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Dynamical Sign Reversal of Magnetic Correlations in Dissipative Hubbard Models

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In quantum magnetism, the virtual exchange of particles mediates an interaction between spins. Here, we show that an inelastic Hubbard interaction fundamentally alters the magnetism of the Hubbard model due to dissipation in spin-exchange processes, leading to sign reversal of magnetic correlations in dissipative quantum dynamics. This mechanism is applicable to both fermionic and bosonic Mott insulators, and can naturally be realized with ultracold atoms undergoing two-body inelastic collisions. The dynamical reversal of magnetic correlations can be detected by using a double-well optical lattice or quantum-gas microscopy, the latter of which enhances the signal of the magnetic correlations because of spin-charge separation in one-dimensional systems. Our results open a new avenue toward controlling quantum magnetism by dissipation.

Quantum magnetism in Mott insulators is one of the central problems in strongly correlated many-body systems [1]. A Mott insulator is described by the Hubbard model, where a strong repulsive interaction between particles precludes multiple occupation and anchors a single spin to each lattice site. While the kinetic motion of particles is frozen in Mott insulators, quantum mechanics allows particles to virtually hop between sites. A second-order process involving virtual exchange of particles leads to an effective spin-spin interaction, providing the fundamental origin of quantum magnetism [1]. Recent developments in quantum simulations of the Hubbard model with ultracold atoms [2] have offered a powerful approach to unveiling low-temperature properties of quantum magnets [3–7]. In particular, quantum-gas microscopy has enabled site-resolved imaging of spin states [8–11], culminating in direct observation of antiferromagnetic correlations and long-range order in the Hubbard model [12–15]. The essential requirement for observing the quantum magnetism is to achieve sufficiently low temperatures comparable with the exchange coupling.

In this Letter, we demonstrate that ultracold atoms undergoing inelastic collisions obey a completely different principle for realizing quantum magnetism; instead of relaxing to low-energy states, those atoms stabilize *high-energy* states due to dissipation caused by inelastic collisions. Inelastic collisions have widely been observed for atoms in excited states [16, 17] and molecules [18, 19], and can be artificially induced by photoassociation [20]. In contrast to standard equilibrium systems which favor low-energy states, the long-time behavior of dissipative systems is governed by the lifetime of each state under dissipation. We show that the spin-exchange mechanism is altered in the presence of inelastic collisions due to dissipation in an intermediate state. As a result, dissipation dramatically changes the magnetism of the Hubbard model; the magnetism is *inverted* from the conventional equilibrium one, leading to the sign reversal of spin correlations through dissipative dynamics.

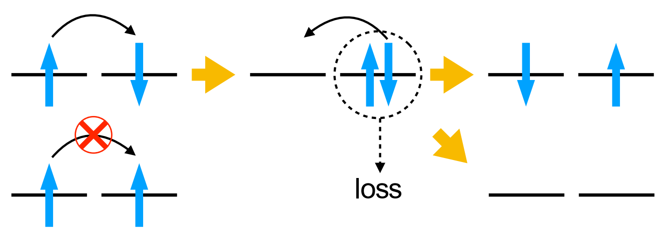

FIG. 1. Schematic illustration of a second-order process mediating the spin-exchange interaction in the dissipative Fermi-Hubbard system. A loss in an intermediate process causes a finite lifetime of the system.

The spin-exchange interaction in the presence of an inelastic interaction, which plays a key role in this Letter, is schematically illustrated in Fig. 1 for the Fermi-Hubbard system. Since an intermediate state in the second-order process involves a doubly occupied site, an antiferromagnetic spin configuration has a finite lifetime due to a particle loss in the intermediate state, whereas a ferromagnetic spin configuration cannot decay due to the Pauli exclusion principle. Because of this dissipative spin-exchange interaction, low-energy states gradually decay, and high-energy spin states will eventually be stabilized. Such stabilization of high-energy states cannot be achieved in conventional equilibrium systems and is reminiscent of negative-temperature states [21, 22] realized in isolated systems [23–32]. In contrast, here dissipation to an environment plays a vital role and thus offers a unique avenue towards the control of magnetism in open systems.

