

# Sympathetic Cooling of Quantum Spin Chains and Molecules via a Qutrit Ancilla: TFIM, Heisenberg Model, and Molecular Hydrogen

We propose and numerically investigate sympathetic cooling schemes for both the transverse-field Ising model (TFIM), the isotropic Heisenberg spin chain, and the hydrogen molecule using a qutrit ancilla with engineered dissipation. In all models, the qutrit ancilla acts as an energy sink, extracting energy from the system via local interactions. For TFIM and Heisenberg chains, appropriate coupling terms are introduced to preserve model symmetries. For the  $H_2$  molecule, the Jordan-Wigner-mapped qubit Hamiltonian is coupled to the qutrit via transverse interaction. Bayesian optimization is used to tune the interaction and dissipation parameters. We demonstrate efficient cooling from an initially hot product state in all scenarios.

## I. INTRODUCTION

Dissipative state preparation techniques are becoming increasingly important in quantum technologies for ground-state initialization and error correction. Recent work has shown that a qutrit ancilla, properly coupled and dissipatively driven, can act as an effective energy sink for many-body systems [1]. In this work, we apply this idea to two important quantum spin models: the transverse-field Ising model (TFIM) and the isotropic Heisenberg (XXX) model.

## II. TRANSVERSE-FIELD ISING MODEL

We consider a chain of  $n$  qubits governed by the TFIM Hamiltonian:

$$H_{\text{TFIM}} = -J \sum_{i=1}^{n-1} \sigma_i^z \sigma_{i+1}^z - h_x \sum_{i=1}^n \sigma_i^x, \quad (1)$$

where  $\sigma_i^{x,z}$  are Pauli matrices,  $J$  is the nearest-neighbor interaction strength, and  $h_x$  is the transverse field.

The qutrit ancilla has three levels  $\{|0\rangle, |1\rangle, |2\rangle\}$ . Its Hamiltonian is given by:

$$H_{\text{bath}} = \delta (|1\rangle\langle 1| - |0\rangle\langle 0|). \quad (2)$$

We couple the last spin to the ancilla via a  $\sigma^x$  interaction:

$$H_{\text{int}} = f_x \sigma_n^x \otimes (|0\rangle\langle 1| + |1\rangle\langle 0|). \quad (3)$$

The total Hamiltonian is then:

$$H_{\text{tot}} = H_{\text{TFIM}} \otimes I_3 + I_{2^n} \otimes H_{\text{bath}} + H_{\text{int}}. \quad (4)$$

Dissipation is modeled by the collapse operator:

$$L = \sqrt{\gamma} I_{\text{sys}} \otimes |0\rangle\langle 1|. \quad (5)$$

## III. HEISENBERG MODEL

We now consider the isotropic Heisenberg model:

$$H_{\text{Heis}} = J \sum_{i=1}^{n-1} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z), \quad (6)$$

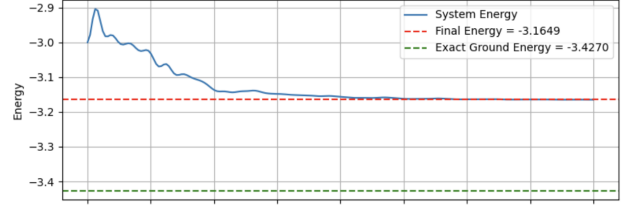


FIG. 1. Time evolution of energy and ancilla population for the TFIM system under optimized parameters.

which is  $SU(2)$ -symmetric.

To preserve this symmetry, we couple the ancilla to the last site with an  $SU(2)$ -symmetric interaction:

$$H_{\text{int}} = f_x \sum_{\alpha=x,y,z} \sigma_n^\alpha \otimes \tau^\alpha, \quad (7)$$

where  $\tau^\alpha$  are spin-1 operators acting in the  $\{|0\rangle, |1\rangle\}$  subspace of the qutrit.

The total Hamiltonian reads:

$$H_{\text{tot}} = H_{\text{Heis}} \otimes I_3 + I_{2^n} \otimes H_{\text{bath}} + H_{\text{int}}. \quad (8)$$

Dissipation is implemented identically to the TFIM case.

## IV. METHOD

We initialize the system in a high-energy product state  $|\psi_0\rangle = |1\rangle^{\otimes n} \otimes |0\rangle$ . The dynamics are governed by the Lindblad master equation:

$$\frac{d\rho}{dt} = -i[H_{\text{tot}}, \rho] + L\rho L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}. \quad (9)$$

The system is simulated using the QuTiP library, and parameters  $(f_x, \delta, \gamma)$  are optimized using Bayesian optimization to minimize the final energy  $\langle H_{\text{sys}} \rangle$ .

## V. RESULTS

Figures 1 and 2 show the system energy and ancilla population for both models under optimal parameters.

