsection.

The relative minus sign in Eq. (9) is thus simply the familiar fermionic exchange sign generated by Wick contractions, closely related to the sign structure appearing in real-time Keldysh expansions of transport kernels [49,50]. The corresponding exchange contribution is present for the spin bath as well, but without this minus sign, so the two baths already differ at the level of the representative fourth-order term. It is important to note, however, that the fourth-order expressions are not used here as a quantitative approximation scheme for the reduced dynamics at arbitrary coupling or memory

time. Beyond second order, a truncated perturbative master equation need not be systematically convergent without further resummation. Their purpose here is instead diagnostic: They identify the lowest order at which the distinct operator algebras of the two baths generate different contributions.

C. Exact diagonalization

Our numerical analysis relies exclusively on exact diagonalization in the many-body basis [51]. In the fermionic model, each mode j can be either occupied or unoccupied, resulting in a Fock-space dimension of $\binom{N_E+1}{n_{\text{exc}}}$ for a fixed total number n_{exc} of occupied modes. In the spin model, each mode is similarly described by two states—occupied ($|\uparrow\rangle$) or unoccupied ($|\downarrow\rangle$)—and hence, for a given fixed number of occupied modes, the Hilbert space dimension remains the same as in the fermionic case. However, the fundamental differences between these representations emerge in the operator algebra rather than in the dimension of the Hilbert space itself.

Once the total Hamiltonian is represented in this many-body basis, it can be diagonalized to yield eigenstates and eigenenergies:

$$H|\Phi_\alpha\rangle = E_\alpha|\Phi_\alpha\rangle. \quad (11)$$

The time evolution of an initial state $|\psi(0)\rangle$ is then computed as

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle = \sum_{\alpha} e^{-iE_\alpha t} |\Phi_\alpha\rangle \langle\Phi_\alpha|\psi(0)\rangle. \quad (12)$$

From $|\psi(t)\rangle$, any observable of interest—such as the system population $\langle O_0^\dagger O_0 \rangle$ —is readily computed.

It is important to note, however, that the computational cost of exact diagonalization depends on the size of the Hilbert space, which scales combinatorially. The dimension is maximal near half filling, where it reaches $\binom{N_E+1}{(N_E+1)/2}$ and scales exponentially with N_E (up to a subexponential prefactor). In contrast, configurations with very low or very high occupied numbers of bath modes correspond to significantly smaller subspaces. Accordingly, we restrict our analysis to small environments, where exact diagonalization remains computationally feasible, enabling direct numerical comparison between the fermionic and spin representations. It should be stressed, however, that this restriction reflects our use of full exact diagonalization. In the present calculations, we already exploit particle-number conservation by working at fixed total occupation.

Larger baths could, in principle, be addressed using Krylov-based propagation, purification-based tensor-network methods, or compressed-environment approaches such as automated compression of environments and treelike process-tensor contraction [33,44,52]. For the present purposes, however, bath sizes up to $N_E = 16$ already suffice to reveal the statistics-dependent deviations at intermediate sizes and the approach to the common ME2 limit.

III. NUMERICAL RESULTS

We begin by comparing the two models for a small bath, where differences are expected to be most pronounced. We

consider $N_E = 3$ bath modes with $n_{\text{exc}} = 2$ initially occupied, the system initially empty, and a uniform coupling $V_j = V = 1$. The bath bandwidth is $\omega_{\text{BW}} = 2$, with equally spaced mode frequencies $\omega_1 = -1$, $\omega_2 = 0$, and $\omega_3 = 1$. To make the algebraic origin of the differences transparent, we write the Hamiltonian in matrix form. Denoting the vacuum by $|0\rangle$, we label the six basis states $|0\rangle, \dots, |5\rangle$ as

$$\begin{aligned} |0\rangle &= c_1^\dagger c_0^\dagger |0\rangle, & |1\rangle &= c_2^\dagger c_0^\dagger |0\rangle, & |2\rangle &= c_3^\dagger c_0^\dagger |0\rangle, \\ |3\rangle &= c_2^\dagger c_1^\dagger |0\rangle, & |4\rangle &= c_3^\dagger c_1^\dagger |0\rangle, & |5\rangle &= c_3^\dagger c_2^\dagger |0\rangle. \end{aligned} \quad (13)$$

Equivalently, we can define the same six states using spin operators. The action of the Hamiltonian, for example,

$$H = \begin{bmatrix} \omega_0 + \omega_1 & 0 & 0 & \mp V_2 & \mp V_3 & 0 \\ 0 & \omega_0 + \omega_2 & 0 & V_1 & 0 & \mp V_3 \\ 0 & 0 & \omega_0 + \omega_3 & 0 & V_1 & V_2 \\ \mp V_2 & V_1 & 0 & \omega_1 + \omega_2 & 0 & 0 \\ \mp V_3 & 0 & V_1 & 0 & \omega_1 + \omega_3 & 0 \\ 0 & \mp V_3 & V_2 & 0 & 0 & \omega_2 + \omega_3 \end{bmatrix}. \quad (15)$$

This compact form makes the algebraic origin of the different dynamics explicit: The two models differ only by these statistics-dependent signs, so their time evolutions already diverge at the level of this finite matrix.