Model.– We consider a dissipative Hubbard model of two-component fermions or bosons realized with ultracold atoms in an optical lattice. The unitary part of the dynamics is governed by the Hubbard Hamiltonian which reads

$$H = -t \sum_{\langle i,j\rangle,\sigma=\uparrow,\downarrow} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) + U \sum_j n^{(f)}_{j\uparrow} n^{(f)}_{j\downarrow} \quad (1)$$

for fermions, and

$$\begin{aligned} H = &- t \sum_{\langle i,j\rangle,\sigma=\uparrow,\downarrow} (b^\dagger_{i\sigma} b_{j\sigma} + \text{H.c.}) + \sum_j U_{\uparrow\downarrow} n^{(b)}_{j\uparrow} n^{(b)}_{j\downarrow} \\ &+ \sum_\sigma \sum_j \frac{U_{\sigma\sigma}}{2} n^{(b)}_{j\sigma}(n^{(b)}_{j\sigma} - 1) \end{aligned} \quad (2)$$

for bosons. Here $c_{j\sigma}$ ($b_{j\sigma}$) is the annihilation operator of a fermion (boson) with spin σ at site j, and $n^{(f)}_{j\sigma} = c^\dagger_{j\sigma} c_{j\sigma}$ ($n^{(b)}_{j\sigma} = b^\dagger_{j\sigma} b_{j\sigma}$). We assume that hopping with an amplitude t occurs between the nearest-neighbor sites and that the on-site elastic interactions are repulsive: $U, U_{\sigma\sigma'} > 0$. We also assume $t > 0$ without loss of generality. Now we suppose that atoms also undergo inelastic collisions; because a large internal energy is converted to the kinetic energy, two atoms after inelastic collisions quickly escape from the trap and are lost. The dissipative dynamics of the density matrix ρ of the system at time τ is described by the following quantum master equation [33]:

$$\frac{d\rho}{d\tau} = i[\rho, H] + \sum_{j,\sigma,\sigma'} \left(L_{j\sigma\sigma'} \rho L^\dagger_{j\sigma\sigma'} - \frac{1}{2}\{L^\dagger_{j\sigma\sigma'} L_{j\sigma\sigma'}, \rho\} \right). \quad (3)$$

The Lindblad operators $L_{j\sigma\sigma'}$ induce two-body losses due to the on-site inelastic collisions, and are expressed as $L_{j\sigma\sigma'} = \sqrt{2\gamma} c_{j\sigma} c_{j\sigma'} \delta_{\sigma,\uparrow}\delta_{\sigma',\downarrow}$ for fermions and $L_{j\sigma\sigma'} = \sqrt{\gamma_{\sigma\sigma'}} b_{j\sigma} b_{j\sigma'}$ for bosons. The coefficients $\gamma, \gamma_{\sigma\sigma'} > 0$ are determined from the loss rates of atoms.

Spin-exchange interaction in dissipative systems.– We first illustrate the basic mechanism that underlies the magnetism of the dissipative Hubbard systems. We consider a strongly correlated regime ($U, U_{\sigma\sigma'} \gg t$) and assume that the initial particle density is set to unity so that a Mott insulating state is realized. For simplicity, we consider the case of the spin SU(2) invariance, i.e., $U_{\uparrow\uparrow} = U_{\downarrow\downarrow} = U_{\uparrow\downarrow} = U$. Then, if doubly occupied states and empty states are ignored, the Fermi (Bose) Hubbard model (1) ((2)) reduces to the antiferromagnetic (ferromagnetic) Heisenberg model $H_{\text{spin}} = J\sum_{\langle i,j\rangle}(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - 1/4)$ ($H_{\text{spin}} = -J\sum_{\langle i,j\rangle}(\boldsymbol{S}_i \cdot \boldsymbol{S}_j + 3/4)$) with the spin-exchange interaction $J = 4t^2/U$ [34, 35].