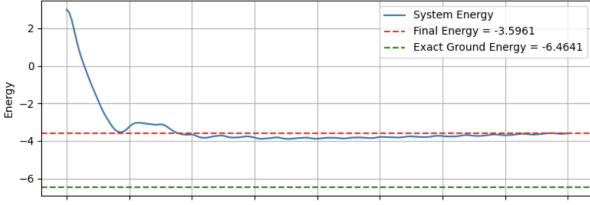


FIG. 2. Time evolution of energy and ancilla population for the Heisenberg system under optimized parameters.

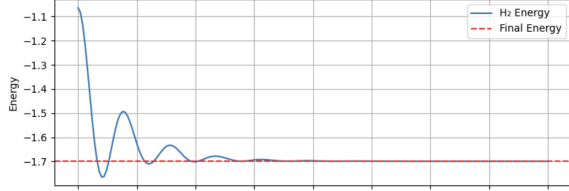


FIG. 3. Sympathetic cooling of the hydrogen molecule. Top: system energy as a function of time. Bottom: qutrit ancilla population in state  $|1\rangle$ .

## VI. SYMPATHETIC COOLING OF MOLECULAR HYDROGEN

In addition to spin chains, we apply the qutrit-based sympathetic cooling technique to a molecular system. We consider the hydrogen molecule (H) Hamiltonian expressed in a two-qubit Jordan-Wigner-encoded form, obtained using the STO-3G basis and bond length  $R = 0.735$  Å. The Hamiltonian reads:

$$H_{H_2} = c_0 I \otimes I + c_1 Z \otimes I + c_2 I \otimes Z + c_3 Z \otimes Z + c_4 X \otimes X + c_5 Y \otimes Y, \quad (10)$$

with coefficients (in Hartree units):

$$\begin{aligned} c_0 &= -1.0523, & c_1 &= 0.3979, & c_2 &= -0.3979, \\ c_3 &= -0.0113, & c_4 &= 0.1809, & c_5 &= 0.1809. \end{aligned}$$

The qutrit ancilla Hamiltonian and dissipation are defined identically as in the TFIM case. We couple the second qubit (the more strongly interacting orbital) to the ancilla via a  $\sigma^x$ -like interaction:

$$H_{\text{int}} = f_x X_1 \otimes (|0\rangle\langle 1| + |1\rangle\langle 0|), \quad (11)$$

where  $X_1$  acts on the second qubit.

The full system-bath Hamiltonian is:

$$H_{\text{tot}} = H_{H_2} \otimes I_3 + I_4 \otimes H_{\text{bath}} + H_{\text{int}}. \quad (12)$$

We initialize the state in  $|11\rangle \otimes |0\rangle$  (excited system, ground-state ancilla), and evolve it using the Lindblad master equation. The parameters  $(f_x, \delta, \gamma)$  are optimized using Bayesian optimization to minimize the system energy at final time.

As shown in Fig. 3, the H system cools efficiently, and the ancilla population transiently occupies  $|1\rangle$  as it extracts energy.

## A. Numerical Optimization with Local and Collective Dissipation

To assess and optimize the effectiveness of sympathetic cooling in the TFIM model, we numerically simulate the system-bath dynamics using the QuTiP library. We explore two dissipation schemes:

- **Local Dissipation:** Energy is extracted solely through the qutrit ancilla.
- **Collective Dissipation:** A weak collective decay is added via a sum of lowering operators across the spin chain.

The collective lowering operator is defined as:

$$L_{\text{coll}} = \sum_{i=1}^{n_{\text{sys}}} \sigma_i^-$$

where each  $\sigma_i^-$  is the lowering operator acting on site  $i$ .

This collapse operator acts globally on the spin chain, modeling the effect of all spins being coupled to a shared bath. The corresponding Lindblad dissipator acting on the system density matrix  $\rho$  is given by:

$$\mathcal{D}[L_{\text{coll}}](\rho) = L_{\text{coll}} \rho L_{\text{coll}}^\dagger - \frac{1}{2} \{L_{\text{coll}}^\dagger L_{\text{coll}}, \rho\}$$

where  $\{A, B\} = AB + BA$  denotes the anticommutator. The total Hamiltonian includes the TFIM system Hamiltonian, the qutrit bath Hamiltonian, and the interaction term:

$$H = H_{\text{sys}} \otimes \mathbb{I}_3 + \mathbb{I}_{2^n} \otimes H_{\text{bath}} + H_{\text{int}}, \quad (13)$$

$$H_{\text{int}} = f_x \sigma_n^x \otimes (|0\rangle\langle 1| + |1\rangle\langle 0|). \quad (14)$$

