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Variational study of two-impurity spin-boson model with a common Ohmic bath: Ground-state phase transitions

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Extensive variational calculations have been carried out to study quantum phase transitions in the ground states of a two-impurity system embedded in a common Ohmic bath of bosons. By means of a trial wave function by the name of the “multi- D_1 ansatz,” quantum criticality in both the impurity system and the Ohmic bosonic bath is investigated with relevant transition points and critical exponents determined accurately. With more than ten thousand variational parameters, our numerical approach produces much better descriptions of the ground states around the transition point, in comparison with previous results from the numerical renormalization group, exact diagonalization, quantum Monte Carlo, and other variational methods. The considerable controversy on the critical coupling in the weak tunneling limit has also been addressed. It is inferred that the ground-state phase transition is of first order in the presence of the strong antiferromagnetic spin-spin coupling, at variance with that in the ferromagnetic regime or in the absence of spin-spin coupling where the transition belongs to the Kosterlitz-Thouless universality class.

I. INTRODUCTION

Considerable attention has been devoted to open quantum systems over the past decades [1–3]. A variety of open quantum systems, together with associated quantum dynamics and phase transitions, have been the subjects of extensive numerical and analytical investigations in a wide range of settings, such as the defect tunneling in solids [4, 5], spontaneous emission in quantum optics [6, 7], charge transfer processes in biological reactions [8, 9], semiconducting quantum dots in nanocavities [10, 11], and quantum tunneling in superconducting circuits [12–14]. The spin-boson model (SBM) describes a single two-level system, e.g., a spin-1/2 particle or a magnetic impurity, linear coupled to environmental degrees of freedom represented by a continuous bath consisting of bosonic field modes [15]. In spite of its apparent simplicity, the system possesses multifaceted properties in statics, dynamics, and quantum criticality, and has often been used as a paradigmatic model for studying open quantum systems.

There exists a ground-state phase transition in SBM separating a nondegenerate delocalized phase from a doubly degenerate localized phase, provided that the coupling between the system and the environment can be characterized by a gapless spectral function $J(\omega) = 2\alpha\omega_c^{1-s}\omega^s$, where α denotes the dimensionless coupling strength, ω_c represents the high frequency cutoff, and s is the spectral exponent [16]. The phase transition is of second order in the sub-Ohmic regime ($0 < s < 1$), and of the Kosterlitz-Thouless type in the Ohmic case

($s = 1$). The latter can be realized in the context of waveguide quantum electrodynamics by coupling a superconducting qubit to a uniform Josephson junction array [17–19]. In recent years, the transition boundary and the critical exponents have been estimated by a variety of approaches, such as the numerical renormalization group (NRG), exact diagonalization (ED), variational matrix product states (VMPS), quantum Monte Carlo (QMC), and variational methods (VM) [20–26]. Results agree in the sub-Ohmic regime, but differ distinctly in the Ohmic regime hinting the difficulty associated with the numerical studies of the Kosterlitz-Thouless transition. Very recently, a variational approach based on a systematic coherent-state expansion has been used to probe the ground-state properties of SBM at $s = 1$ [27].

Variants of the standard SBM have also been intensively studied [25, 28–32]. The two-impurity SBM, for example, is one of the prominent SBM generalizations, as it is essential for studying quantum logical operations involving two qubits in quantum computations [33–35]. In addition, the presence of a second impurity allows us to address the interplay between quantum control and dissipation represented by the spin-spin and spin-bath interactions, respectively, giving rise to a much richer phase diagram [36]. For the single-impurity SBM with an Ohmic bath, the Kosterlitz-Thouless transition point of $\alpha_c \approx 1$ is generally accepted in the weak tunneling limit, which can be estimated by mapping onto the anisotropic Kondo model with bosonization techniques [1, 16, 37]. In contrast, the value of α_c for the two-impurity SBM attached a common Ohmic bath is still under contention. Specifically, $\alpha_c = 0.5$ was predicted variationally in the absence of both bias and spin-spin coupling [38], very different from $\alpha_c \approx 0.18$ obtained in NRG calculations, 0.22 in QMC simulations, and 0.16 from nonequilibrium

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quantum dynamics with a tunneling constant of 0.025 [36, 39, 40]. Very recently, $\alpha_c = 0.125$ was arrived at by means of the variational treatment based on a new ansatz and mean-field approximation [41]. It follows that an accurate determination of the transition point is needed for the two-impurity model. More importantly, it should be addressed whether the transition belongs to the Kosterlitz-Thouless universality class in the presence of the impurity-impurity coupling.