Here we employ a quantum-trajectory method [36–38] to investigate the dynamics described by Eq. (3) [39]. The dynamics is decomposed into a non-unitary Schrödinger evolution under an effective non-Hermitian Hamiltonian $H_{\text{eff}} \equiv H - \frac{i}{2}\sum_{j,\sigma,\sigma'} L^\dagger_{j\sigma\sigma'} L_{j\sigma\sigma'}$ and stochastic quantum-jump processes which induce particle losses with the jump operators $L_{j\sigma\sigma}$. The non-Hermitian Hamiltonian H_{eff} is obtained if we replace the Hubbard interactions U and $U_{\sigma\sigma'}$ with $U - i\gamma$ and $U_{\sigma\sigma'} - i\gamma_{\sigma\sigma'}$, respectively, thereby making the interaction coefficients complex-valued due to the inelastic interactions. In each quantum trajectory, the system evolves under the non-Hermitian Hubbard model during a time interval between loss events [40, 41]. Each quantum trajectory is characterized by the number of loss events. Let us first consider a trajectory that does not involve any loss event; along this trajectory, the particle number stays constant. Since the double occupancy is still suppressed due to the large Hubbard interaction U, the dynamics is constrained to the Hilbert subspace of the spin Hamiltonian. The effective spin Hamiltonian, which governs the dynamics in the quantum trajectory, is derived from the non-Hermitian Hubbard model through the second-order perturbation theory, giving

$$H_{\text{eff}} = \eta(J_{\text{eff}} + i\Gamma) \sum_{\langle i,j\rangle} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{1-2\eta}{4} \right), \quad (4)$$

where $J_{\text{eff}} = 4Ut^2/(U^2+\gamma^2)$, $\Gamma = 4\gamma t^2/(U^2+\gamma^2)$, and $\eta = +1$ ($\eta = -1$) for fermions (bosons). Here we assume spin-independent dissipation $\gamma_{\sigma\sigma'} = \gamma$ for bosonic atoms (see Supplemental Material [39] for a general case). Equation (4) shows that the spin-spin interactions are affected by dissipation even if the double occupancy is suppressed by the strong repulsion, since the virtual second-order process involves a doubly occupied site (see Fig. 1). In fact, the energy denominators in $J_{\text{eff}} = \text{Re}\left[\frac{4t^2}{U-i\gamma}\right]$ and $\Gamma = \text{Im}\left[\frac{4t^2}{U-i\gamma}\right]$ reflect the dissipation in the intermediate state. The eigenenergy of the Hamiltonian (4) is given by $E_n = (J_{\text{eff}} + i\Gamma)E^{(0)}_n/J$, where $E^{(0)}_n \leq 0$ is the eigenenergy of the Heisenberg Hamiltonian H_{spin}. Thus, the decay rate of the n-th eigenstate, which is given by the imaginary part of the energy, is proportional to $E^{(0)}_n$: $-\text{Im}[E_n] = -(\Gamma/J)E^{(0)}_n \geq 0$. Since $E^{(0)}_n \leq 0$, this indicates that lower-energy states have larger decay rates with shorter lifetimes. Therefore, after a sufficiently long time, only the high-energy spin states survive. This implies that the dissipative Fermi (Bose) Hubbard system develops ferromagnetic (antiferromagnetic) correlations. The mechanism can intuitively be understood from Fig. 1 for the Fermi-Hubbard system as no decay occurs for a ferromagnetic spin configuration. For the Bose-Hubbard system, while additional spin-exchange processes due to the absence of the Pauli exclusion principle for ferromagnetic spin configurations lead to a ferromagnetic Heisenberg interaction for a closed system, dissipation during the exchange processes renders ferromagnetic states to decay faster than antiferromagnetic states in the dissipative system.