Figure 2 shows the resulting system population $n_s(t)$ from exact diagonalization for the two models. We can see that even for this minimal bath, the two models display distinct oscillation and relaxation patterns.

In this model, if $n_{\text{exc}} = 1$ or $n_{\text{exc}} = N_E$, then every nonzero off-diagonal element only transfers that single excitation between the system and one bath mode. No process ever exchanges two indistinguishable bath particles, so no

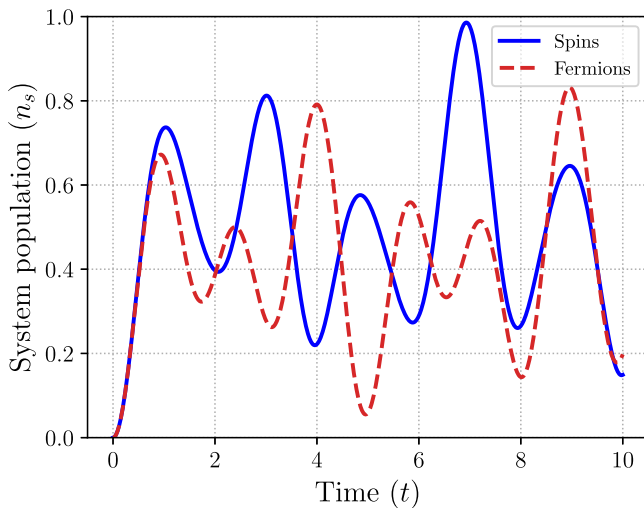


FIG. 2. Population dynamics from exact diagonalization for $N_E = 3$, $n_{\text{exc}} = 2$, uniform coupling $V = 1$, and $\omega_{\text{BW}} = 2$ with mode frequencies $\{-1, 0, 1\}$. Fermionic results (red dashed) vs spins (blue).

on $|0\rangle$, is

$$\begin{aligned} H|0\rangle &= H c_1^\dagger c_0^\dagger |0\rangle = (\omega_0 + \omega_1) |0\rangle + V_2 \underbrace{c_2^\dagger c_0^\dagger c_1^\dagger c_0^\dagger |0\rangle}_{=-|3\rangle} \\ &\quad + V_3 \underbrace{c_3^\dagger c_0^\dagger c_1^\dagger c_0^\dagger |0\rangle}_{=-|4\rangle}, \end{aligned} \quad (14)$$

where the minus signs are replaced by plus signs for spins because operators on different sites commute.

Collecting all matrix elements in this basis yields the following statistics-aware Hamiltonian matrix. Entries whose sign depends on operator reordering are written with $\mp$; take the upper ($-$) sign for fermions and the lower ($+$) sign for spins:

anticommutation sign arises. Consequently, the fermionic and spin Hamiltonians are identical in these cases, and the dynamics coincide.

We now turn to parameter choices relevant for larger environments. For an (effectively) infinite bath with equidistantly spaced modes, all coupled with the same constant $V_k \equiv V$, Born-Markov master equations predict a golden-rule rate [28,29,53]

$$\gamma = 2\pi |V|^2 \rho(\omega_0), \quad (16)$$

where $\rho(\omega_0)$ is the mode density at the system frequency. In our discrete bath with N_E modes uniformly spanning a bandwidth ω_{BW} , $\rho(\omega_0) = N_E/\omega_{\text{BW}}$. We therefore parametrize the coupling by

$$V = \sqrt{\frac{\gamma}{2\pi \rho(\omega_0)}} = \sqrt{\frac{\gamma \omega_{\text{BW}}}{2\pi N_E}}. \quad (17)$$

This scaling is the discrete analog of the standard continuum-limit prescription in Born-Markov theory. Indeed, the bath kernels entering the second-order master equation contain sums of the form $\sum_k |V_k|^2 e^{-i(\omega_0 - \omega_k)\tau}$, which become $\int d\omega \rho(\omega) |V(\omega)|^2 e^{-i(\omega_0 - \omega)\tau}$ as the mode spacing tends to zero. Choosing $V \propto N_E^{-1/2}$ at fixed bandwidth therefore keeps $\rho(\omega_0)|V|^2$, and hence the characteristic rate γ , finite as $N_E \rightarrow \infty$. In the following results, we set $\omega_{\text{BW}} = 4\gamma$, with the bath frequencies uniformly spaced within ω_{BW} .