In previous studies on quantum phase transitions in SBM, attention was mainly focused on the spin-related observations, especially for the spontaneous magnetization, a nature order parameter [24, 42–45]. The Bethe Ansatz solution of the anisotropic Kondo model, believed to be equivalent to the Ohmic single-spin model, shows that the spin coherence $\langle \sigma_x \rangle$ decreases monotonically with the coupling α , and remains continuous and finite at the Kosterlitz-Thouless transition. In contrast, a discontinuous reduction in the spin magnetization occurs at the transition point α_c from $\langle \sigma_z \rangle = 0$ in the delocalized phase to $\langle \sigma_z \rangle = -1$ (or 1) in the localized phase [16]. Even under a tiny bias, however, the discontinuity in the magnetization is replaced by a smooth crossover, which may result in a significant reduction of the critical coupling α_c . Those results have been numerically confirmed by applying the NRG and VM approaches to the spin-boson model [27, 42]. For the two-impurity SBM, unfortunately, small but finite bias values, e.g., $10^{-8}\omega_c$ and $10^{-5}\omega_c$, were sometimes chosen to trigger the phase transition. Therefore, results such as $\alpha_c \approx 0.18$ and 0.125 are possibly underestimated [36, 41]. Moreover, the abrupt jumps in the magnetization has not been reproduced numerically in the absence of the bias. Beyond the magnetization, the bath observables provide a direct observation of the quantum criticality intrinsic to the environment possessing many-body effects. The critical properties of the sub-Ohmic bath have recently been explored with the help of a variational approach in which the complete spin-environment wave function of the ground state can be determined [46]. However, whether they are good indicators for phase transition detection in the Ohmic SBM remains an open issue.

In this paper, a numerical variational method (NVM) is devised to study the ground-state phase transition of the two-impurity SBM in a common Ohmic bath. Using the generalized trial wave function composed of coherent-state expansions, which has been proven successful in treating the ground-state phase transitions and quantum dynamics of quantum many-body systems [29, 30, 47–50], we systematically investigate the ground-state energy, magnetization, and spin coherence as well as the observables related to the Ohmic bath. The transition point and critical exponents are accurately determined, and phase diagram spanned by the spin-spin and spin-bath couplings is identified, in comparison with those obtained from NRG and QMC. The rest of the paper is organized as follows. In Sec. II, the two-impurity model and NVM is described. In Sec. III, the numerical results

are presented for the validity of NVM, quantum criticality of the Ohmic bath, and phase diagram. Finally, they are discussed at length before drawing conclusions in Sec. VI.

II. MODEL AND METHOD

For completeness and further reference, we first introduce the standard Hamiltonian of SBM,

$$\hat{H} = \frac{\varepsilon}{2}\sigma_z - \frac{\Delta}{2}\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \frac{\sigma_z}{2} \sum_k \lambda_k (b_k^\dagger + b_k), \quad (1)$$

where ε is an energy bias, Δ denotes the bare tunneling amplitude, σ_x and σ_z represent the Pauli spin-1/2 operators, $b_k^\dagger$ (b_k) is the bosonic creation (annihilation) operator of the k -th bath mode whose frequency is ω_k , and λ_k signifies the coupling amplitude between the spin and environment. By dividing the phonon frequency domain $[0, \omega_c]$ into M intervals $[\Lambda_k, \Lambda_{k+1}]\omega_c$ ($k = 0, 1, \dots, M-1$), we calculate the coupling strength λ_k and bosonic frequency ω_k in Eq. (1) with a coarse-grained treatment of the continuous spectral density function $J(\omega) = \sum_k \lambda_k^2 \delta(\omega - \omega_k)$ [20, 23, 29, 46, 51],

$$\lambda_k^2 = \int_{\Lambda_k \omega_c}^{\Lambda_{k+1} \omega_c} dt J(t), \quad \omega_k = \lambda_k^{-2} \int_{\Lambda_k \omega_c}^{\Lambda_{k+1} \omega_c} dt J(t)t. \quad (2)$$