Double-well systems.– A minimal setup to demonstrate the basic principle described above is a two-site system. It can be experimentally realized with an ensemble of double wells created by optical superlattices [3, 4], and magnetic correlations between the left and right wells

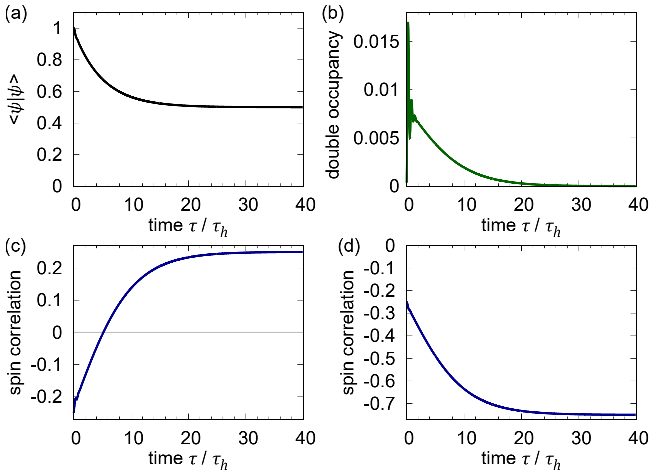

FIG. 2. (a) Time evolution of the squared norm $\langle\psi(\tau)|\psi(\tau)\rangle$ and (b) that of the double occupancy $\langle\psi(\tau)|\,\frac{1}{2}(n^{(a)}_{1\uparrow}n^{(a)}_{1\downarrow}+n^{(a)}_{2\uparrow}n^{(a)}_{2\downarrow})\,|\psi(\tau)\rangle\,/\,\langle\psi(\tau)|\psi(\tau)\rangle$ ($a=f$ or b). Note that these quantities take the same values for the Fermi and Bose Hubbard models. (c) Time evolution of the spin correlation $\langle\psi(\tau)|\,\boldsymbol{S}_1\cdot\boldsymbol{S}_2\,|\psi(\tau)\rangle\,/\,\langle\psi(\tau)|\psi(\tau)\rangle$ of the Fermi-Hubbard model and (d) that of the Bose-Hubbard model. The parameters are set to $U/t=10$ and $\gamma/t=3$. The unit of time is the inverse hopping rate $\tau_h=1/t$.

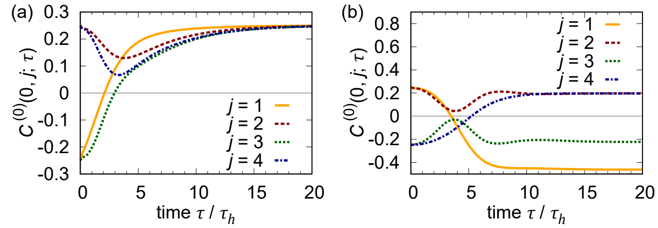

FIG. 3. Dynamics of the spin correlations $C^{(0)}(0,j;\tau)$ for the dissipative 8-site Fermi [(a)] and 6-site Bose [(b)] Hubbard systems in the absence of quantum-jump events. The parameters are set to $U/t=10$ and $\gamma/t=10$. The unit of time is the inverse hopping rate $\tau_h=1/t$.

can be measured from singlet-triplet oscillations [4, 5, 7]. We consider an ensemble of double wells in which two particles with opposite spins occupy each double well. During the dissipative dynamics, a double well in which a loss event takes place becomes empty. Therefore, when a magnetic correlation is measured at time τ, signals come from double wells where particles are still not lost. Such wells are faithfully described by the quantum trajectory without loss events.