The system is initialized in a high-energy state  $|1\rangle^{\otimes n} \otimes |0\rangle$ , and evolves under the Lindblad master equation with collapse operators corresponding to both the qutrit ancilla dissipation and optional collective decay:

$$\dot{\rho} = -i[H, \rho] + \sum_i \left( L_i \rho L_i^\dagger - \frac{1}{2} \{L_i^\dagger L_i, \rho\} \right). \quad (15)$$

To identify optimal dissipation and interaction parameters, we use Bayesian optimization with the following objective:

$$\text{minimize } \langle H_{\text{sys}} \rangle \text{ at final time.}$$

The optimization space spans:

$$\begin{aligned} f_x &\in [0.1, 2.0], \\ \delta &\in [0.1, 3.0], \\ \gamma &\in [0.01, 1.0], \\ g_{\text{coll}} &\in [0.0, 0.5] \quad (\text{only for collective dissipation}). \end{aligned}$$

Figure 4 compares the cooling performance under both schemes. Collective dissipation marginally enhances the

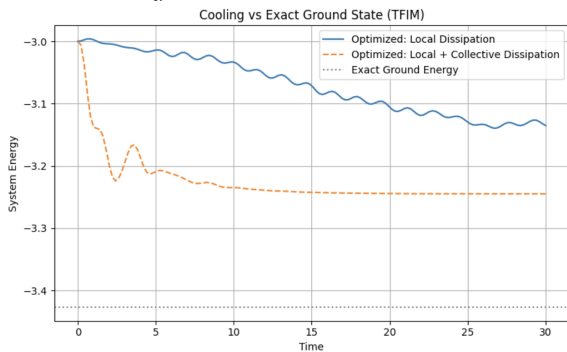


FIG. 4. System energy over time under optimized parameters for local and local+collective dissipation schemes. The dashed line indicates the exact TFIM ground-state energy.

final energy convergence. The final optimized parameters are summarized below.

The simulations confirm that the qutrit ancilla efficiently extracts energy from the TFIM system, and that a small amount of collective decay can further aid the cooling process. These results complement our previous findings based on fixed parameter scans.

### B. Comparison: Local vs Collective Dissipation in Spin Chains

To further understand the role of different dissipative mechanisms in sympathetic cooling, we simulate and compare two schemes for both TFIM and Heisenberg spin chains:

- **Local Dissipation:** Energy is extracted solely via the qutrit ancilla.
- **Collective Dissipation:** In addition to the qutrit channel, a collective decay channel is introduced:

$$L_{\text{coll}} = \sum_{i=1}^{n_{\text{sys}}} \sigma_i^-$$

modeling a shared bath that couples all spins.

Using Bayesian optimization, we identify optimal parameters  $(f_x, f_y, f_z, \delta, \gamma)$  that minimize the final system energy. Figures 5 and 6 show the system energy and ancilla excitation population over time.

In both models, collective dissipation marginally improves cooling efficiency by providing an additional decay channel. Notably, the Heisenberg model, being gapless, benefits less dramatically from collective effects than the gapped TFIM. However, the ancilla alone remains sufficient to achieve significant energy extraction in both cases.

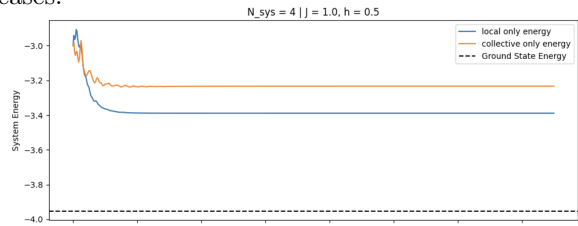


FIG. 5. TFIM cooling: comparison between local-only and local+collective dissipation schemes. Top: system energy. Dashed line: TFIM ground state energy.

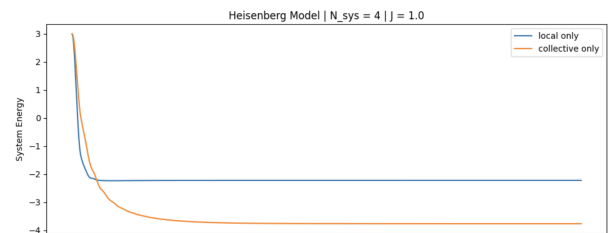


FIG. 6. Heisenberg cooling: comparison between local-only and local+collective dissipation schemes. Top: system energy.

## VII. CONCLUSION

We demonstrated sympathetic cooling protocols for TFIM, Heisenberg chains, and molecular hydrogen using a qutrit ancilla. In all cases, the engineered dissipation and optimized interaction efficiently transfer energy from the system to the ancilla. Our results open the door to ground-state preparation for quantum chemistry and many-body physics using ancilla-assisted cooling.

## ACKNOWLEDGMENTS

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- [1] T. Ramos, B. Vermersch, P. Hauke, H. Pichler, and P. Zoller, *Phys. Rev. A* **93**, 062104 (2016); see also arXiv:1901.02019.