For convergence, we set the cutoff frequency $\omega_c = 1$. A logarithmic discretization procedure with the parameter $\Lambda_k = \Lambda^{k-M}$ is usually adopted for the sub-Ohmic regime ($s < 1$) presenting a second-order phase transition. However, in a more prominent case with Ohmic spectrum, i.e., $s = 1$, the continuum limit $\Lambda \rightarrow 1$ is required to obtain an accurate quantum criticality of the Kosterlitz-Thouless transition, while $\Lambda = 1.4 \sim 2.0$ is used in earlier numerical works [27, 36, 51]. A linear discretization procedure with $\Lambda_k = k/M$ is a possible alternative, for the bosonic modes at different frequencies are equally important.

In this paper, we primarily aim to study the two-impurity SBM for which the Hamiltonian is given by

$$\begin{aligned} \hat{H} = & \frac{\varepsilon}{2}(\sigma_1^z + \sigma_2^z) - \frac{\Delta}{2}(\sigma_1^x + \sigma_2^x) + \sum_k \omega_k b_k^\dagger b_k \\ & + \frac{\sigma_1^z + \sigma_2^z}{2} \sum_k \lambda_k (b_k^\dagger + b_k) + \frac{K}{4} \sigma_1^z \sigma_2^z, \end{aligned} \quad (3)$$

where the subscripts of σ_i ($i = 1, 2$) correspond to qubits 1 and 2, and K is the Ising-type qubit-qubit interaction. First of all, a simple case in the absence of bias and spin-spin interaction $K = \varepsilon = 0$ is investigated for understanding the ground-state quantum phase transition in the Ohmic environment. The transition point is determined accurately, and critical properties of the Ohmic bath are identified. After that, both of the ferromagnetic ($K < 0$) and antiferromagnetic ($K > 0$) situations as well as the biased cases ($\varepsilon > 0$) are studied, and the phase diagram is given in Subsection C of Sec. III.

As one of successful approaches that enables direct access to the ground-state wave function, the variational method has recently been adopted to study SBM, where the form of the trial wave function plays a vital role in obtaining the ground state [29, 42, 46]. In this work, a systematic coherent-state expansion, termed as the “multi- D_1 ansatz”, is used as the variational ansatz, which has been proved to be efficient in tackling the ground-state phase transitions and quantum dynamics of SBM and its variant [29, 30, 48].

$$\begin{aligned}
|\Psi\rangle = & |\uparrow\uparrow\rangle \sum_{n=1}^N A_n \exp \left[\sum_{k=1}^M \left(f_{n,k} b_k^\dagger - \text{H.c.} \right) \right] |0\rangle_b \\
& + |\uparrow\downarrow\rangle \sum_{n=1}^N B_n \exp \left[\sum_{k=1}^M \left(g_{n,k} b_k^\dagger - \text{H.c.} \right) \right] |0\rangle_b \quad (4) \\
& + |\downarrow\uparrow\rangle \sum_{n=1}^N C_n \exp \left[\sum_{k=1}^M \left(h_{n,k} b_k^\dagger - \text{H.c.} \right) \right] |0\rangle_b \\
& + |\downarrow\downarrow\rangle \sum_{n=1}^N D_n \exp \left[\sum_{k=1}^M \left(p_{n,k} b_k^\dagger - \text{H.c.} \right) \right] |0\rangle_b,
\end{aligned}$$

where H.c. denotes Hermitian conjugate, $\uparrow$ ($\downarrow$) stands for the spin up (down) state, and $|0\rangle_b$ is the vacuum state of the bosonic bath. The variational parameters $f_{n,k}$, $g_{n,k}$, $h_{n,k}$, and $p_{n,k}$ represent the displacements of the coherent states correlated to the spin configurations $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$ respectively, and A_n , B_n , C_n , and D_n are weights of the coherent states. The subscripts n and k correspond to the ranks of the coherent superposition and effective bath mode, respectively.