Figure 2 shows the time evolutions of (a) the squared norm of the state $\langle\psi(\tau)|\psi(\tau)\rangle$, (b) the double occupancy $\langle\psi(\tau)|\,\frac{1}{2}(n^{(a)}_{1\uparrow}n^{(a)}_{1\downarrow}+n^{(a)}_{2\uparrow}n^{(a)}_{2\downarrow})\,|\psi(\tau)\rangle\,/\,\langle\psi(\tau)|\psi(\tau)\rangle$ ($a=f,b$), and (c) (d) the spin correlation $\langle\psi(\tau)|\,\boldsymbol{S}_1\cdot\boldsymbol{S}_2\,|\psi(\tau)\rangle\,/\,\langle\psi(\tau)|\psi(\tau)\rangle$ obtained from a numerical solution of the Schrödinger equation $i\partial_\tau\,|\psi(\tau)\rangle=H_{\rm eff}\,|\psi(\tau)\rangle$. Here $H_{\rm eff}$ is the two-site non-Hermitian Fermi (Bose) Hubbard model and the initial state is assumed to be $c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}\,|0\rangle$ ($b^\dagger_{1\uparrow}b^\dagger_{2\downarrow}\,|0\rangle$), where $|0\rangle$ is the particle vacuum. The results clearly show that the dissipative Fermi (Bose) Hubbard system develops a ferromagnetic (antiferromagnetic) correlation which is eventually saturated at 0.25 (-0.75), indicating a formation of the highest-energy spin state $(|\uparrow\rangle_1\,|\downarrow\rangle_2+|\downarrow\rangle_1\,|\uparrow\rangle_2)/\sqrt{2}$ ($(|\uparrow\rangle_1\,|\downarrow\rangle_2-|\downarrow\rangle_1\,|\uparrow\rangle_2)/\sqrt{2}$) of the Heisenberg model. We note that the double occupancy in the dynamics is almost negligible and further suppressed by an increase in the dissipation γ (see Supplemental Material for the dependence on γ [39]); the latter is due to the continuous quantum Zeno effect [18–20] by which strong dissipation inhibits hopping to an occupied site. Nevertheless, virtual hopping is allowed, leading to the growth in the spin correlation.

Another important feature is that the squared norm stays constant after the spin correlation is saturated. Since the squared norm corresponds to the probability of the lossless quantum trajectory [38], the saturation signals that the system enters a dark state that is immune to dissipation. This property explains why the highest-energy spin state is realized in the long-time limit; the spin-symmetric (spin-antisymmetric) state of fermions (bosons) is actually free from dissipation and thus has the longest lifetime, since in this spin configuration both Fermi and Bose statistics dictate antisymmetry of the real-space wavefunction and thus allow no double occupancy [42].

Extracting spin correlations from conditional correlators.– Having established the basic mechanism of the magnetism induced by dissipation, we now include the effect of quantum jumps, which create holes due to particle loss. One might think that the created holes scramble the background spin configuration and disturb the development of the spin correlation. Below we show that this issue can be circumvented by using quantum-gas microscopy for the one-dimensional Hubbard models.

We first show in Fig. 3 the time evolution of the one-dimensional dissipative Hubbard models in quantum trajectories without quantum-jump events. The system size is $N=8$ ($N=6$) for the Fermi (Bose) system. The initial states are chosen to be a Néel state $|\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\rangle$ for the Fermi system, and a ferromagnetic domain-wall state $|\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\rangle$ for the Bose system, in accordance with the equilibrium spin configuration of each system without dissipation. After the dissipation is switched on at $\tau=0$, the Fermi (Bose) system in Fig. 3 (a) (Fig. 3 (b)) clearly develops a ferromagnetic (antiferromagnetic) spin correlation $C^{(0)}(i,j;\tau)\equiv\langle\psi(\tau)|\,\boldsymbol{S}_i\cdot\boldsymbol{S}_j\,|\psi(\tau)\rangle\,/\,\langle\psi(\tau)|\psi(\tau)\rangle$, whose sign is reversed from that of the initial state, and the correlation is eventually saturated at a value consistent with the highest-energy state of the antiferromagnetic (ferromagneic) Heisenberg chain.