Representative population dynamics for $N_E = 4, 8, 16$ are shown in Fig. 3. The system is initially unoccupied, and the bath is always half filled.

The master-equation results provide an analytic reference for the observed convergence. The black solid curves in Fig. 3 correspond to the second-order master equation [28,54,55] derived in Sec. II, which, to second order in the system-bath coupling, is identical for fermions and spins. For small baths [panel (a)], both fermionic and spin results deviate

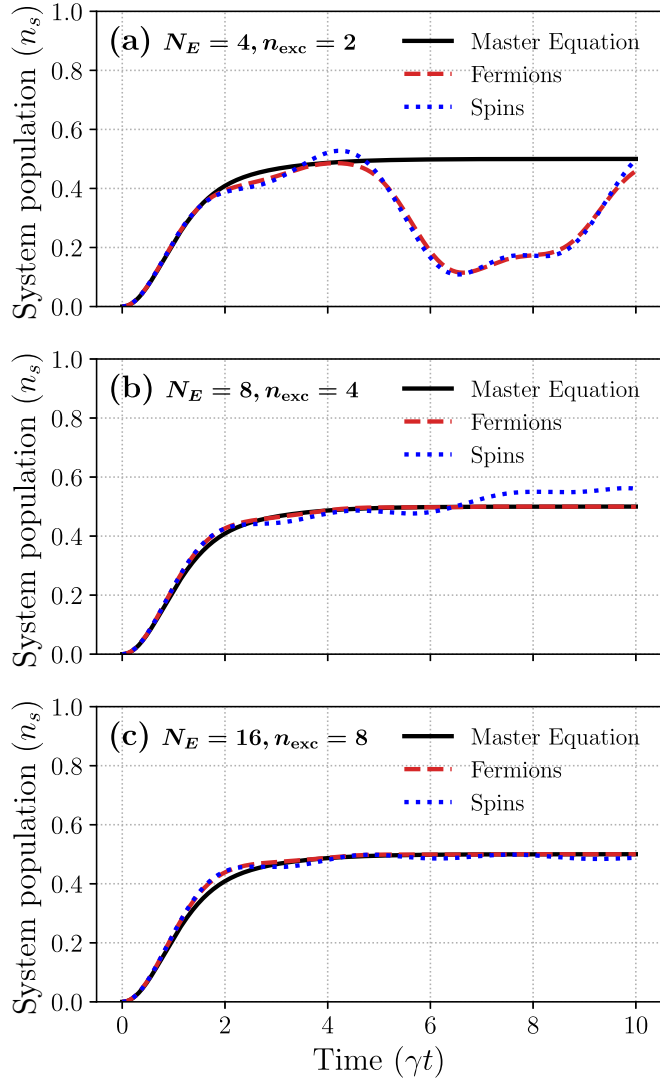


FIG. 3. System population $n_s(t)$ with bandwidth $\omega_{BW} = 4\gamma$ for (a) $N_E = 4$, $n_{exc} = 2$, (b) $N_E = 8$, $n_{exc} = 4$, and (c) $N_E = 16$, $n_{exc} = 8$. Black solid ME2; red dashed fermionic bath; and blue dotted spin bath. As N_E increases, the fermionic and spin results converge and approach the ME2 prediction, reflecting the Markovian limit.

noticeably from the ME2 prediction, reflecting the importance of higher-order exchange processes neglected by the master equation. These deviations are strongly influenced by interference pathways between multiple bath excitations. As the bath size increases [panels (b) and (c)], both exact-diagonalization results approach the ME2 prediction, confirming that higher-order corrections become negligible when N_E is large and the per-mode coupling decreases as $1/\sqrt{N_E}$. By $N_E = 16$, the agreement is nearly quantitative, indicating that the dynamics can be fully captured by second-order processes in this effectively continuous-bath limit.

This convergence can also be interpreted in terms of bath statistics: The fermionic bath is Gaussian by construction, with all higher-order correlations reducible to products of two-point functions via Wick's theorem. The spin bath, in contrast, is generally non-Gaussian at finite bath size and does not admit a simple Wick reduction [56,57]. However, as N_E