Recently, it has been reported that the variational treatment based on Silbey-Harris ansatz fails for the ground-state phase transition of SBM, since the imposed constraints $f_{n,k} = -p_{n,k}$ and $A_n = D_n$ are broken in the localized phase or the biased case [24, 42, 52]. Here the multi- D_1 ansatz goes beyond that of Silbey and Harris. Moreover, the number of the flexible variational parameters is much larger than that in Silbey-Harris one and its recent extension [30]. For example, it has more than 12 000 variational parameters if $M = 500$ and $N = 6$. The sophistication of the trial wave function ensures it is possible to obtain an accurate description of the ground state around the transition point, for the existence of huge quantum fluctuations and entanglements in the environment, though the variational procedure becomes quite difficult.

Numerical variational method (NVM) is then utilized to search for the ground state by minimizing the system energy E with respect to variational parameters. With the multi- D_1 ansatz defined in Eq. (4) at hand, $E = \mathcal{H}/\mathcal{N}$ can be calculated with the Hamiltonian expectation $\mathcal{H} = \langle \psi | \hat{H} | \psi \rangle$ and norm of the wave function $\mathcal{N} = \langle \psi | \psi \rangle$. A set of self-consistency equations are then derived

$$\frac{\partial \mathcal{H}}{\partial x_i} - E \frac{\partial \mathcal{N}}{\partial x_i} = 0, \quad (5)$$

where x_i ($i = 1, 2, \dots, 4NM + 4N$) denotes any variational parameter. For each set of the model parameters, more than 100 initial states are used with different (A_n , B_n , C_n , and D_n) uniformly distributed within an interval $[-1, 1]$, and ($f_{n,k}$, $g_{n,k}$, $h_{n,k}$, and $p_{n,k}$) obeying classical displacement law $\pm \lambda_k / \omega_k$. Meanwhile, the simulated annealing algorithm is employed in variational calculations in order to escape from metastable states. The termination criterion of the iteration procedure is $\max\{x_i^* - x_i\} < 1 \times 10^{-10}$. Thus, one can obtain the ground-state solution $|\Psi_g\rangle$ with the minimum energy E_g . The reader is referred to “Appendix A” for more details.

Besides the ground-state energy E_g as well as spin coherence and magnetization $\langle \sigma_{x,z} \rangle = \langle \Psi_g | \sigma_{x,z} | \Psi_g \rangle$, the observables related to the Ohmic bath defined in “Appendix B” are also evaluated as indicators to characterize ground-state phase transition for the two-impurity model, including the variances of phase space variables ΔX_b and ΔP_b , the correlation functions Cor_X and Cor_P , renormalized tunneling Δ_r , and average displacements and coherent-state weights $\bar{f}_k$, $\bar{p}_k$, $\bar{A}$, and $\bar{D}$ [27, 46].

Finally, convergence tests of variational results are performed against the numbers of effective bath modes M and coherent-superposition states N . A linear discretization procedure is used in this work for the Ohmic spectrum with $s = 1$. The results in “Appendix C” show that $M = 500$ and $N = 6$ are sufficient in NVM to rebuild the ground state of the two-impurity model. Therefore, main results are presented with this setting unless noted otherwise.

III. NUMERICAL RESULTS

A. Validity of variational calculations

Using large-scale NVM simulations, we study the ground-state phase transition of the two-impurity SBM in the Ohmic regime, and compare our results with those from exact diagonalization (ED) [23, 29]. As the ED technique is CPU-time and memory consuming, we adopt the logarithmic discretization (instead of the linear one) in the ED procedure, together with a discretization factor of $\Lambda = 2$, an effective bath-mode number of $M = 12$, and a bosonic truncated number of $N_{\text{tr}} = 4$. Without loss of generality, we focus on the case of $K = \varepsilon = 0$, $\Delta = 0.025$, and $s = 1$.