Quantum-gas microscopy enables a high-precision measurement of the particle number at the single-site

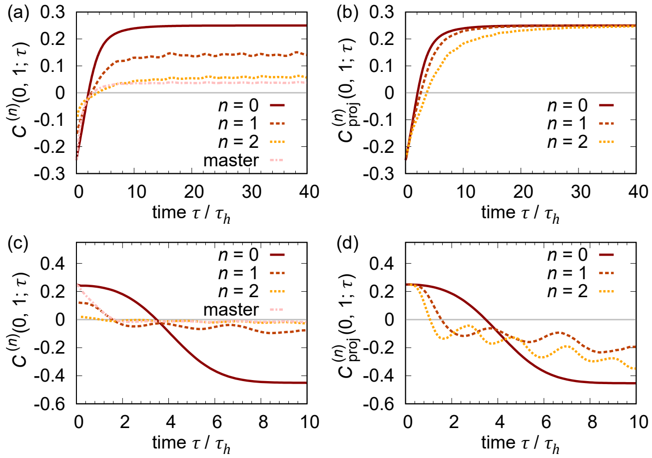

FIG. 4. (a) (c) Dynamics of spin correlations $C^{(n)}(0,1;\tau)$ averaged over quantum trajectories that involve n quantum jumps. The label “master” corresponds to $C(0,1;\tau)$, in which the correlation is calculated from the full density matrix of the solution to the master equation. (b) (d) Dynamics of conditional correlators $C^{(n)}_{\mathrm{proj}}(0,1;\tau)$ after elimination of the effect of holes by additional projection. (a) and (b) show the results for the dissipative Fermi-Hubbard model, and (c) and (d) show those for the dissipative Bose-Hubbard model. The parameters and the initial states are the same as in Fig. 3. The unit of time is the inverse hopping rate $\tau_h = 1/t$.

resolution [8–11]. Given a single-shot image of an atomic gas, the occupation number of each site is identified to be zero, one, or two. From this information, one can find the number of quantum jumps that have occurred by the time of the measurement. Accordingly, one can take an ensemble average over quantum trajectories with a given number of quantum jumps [43]. The density matrix conditioned on the number of quantum jumps from the initial time to τ is given by $\rho^{(n)}(\tau) \equiv \mathcal{P}^{(n)}\rho(\tau)\mathcal{P}^{(n)}/\mathrm{Tr}[\mathcal{P}^{(n)}\rho(\tau)\mathcal{P}^{(n)}]$. Here $\mathcal{P}^{(n)}$ is a projection onto the sector in which n quantum jumps have occurred. Then, one can calculate the correlation function $C^{(n)}(i,j;\tau) \equiv \mathrm{Tr}[\rho^{(n)}(\tau)\boldsymbol{S}_i \cdot \boldsymbol{S}_j]$ [39].

Figure 4(a) (4(c)) shows the dynamics of the magnetic correlation $C^{(n)}(0,1;\tau)$ of the dissipative Fermi (Bose) Hubbard system. For comparison, we also show $C(0,1;\tau) \equiv \mathrm{Tr}[\rho(\tau)\boldsymbol{S}_0 \cdot \boldsymbol{S}_1]$ where the average is taken over all quantum trajectories so as to give the solution of the master equation (3). The result indicates that the sign reversal of the magnetic correlations is still seen in the presence of quantum jumps, and the magnitude of the correlation increases with decreasing the number of quantum jumps.

The correlation function $C^{(n)}(i,j;\tau)$ includes the effect of holes produced by quantum jumps. However, one can remove the effect of holes and extract the contribution from spins remaining in the system by imposing a further condition with the following conditional correlator [39]:

$$C^{(n)}_{\mathrm{proj}}(j,j+1;\tau) \equiv \frac{\mathrm{Tr}[P_jP_{j+1}\rho^{(n)}(\tau)P_jP_{j+1}\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}]}{\mathrm{Tr}[P_jP_{j+1}\rho^{(n)}(\tau)P_jP_{j+1}]}, \tag{5}$$