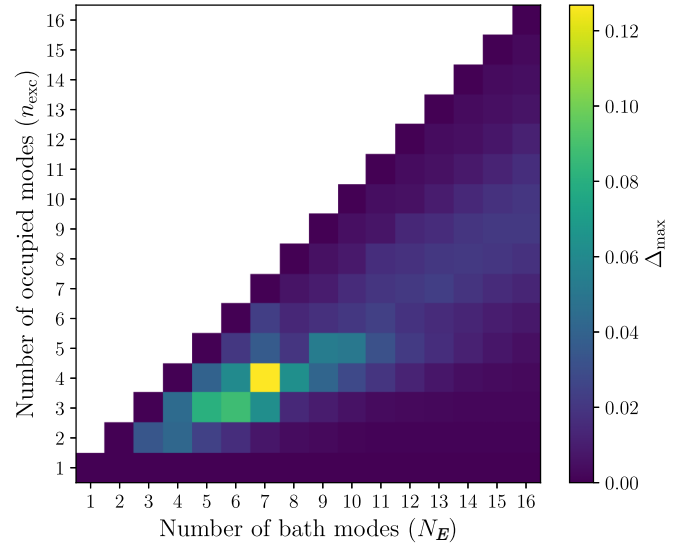


FIG. 4. Maximum population difference $\Delta_{\max}$ between fermions and spins with $\omega_{BW} = 4\gamma$, plotted as a function of N_E (x axis) and the number of occupied bath modes n_{exc} (y axis). Differences peak at moderate bath sizes and near half filling, while vanishing for very small or large N_E .

grows, while the individual couplings scale as $V_k \propto N_E^{-1/2}$, the contribution of such higher-order terms to the reduced dynamics becomes progressively less important. The large-bath agreement with ME2 can therefore be understood as arising from the suppression of higher-order spin-bath corrections in this scaling limit. This convergence, however, does not by itself imply a general equivalence with a genuine bosonic bath. The point of Fig. 3 is that, in the scaling limit considered here, the exact fermionic and spin many-body dynamics both approach the common second-order master-equation limit. At that level, the reduced dynamics depend only on the two-point bath correlation functions entering Eq. (6). In this restricted sense, any suitably engineered environment—including, in principle, a bosonic one—could reproduce the same ME2 dynamics if it generated the same kernels $C_1(\tau)$ and $C_2(\tau)$.

To systematically quantify the discrepancy between the two models, we define

$$\Delta_{\max} = \max_{\gamma t \in [0,10]} |n_S^{(\text{fermion})}(t) - n_S^{(\text{spin})}(t)|, \quad (18)$$

the maximum absolute difference in system population over time. Figure 4 shows a heatmap of $\Delta_{\max}$ plotted against bath size N_E and number of initially occupied bath modes n_{exc} . Note that the absolute magnitudes here are smaller than those in Fig. 2. This is because we now use a coupling defined in Eq. (17), which is relatively smaller than the unscaled coupling $V = 1$ used in Fig. 2.

The largest discrepancies occur for moderate bath sizes ($4 \lesssim N_E \lesssim 8$) and near half filling. In this regime, multiple bath modes participate in multiloop exchange processes, with contributions that are strongly affected by fermionic antisymmetric operator ordering. For very small or very large bath sizes, $\Delta_{\max}$ decreases: In small baths, only a limited number of exchange pathways exist, while in large baths the weak per-mode coupling suppresses higher-order contributions, leaving only second-order processes. When the bath is nearly empty

or almost completely filled, $\Delta_{\max}$ is also small, since the number of available exchange pathways is minimal, leading to identical dynamics for fermions and spins.

IV. CONCLUSIONS

We compared a minimal resonant-level model coupled to either a fermionic or a spin bath using exact diagonalization and an analytically tractable second-order master equation. Importantly, the reduced dynamics are already sensitive to operator ordering, despite the model being strictly quadratic. The two descriptions agree at second order—where only two-point correlators enter—but differ once higher-order processes contribute. In small and moderately sized baths, especially near half filling, antisymmetric fermionic operator algebra introduces exchange minus signs that suppress certain multiexcitation pathways, while commuting spin operators make those pathways add constructively, yielding different dynamics.

As the bath size increases while the per-mode coupling decreases as $V \propto N_E^{-1/2}$ for a fixed Markovian rate γ , higher-order corrections become negligible and both models converge to the ME2 prediction. The convergence can therefore be understood as arising from the suppression of higher-order spin-bath corrections in this scaling limit.

Practically, spin-bath simulations are reliable for large, weakly coupled environments, but for smaller or more strongly coupled baths—particularly near half filling—a fully fermionic treatment is required to capture exchange-statistics-driven effects in the reduced dynamics. This also clarifies the scope for simplified bath representations in numerical impurity solvers: For approaches such as fork tensor-product states (FTPS), fermionic TEDOPA, or fermionic process-tensor formulations [42,43,58], replacing a fermionic reservoir by a commuting spin bath may be justified only in the large, weakly coupled regime identified here, whereas whenever higher-order exchange-sensitive contributions remain appreciable, the full fermionic structure must be retained.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: SECOND-ORDER MASTER EQUATION