Fig. 1(a) shows the ground-state energy E_g as a function of the coupling strength α . For the α values considered here, E_g of NVM is a slightly lower than that of ED. It is concluded that in the Ohmic regime our NVM with linear discretization yields a better approximation to the ground state energy, than the ED approach with logarithmic discretization with $\Lambda = 2$. The latter becomes exact only in the limit $\Lambda \rightarrow 1$, which cannot be achieved with computational resources currently available. In the inset of Fig. 1(a), the second derivative of E_g is plotted for further comparison. There is agreement

Figure 1. The ground-state energy E_g in (a) and magnetization $\langle \sigma_z \rangle$ in (b) of the Ohmic two-impurity SBM with $s = 1$ as a function of the coupling strength α at $\epsilon = K = 0$ and $\Delta = 0.025$. The numbers of effective bath modes and coherent-superposition states, $M = 500$ and $N = 6$, are used in the numerical variational method (NVM), and the truncated number $N_{tr} = 4$ is set in the exact-diagonalization (ED) procedure. In the inset of (a), the second derivative of E_g is shown for ED and NVM, and an exponential fit is presented with the dashed line. In (b), a bias case of $\epsilon = 10^{-4}$ is given with stars.

Figure 2. (a) The spin coherence $\langle \sigma_x \rangle$ obtained by ED and NVM against the dissipation α at $\epsilon = K = 0$, $s = 1$, and $\Delta = 0.025$. The criterion $\langle \sigma_x \rangle = \Delta/\omega_c$ is plotted with the dash-dotted line, and $\Delta/\langle \sigma_x \rangle$ is shown in the inset. (b) The ground-state energy E_g and spin coherence $\langle \sigma_x \rangle$ obtained from different variational works, i.e., VM1 in Ref.[38], VM2 in Ref.[41], and NVM in this work, in the biased case of $\epsilon = 10^{-5}$, $s = 1$, $K = 0$, and $\Delta = 0.1$. A sharp kink of spin coherence is marked by the arrow.

between solid squares (ED) and pluses (NVM), and we obtain an exponential behavior of $\partial^2 E_g / \partial \alpha^2$ by fitting the data to $y = a \exp(-bx)$, yielding a decay exponent of $b = 23.2(2)$. This lends support to a quantum phase transition of the Kosterlitz-Thouless type for the two-impurity SBM in the presence of an Ohmic bath, as there is no discontinuity in derivatives of E_g of any order. In

addition, magnetization $\langle \sigma_z \rangle$ as a function of α calculated by ED (NVM) is depicted in Fig. 1(b) with circles (triangles). For simplicity, only one branch of the doubly degenerate ground states is presented for $\langle \sigma_z \rangle \leq 0$, and the other can be obtained easily by projecting the operator $\mathcal{P}_x = \sigma_x \exp(i\pi \sum b_k^\dagger b_k)$ onto $|\Psi_g\rangle$. In both curves, abrupt jumps from $\langle \sigma_z \rangle = 0$ to -1 occur exactly at the

Figure 3. Time evolution of the ground-state energy E_g , magnetization $\langle\sigma_z\rangle$, and spin coherence $\langle\sigma_x\rangle$ for the coupling strength $\alpha = 0.292$ at $\varepsilon = K = 0$, $s = 1$, and $\Delta = 0.025$, where t denotes the number of iterations.

Kosterlitz-Thouless transition, same as in the single-spin SBM [16]. The transition point $\alpha_c \approx 0.32$ of NVM is then located by the discontinuity, greater than $\alpha_c \approx 0.26$ from ED results. In a biased case, e.g., $\varepsilon = 1 \times 10^{-4}$, the sharp transition is softened to a smooth crossover, consistent with the results in Refs. [27, 38, 42].

The spin coherence $\langle\sigma_x\rangle$ as a function of α is also investigated for ED and NVM in Fig. 2(a). The NVM coherence exhibits a monotonic, smooth decrease, while that of ED manifests a strong suppression in the entire α range. A sudden drop to zero is found for the ED coherence when $\alpha \geq \alpha_c$, at variance with the prediction that the coherence should be a continuous function of α retaining a finite value Δ/ω_c at the Kosterlitz-Thouless transition in the presence of an Ohmic bath [16, 27]. With this criterion, the NVM critical point of $\alpha_c \approx 0.3$ is indicated by the intersection of the triangles and the dot-dashed line, close to that obtained from the NVM magnetization curve in Fig. 1(b). In the inset, $\Delta/\langle\sigma_x\rangle$ calculated by NVM exhibits linear behavior conforming to the expression of $\Delta/\langle\sigma_x\rangle = (2\alpha - 1)\omega_c$ obtained via the Bethe Ansatz solution for the single-spin model [16], although our slope is 3.83(3). In contrast, the ED result deviates from the linear relation substantially, again pointing to the advantages of NVM.