where P_j is a projector onto states in which site j is singly occupied. More generally, one can use a correlation function $C^{(n)}_{\mathrm{proj}}(j,j+d;d_h;\tau) \equiv \mathrm{Tr}[P_jQ_{d_h}P_{j+d}\rho^{(n)}(\tau)P_jQ_{d_h}P_{j+d}\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+d}]/\mathrm{Tr}[P_jQ_{d_h}P_{j+d}\rho^{(n)}(\tau)P_jQ_{d_h}P_{j+d}]$, where Q_{d_h} is another projector onto states with d_h holes and $d-d_h-1$ singly occupied sites between sites j and $j+d$. Such conditional correlators have been measured with quantum-gas microscopy [44, 45] by collecting images that match the conditions.

Numerical results of the conditional correlators $C^{(n)}_{\mathrm{proj}}(0,1;\tau)$ for the Fermi (Bose) Hubbard system are shown in Fig. 4(b) (4(d)). Notably, the magnetic correlations are significantly enhanced from those without projection and even saturated at the same maximum value as in the case without quantum jumps for the Fermi-Hubbard system. While saturation is not achieved in the Bose-Hubbard system since the numerical simulation is limited to $\tau/\tau_h \lesssim 10$ for sufficient statistical convergence, similar saturation behavior can be seen at a single-trajectory level [39]. Nevertheless, a significant increase in the antiferromagnetic correlation is clearly observed by comparison between Figs. 4(c) and 4(d).

The underlying physics behind these results is spin-charge separation in one-dimensional systems [46]. In the strongly correlated Hubbard chain, the created holes move freely as if they were non-interacting, while the background spin state remains the same as that of the Heisenberg chain [47]. In particular, given an eigenstate of the one-dimensional Hubbard chain, one can reconstruct an eigenstate of the Heisenberg model by eliminating holes involved in individual particle configurations that are superposed in the quantum state [45, 47, 48]. Thus, the conditional correlators $C^{(n)}_{\mathrm{proj}}(j,j+1;\tau)$ and $C^{(n)}_{\mathrm{proj}}(j,j+d;d_h;\tau)$ capture the essential features of spin correlations in the background Heisenberg model, which are equivalent to those in the case without holes at least in the highest-energy spin state that can be achieved in the long-time limit. This explains the saturated value of the conditional spin correlation that exactly coincides with that in the trajectory without loss events shown in Fig. 3. Although the original argument on the spin-charge separation in eigenstates of the Hubbard model was limited to the fermion case [45, 47, 48], our numerical results indicate that this mechanism also works for the Bose-Hubbard system.

Summary and future perspectives.– We have shown that an inelastic Hubbard interaction alters the spin-exchange process due to a finite lifetime of the intermediate state, leading to novel quantum magnetism opposite to the conventional equilibrium magnetism. Rather than stabilizing low-energy states, high-energy spin states have longer lifetimes and are thus realized in dissipative systems. The Hubbard models with inelastic interactions can be realized with various types of ultracold atoms with internal excited states. A possible experimental platform is a system of ytterbium atoms having long-lived excited states for which the decay to the ground state due to spontaneous emission is negligible [16, 17]. Furthermore, inelastic collisions can be artificially induced by using photoassociation techniques [20], which will enable the control of quantum magnetism with dissipation.

Our work raises interesting questions for future investigation. First, while we have shown that the effect of holes can be eliminated in one-dimensional systems due to spin-charge separation, it cannot in two (or higher) dimensions. Second, since the Bose-Hubbard system develops antiferromagnetic correlations due to dissipation, geometric frustration in the lattice may realize quantum spin liquids and topological order, which have not yet been realized in cold-atom experiments due to the difficulty of cooling. Third, if the spin SU(2) symmetry is relaxed, eigenstates of the non-Hermitian spin Hamiltonian with the complex-valued spin-exchange couplings are no longer the same as those of the original Hermitian spin Hamiltonian. It is therefore worthwhile to explore novel quantum magnetism in these non-Hermitian spin Hamiltonians [49].

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