Consider the total Hamiltonian defined in Sec. II as $H = H_S + H_E$, where H_E bundled together the free bath and the system-bath coupling. For the master-equation derivation, it is convenient to split this into a free part and an interaction:

$$H = H_S + H_B + H_{SB}, \quad (\text{A1})$$

where the system Hamiltonian is

$$H_S = \omega_0 O_0^\dagger O_0, \quad (\text{A2})$$

the bath Hamiltonian is

$$H_B = \sum_k \omega_k O_k^\dagger O_k, \quad (\text{A3})$$

and the system-bath interaction is given by

$$H_{SB} = \sum_k (V_k O_0^\dagger O_k + V_k^* O_k^\dagger O_0). \quad (\text{A4})$$

Here, O_0 may represent either a fermionic annihilation operator c_0 or a spinlike lowering operator σ_0 . Likewise, O_k is the corresponding bath operator (c_k or σ_k), with $\hbar = 1$ throughout.

Moving to the interaction picture, the free evolution of the system and bath operators is

$$O_0(t) = e^{-i\omega_0 t} O_0, \quad (\text{A5})$$

$$O_k(t) = e^{-i\omega_k t} O_k, \quad (\text{A6})$$

and thus the interaction Hamiltonian becomes

$$\tilde{H}_{SB}(t) = \sum_k [V_k e^{i(\omega_0 - \omega_k)t} O_0^\dagger O_k + \text{H.c.}]. \quad (\text{A7})$$

Assuming an initially factorized system-bath state, the second-order contribution to the master equation for the reduced density matrix $\rho_S(t)$ is

$$\frac{d\rho_S(t)}{dt} = - \int_0^t dt' \text{Tr}_B [\tilde{H}_{SB}(t), [\tilde{H}_{SB}(t'), \rho_S(t') \otimes \rho_B]]. \quad (\text{A8})$$

As noted in Sec. II B 1, although a fully general fermionic reduced-state formalism distinguishes even- and odd-parity components [39], in the present single-mode, number-conserving setting these sectors remain decoupled, so the standard reduced operator $\rho_S(t)$ is sufficient. Expanding the nested commutators and discarding vanishing terms, one obtains

$$\begin{aligned} \frac{d\rho_S(t)}{dt} = & - \sum_k |V_k|^2 \int_0^t dt' [e^{i\omega_k(t-t')} \langle O_k^\dagger O_k \rangle e^{-i\omega_0(t-t')} [O_0, O_0^\dagger \rho_S(t')] + e^{i\omega_k(t-t')} \langle O_k O_k^\dagger \rangle e^{-i\omega_0(t-t')} [\rho_S(t') O_0^\dagger, O_0] \\ & + e^{-i\omega_k(t-t')} \langle O_k O_k^\dagger \rangle e^{i\omega_0(t-t')} [O_0^\dagger, O_0 \rho_S(t)] + e^{-i\omega_k(t-t')} \langle O_k^\dagger O_k \rangle e^{i\omega_0(t-t')} [\rho_S(t) O_0, O_0^\dagger]]. \end{aligned} \quad (\text{A9})$$

We assume the bath is in thermal equilibrium, governed by a Fermi-Dirac distribution:

$$f(\omega_k) = \frac{1}{e^{\beta(\omega_k - \mu)} + 1}.$$

Then, the correlation functions are

$$\langle O_k O_j^\dagger \rangle = \delta_{kj} [1 - f(\omega_k)], \quad (\text{A10})$$

$$\langle O_k^\dagger O_j \rangle = \delta_{kj} f(\omega_k). \quad (\text{A11})$$

Defining

$$C_1(\tau) = \sum_k |V_k|^2 e^{-i(\omega_0 - \omega_k)\tau} f(\omega_k), \quad (\text{A12})$$

$$C_2(\tau) = \sum_k |V_k|^2 e^{-i(\omega_0 - \omega_k)\tau} [1 - f(\omega_k)], \quad (\text{A13})$$

and letting $\tau = t - t'$, one can rewrite the master equation compactly as

$$\begin{aligned} \frac{d\rho_S(t)}{dt} = & - \int_0^t dt' (C_1(\tau) [O_0, O_0^\dagger \rho_S(t')] \\ & + C_2(\tau) [\rho_S(t') O_0^\dagger, O_0] + \text{H.c.}). \end{aligned} \quad (\text{A14})$$

Crucially, this second-order master equation depends only on bath correlation functions, which are entirely specified by the bath statistics and do not hinge on the (anti)commuting nature of O_k . As a result, the same expression holds whether O_0 and O_k are fermionic annihilation operators or spinlike lowering operators.