To further confirm the validity of NVM, we compare our variational results based on the multi- D_1 ansatz with those from other variational studies, named as “VM1” [38] and “VM2” [41] for convenience, in which the Silbey-Harris ansatz and its extension were utilized in combination with unitary transformations with variational parameters. In Fig. 2(b), a biased case with

$\varepsilon = 1 \times 10^{-5}$, $K = 0$, $\Delta = 0.1$, and $s = 1$ is considered. Shown in Fig. 2(b) as functions of α are the ground-state energy E_g and the spin coherence $\langle\sigma_x\rangle$ calculated by VM1 (circles), VM2 (stars), and NVM (triangles). The NVM result has lower ground-state energy and larger spin coherence, implying that the ground state obtained by our ansatz is indeed the most accurate among the three. Moreover, the arrow in the inset indicates a kink in $\langle\sigma_x\rangle$ calculated by VM2, against the usual expectation that $\langle\sigma_x\rangle$ decays monotonically and smoothly around the Kosterlitz-Thouless transition [27]. The increase of the spin coherence as α goes above 0.14 is counterintuitive, since strong environment-induced dissipation will destroy the quantum entanglement that preserves the spin coherence.

In fact, numerous metastable states exist in the vicinity of the ground state around the Kosterlitz-Thouless transition. Taking $\alpha = 0.292$ as an example, time evolution of E_g , $\langle\sigma_z\rangle$, and $\langle\sigma_x\rangle$ is presented in Fig. 3. A huge change in the magnetization appears from $\langle\sigma_z\rangle = -0.85$ (a metastable state) to 0 (the ground state), while the decrement in E_g (or the increment in $\langle\sigma_x\rangle$) is only a paltry amount of 3×10^{-7} (3×10^{-5}). It follows that a certain high accuracy in computation is required to capture the ground state, beyond what can be afforded by the usual numerical methods in recent studies [36, 38–41]. If a metastable state is mistaken as the ground state, the critical point is underestimated substantially, such as the biased ED results presented in Fig. 1(b). However, a non-zero bias value of $10^{-8}\omega_c$ is considered in previous NRG calculations, indicating that the reported value of the critical point in Ref. [36], $\alpha_c \approx 0.18$, is

Figure 4. The renormalized tunneling Δ_r , correlation functions Cor_X and $-\text{Cor}_P$, and departure from the minimum uncertainty, $\Delta X_b \Delta P_b - 1/4$ are shown with respect to the coupling strength α . Dashed lines represent exponential fits.

smaller than the exact one. To the best of our knowledge, the metastable states of the two-impurity models near the Kosterlitz-Thouless transition are discussed here for the first time, made possible only by the accuracy of the ground state obtained by our numerical calculations. In the iterative process of NVM in this work, the system always gets trapped in metastable states in the α range of $[0.28, 0.35]$. To eliminate the inaccuracy due to metastable states near the quantum transition, additional hundreds of samples are then needed to achieve the true ground state, for each set of the model coefficients (α , Δ , ε , and K). In addition, some data from the metastates have to be discarded according to the criterion that the absolute value of $\langle \sigma_z \rangle$ monotonically increases with α , and the sharp jump in $\langle \sigma_z \rangle$ is unique.