APPENDIX B: FOURTH-ORDER MASTER EQUATION

In this Appendix, we carefully look at a fourth-order contribution to the perturbative master equation, explicitly

$$\mathcal{D}^{(4)}(t) = (-i)^4 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 \text{Tr}_B[\tilde{H}_{SB}(t_1), [\tilde{H}_{SB}(t_2), [\tilde{H}_{SB}(t_3), [\tilde{H}_{SB}(t_4), \rho_S(t_4) \otimes \rho_B]]]]]. \quad (\text{B3})$$

The nested time integrals explicitly enforce the causal ordering $t_1 > t_2 > t_3 > t_4$, which is equivalent to the action of the standard time-ordering operator $\mathcal{T}$ in the Dyson series. Thus, $\mathcal{T}$ does not appear explicitly in Eq. (B3). Although the nested commutators generate 16 distinct terms, we now focus on one representative nonvanishing term. In particular, we consider

$$\text{Tr}_B[\tilde{H}_{SB}(t_1) \tilde{H}_{SB}(t_2) \tilde{H}_{SB}(t_3) \tilde{H}_{SB}(t_4) \rho_S(t) \otimes \rho_B], \quad (\text{B4})$$

which describes a sequence of four interactions between the system and the bath. Substituting Eq. (B1) into this product

addressing the crucial aspects of operator ordering in the bath correlation functions. Equivalently, the multitime bath objects evaluated below can be regarded as branch-resolved components of contour-ordered correlators on the Keldysh contour; the explicit real-time expressions written here are the components selected by the nested commutator structure of the fourth-order master-equation expansion [36,49]. The starting point is the total Hamiltonian in the interaction picture:

$$\tilde{H}_{SB}(t) = \sum_k [V_k O^\dagger O_k e^{i\Delta_k t} + V_k^* O_k^\dagger O e^{-i\Delta_k t}], \quad (\text{B1})$$

with

$$\Delta_k = \omega_0 - \omega_k,$$

where O and $O^\dagger$ denote system operators, while O_k and $O_k^\dagger$ act on the bath. Our goal is to analyze the perturbative expansion of the master equation to fourth order in H_{SB} , focusing on a representative terms that yield nonzero contributions under the bath trace. We retain an abstract operator notation for O and O_k until we later specify whether the bath operators are fermionic or spin.

The reduced dynamics of the system can be obtained from the Liouville-von Neumann equation via a perturbative expansion. Specifically, the time evolution of the system density matrix $\rho_S(t)$ may be written as

$$\frac{d\rho_S(t)}{dt} = \sum_{n=1}^{\infty} \mathcal{D}^{(n)}(t), \quad (\text{B2})$$

where $\mathcal{D}^{(n)}(t)$ denotes the n th-order contribution in the system-bath coupling. At fourth order, the contribution takes the schematic form

and simplifying yields 16 terms, only some of which survive under the bath trace.

At a given time t_i , we write

$$\tilde{H}_{SB}(t_i) = \sum_{k_i} [V_{k_i} O^\dagger O_{k_i} e^{i\Delta_{k_i} t_i} + V_{k_i}^* O_{k_i}^\dagger O e^{-i\Delta_{k_i} t_i}], \quad (\text{B5})$$

with $\Delta_{k_i} = \omega_0 - \omega_{k_i}$. Substituting Eq. (B5) into the nested commutators yields a product of four such interaction Hamiltonians. After simplifying, one encounters another 16 terms, and we focus on a representative nonvanishing term:

$$\mathcal{K}(t_1, t_2, t_3, t_4) = \sum_{k_1, k_2, k_3, k_4} [V_{k_1} V_{k_2}^* V_{k_3} V_{k_4}^* e^{i(-\Delta_{k_1} t_1 + \Delta_{k_2} t_2 + \Delta_{k_3} t_3 - \Delta_{k_4} t_4)} O_{k_1}^\dagger O O_{k_2}^\dagger O_{k_3} O_{k_4}^\dagger O \rho_S \otimes \rho_B]. \quad (\text{B6})$$

To isolate the essential operator structure pertaining to the bath, we may rewrite $\mathcal{K}$ in the form

$$\mathcal{K}(t_1, t_2, t_3, t_4) = \sum_{k_1, k_2, k_3, k_4} [V_{k_1} V_{k_2}^* V_{k_3} V_{k_4}^* e^{i(-\Delta_{k_1} t_1 + \Delta_{k_2} t_2 + \Delta_{k_3} t_3 - \Delta_{k_4} t_4)} (O O^\dagger O^\dagger O) \rho_S \times \mathcal{C}_{\text{bath}}], \quad (\text{B7})$$

TABLE I. Systematic classification of the six fourth-order fermionic bath correlators containing two creation and two annihilation operators for the product state in Eq. (B9). The first three columns assume $k \neq q$; the last column gives the case where all indices are equal, $k_1 = k_2 = k_3 = k_4 = k$. The corresponding spin-bath values are obtained by replacing the exchange-generated minus signs by plus signs, while leaving the zero and same-mode entries unchanged.

Operator ordering	$(k_1 = k_2 = k)(k_3 = k_4 = q)$	$(k_1 = k_3 = k)(k_2 = k_4 = q)$	$(k_1 = k_4 = k)(k_2 = k_3 = q)$	$(k_1 = k_2 = k_3 = k_4 = k)$
$c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3} c_{k_4}$	0	$-f_k f_q$	$+f_k f_q$	0
$c_{k_1}^\dagger c_{k_2} c_{k_3}^\dagger c_{k_4}$	$f_k f_q$	0	$f_k(1 - f_q)$	f_k
$c_{k_1}^\dagger c_{k_2} c_{k_3} c_{k_4}^\dagger$	$f_k(1 - f_q)$	$-f_k(1 - f_q)$	0	0
$c_{k_1} c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4}$	$(1 - f_k) f_q$	$-(1 - f_k) f_q$	0	0
$c_{k_1} c_{k_2}^\dagger c_{k_3} c_{k_4}^\dagger$	$(1 - f_k)(1 - f_q)$	0	$(1 - f_k) f_q$	$1 - f_k$
$c_{k_1} c_{k_2} c_{k_3}^\dagger c_{k_4}^\dagger$	0	$-(1 - f_k)(1 - f_q)$	$+(1 - f_k)(1 - f_q)$	0

where the bath-dependent part is

$$\mathcal{C}_{\text{bath}} = \text{Tr}_B [O_{k_1}^\dagger O_{k_2} O_{k_3} O_{k_4}^\dagger \rho_B]. \quad (\text{B8})$$

From this point onward, we focus on the evaluation of $\mathcal{C}_{\text{bath}}$, while understanding that the time-dependent phases from Eq. (B6) factor out.

To determine which index combinations $\{k_1, k_2, k_3, k_4\}$ yield a nonzero trace, we assume a product-state bath density matrix,

$$\rho_B = \bigotimes_{k=1}^N \rho_B^{(k)}, \quad \rho_B^{(k)} = (1 - f_k) |0\rangle_k \langle 0| + f_k |1\rangle_k \langle 1|, \quad (\text{B9})$$

with $f_k \equiv f(\omega_k)$. Therefore, only terms with an equal number of creation and annihilation operators on each mode contribute to the trace. Each factor $\hat{H}_{SB}(t_i)$ contributes either $O^\dagger O_{k_i}$ or $O_{k_i}^\dagger O$, so four interaction Hamiltonians generate $2^4 = 16$ bath-operator strings. For the number-diagonal product state in Eq. (B9), only the six strings with two bath creation and two bath annihilation operators survive under the bath trace. Up to relabeling, their nonzero contributions reduce to the index patterns $k_1 = k_2, k_3 = k_4, k_1 = k_3, k_2 = k_4, k_1 = k_4, k_2 = k_3$, and $k_1 = k_2 = k_3 = k_4$. The mode frequencies enter only through the phase factors in Eq. (B6), so the fermion-spin distinction is determined entirely by the algebraic evaluation of the bath trace. Table I summarizes the corresponding fermionic four-point traces.

For a fermionic bath, where $\{c_k, c_{k'}^\dagger\} = \delta_{kk'}$, we evaluate representative contributions explicitly. Three illustrative cases are given as follows:

Case 1: $k_1 = k_2, k_3 = k_4$, and $k_1 \neq k_3$.

$$\begin{aligned} \mathcal{C}_{\text{fermion}}^{(1)} &= \delta_{k_1, k_2} \delta_{k_3, k_4} \text{Tr}[c_{k_1}^\dagger c_{k_1} \rho_B^{(k_1)}] \text{Tr}[c_{k_3} c_{k_3}^\dagger \rho_B^{(k_3)}] \\ &= \delta_{k_1, k_2} \delta_{k_3, k_4} f_{k_1} (1 - f_{k_3}). \end{aligned} \quad (\text{B10})$$

Case 2: $k_1 = k_3, k_2 = k_4$, and $k_1 \neq k_2$.

$$\begin{aligned} \mathcal{C}_{\text{fermion}}^{(2)} &= -\delta_{k_1, k_3} \delta_{k_2, k_4} \text{Tr}[c_{k_1}^\dagger c_{k_1} \rho_B^{(k_1)}] \text{Tr}[c_{k_2} c_{k_2}^\dagger \rho_B^{(k_2)}] \\ &= -\delta_{k_1, k_3} \delta_{k_2, k_4} f_{k_1} (1 - f_{k_2}). \end{aligned} \quad (\text{B11})$$

Case 3: $k_1 = k_4, k_2 = k_3$, and $k_1 \neq k_2$.

$$\mathcal{C}_{\text{fermion}}^{(3)} = \text{Tr}[c_{k_1}^\dagger c_{k_1} \rho_B^{(k_1)}] \text{Tr}[c_{k_2} c_{k_2} \rho_B^{(k_2)}] = 0. \quad (\text{B12})$$

Summing the nonzero contributions for the ordering in Eq. (B8), we obtain

$$\begin{aligned} \mathcal{C}_{\text{fermion}} &= \delta_{k_1, k_2} \delta_{k_3, k_4} (1 - \delta_{k_1, k_3}) f_{k_1} (1 - f_{k_3}) \\ &\quad - \delta_{k_1, k_3} \delta_{k_2, k_4} (1 - \delta_{k_1, k_2}) f_{k_1} (1 - f_{k_2}). \end{aligned} \quad (\text{B13})$$

For completeness, Table I shows that for other orderings with two creation and two annihilation operators, terms with equal indices need not vanish. For the ordering in Eq. (B8), however, both the crossed case and the fully equal case are zero.

For spin baths, with $[\sigma_k, \sigma_{k'}^\dagger] = \delta_{kk'}$, the same index patterns contribute, but no minus sign appears:

$$\begin{aligned} \mathcal{C}_{\text{spin}} &= \delta_{k_1, k_2} \delta_{k_3, k_4} (1 - \delta_{k_1, k_3}) f_{k_1} (1 - f_{k_3}) \\ &\quad + \delta_{k_1, k_3} \delta_{k_2, k_4} (1 - \delta_{k_1, k_2}) f_{k_1} (1 - f_{k_2}). \end{aligned} \quad (\text{B14})$$

For the ordering in Eq. (B8), this differs from Eq. (B13) only by the sign of the exchange contribution. However, even if these terms are neglected or vanish, the fermionic and spin correlations remain distinct: The fermionic case carries a relative minus sign from anticommutation in the exchange pattern $k_1 = k_3, k_2 = k_4$, whereas spin operators commute on different sites. Thus, the representative fourth-order terms in the master equation differ for the two types of baths, even when their spectral densities and occupations are identical.

APPENDIX C: SINGLE-BODY DIAGONALIZATION FOR FERMIONS VERSUS SPIN MODELS

A key simplification of the fermionic formulation is that the Hamiltonian is quadratic in creation and annihilation operators,

$$H = \sum_{i,j} A_{ij} c_i^\dagger c_j,$$

with

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i, c_j\} = 0.$$

The single-particle problem defined by the Hermitian matrix A can be diagonalized via a unitary transformation

$$c_i = \sum_{\alpha} P_{i\alpha} d_{\alpha}, \quad c_i^\dagger = \sum_{\alpha} d_{\alpha}^\dagger P_{i\alpha}^*.$$

The new operators obey

$$\{d_{\alpha}, d_{\beta}^\dagger\} = (P^\dagger P)_{\alpha\beta} = \delta_{\alpha\beta}, \quad \{d_{\alpha}, d_{\beta}\} = 0,$$

so the fermionic algebra is preserved. In the new modes d_α , the Hamiltonian becomes diagonal,

$$H = \sum_{\alpha} \lambda_{\alpha} d_{\alpha}^{\dagger} d_{\alpha}.$$

Population dynamics and correlation functions can then be computed directly from this single-particle diagonalization without constructing the full many-body Hilbert space.

For the spin model, the bath modes are described by ladder operators $\{\sigma_i^-, \sigma_i^+\}$ obeying

$$\{\sigma_i^-, \sigma_i^+\} = 1, \quad [\sigma_i^{\pm}, \sigma_j^{\pm}] = 0 \quad (i \neq j).$$

These relations mix commutation and anticommutation depending on whether operators act on the same or different

sites. If one attempts a basis transformation

$$\sigma_i^- = \sum_{\alpha} P_{i\alpha} d_{\alpha}, \quad \sigma_i^+ = \sum_{\alpha} d_{\alpha}^{\dagger} P_{i\alpha}^*,$$

the resulting mode operators satisfy

$$\{d_{\alpha}, d_{\beta}^{\dagger}\} = (P^{\dagger} P)_{\alpha\beta} + 2 \sum_{k \neq \ell} P_{k\alpha}^* P_{\ell\beta} \sigma_{\ell}^+ \sigma_k^-,$$

where the second term is operator valued. This means the transformed operators do *not* obey simple canonical anticommutation relations, and the Hamiltonian cannot be reduced to a diagonal sum of commuting bilinear terms. As a result, the efficient single-particle diagonalization applicable to fermions does not carry over to the spin model, which must be treated by explicit many-body diagonalization or other approximation schemes.

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