B. Quantum criticality of the Ohmic bath

In this subsection, we systematically study the ground-state properties of the Ohmic bath for the Kosterlitz-Thouless transition. Fig. 4 displays α -dependent bath-related observables as defined in Appendix B, which include the renormalized tunneling Δ_r , the correlation functions Cor_X and $-\text{Cor}_P$, and a measure of deviation from the uncertainty minimum, $\Delta X_b \Delta P_b - 1/4$. Note that for clarity only the bath mode with the lowest frequency $\omega_{k=0}$ is considered here for the variance of the phase space variables, and two bath modes with $l = 0$ and $k = 1$ for the correlation functions. In the delocalized phase (small α), the renormalized tunneling quickly decays as α increases, and the curve is fitted using the dashed line of $\Delta_r \propto \exp(-27.2\alpha)$. In the localized phase

(large α), however, it gradually increases to a nonzero value, in contrast to the usual assumption of $\Delta_r = 0$ [38, 42]. This deviation could be caused by the breaking of the symmetry constraint $f_{n,k} = -p_{n,k}$ which is imposed artificially in previous study on the ground-state phase transition of SBM [27, 38]. The transition point $\alpha_c = 0.316(1)$ is then determined according to the sudden jump of Δ_r . An exponential damping of $-\text{Cor}_P$ is found for $\alpha < \alpha_c$ with the slope being comparable with that of Δ_r . In contrast, there are increases in the correlation function Cor_X and the deviation from the uncertainty minimum, $\Delta X_b \Delta P_b - 1/4$. For $\alpha > \alpha_c$, however, the correlation functions Cor_P and Cor_X vanish, and so does the departure of the uncertainty from $1/4$. It is inferred that the bath modes in the localized phase are independent, and behave as a single-coherent state where $\Delta X_b = \Delta P_b = 1/2$.

In Fig. 5, the offsets $2\Delta X_b - 1$ and $1 - 2\Delta P_b$ are plotted with respect to the frequency of the bath mode ω_k for various couplings α . In Fig. 5(a), perfect power-law decay is found in $2\Delta X_b - 1$ for $\alpha = 0.315$ (top blue curve) with a critical exponent of $1.00(1)$. A scaling property of $\Delta X_b = 0.0025/\omega_k + 1/2$ is then uncovered with a power-law fit. For cases of weaker coupling, such as $\alpha = 0.05$ and 0.1 , almost parallel curves are found slightly below (and qualitatively similar to) that of $\alpha = 0.315$. For coupling strengths larger than $\alpha_c = 0.316(1)$, e.g., $\alpha = 0.40$ and 0.50 , $2\Delta X_b - 1$ becomes negligibly small, signaling $\Delta X_b = 1/2$ in the localized phase. Similar power-law decay of $1 - 2\Delta P_b$ is found in Fig. 5(b) for $\alpha < \alpha_c$, where the top curve corresponds to $\alpha = 0.10$. An exponent of $1.83(2)$ can be obtained from the slope. If $\alpha > \alpha_c$, such as $\alpha = 0.32, 0.40$, and 0.50 , both $1 - 2\Delta P_b$ and $2\Delta X_b - 1$

Figure 5. The variances of the phase space variables deviating from the equal uncertainty $\Delta X_b = \Delta P_b = 1/2$ for different coupling strengthes α on a log-log scale at $\varepsilon = K = 0$, $s = 1$, and $\Delta = 0.025$. The dashed lines show power-law fits.

Figure 6. The correlation functions Cor_X in (a) and $-\text{Cor}_P$ in (b) between two bath modes as a function of the bosonic frequency ω_k for different values of α on a log-log scale. Other parameters $\varepsilon = K = 0$, $s = 1$, and $\Delta = 0.025$ are set. And dashed lines represent power-law fits.

increase with the frequency if $\omega_k < \omega^*$, followed by leveling off in the high-frequency regime (i.e., $\omega_k > \omega^*$) with a characteristic scale of $\omega^* \approx 0.1$. This nonmonotonic behavior has also been reported for the ω_k -dependent average displacement and the squeezing amplitude in the noncritical regime of the sub-Ohmic single-spin SBM [46].

We next investigate the frequency dependence of the correlation functions Cor_X and $-\text{Cor}_P$ as defined in Eqs. (B5) and (B6), respectively, where the lowest-frequency bosonic mode $l = 0$ is fixed for convenience.

As presented in Fig. 6, Cor_X and $-\text{Cor}_P$ behave quite similarly with ΔX_b and $1 - 2\Delta P_b$, respectively, with exponents values of 0.500(3) and 1.50(2). It follows that $\text{Cor}_X \sim 1/\sqrt{\omega_k}$ and $\text{Cor}_P \sim -1/\omega_k^{3/2}$ in the delocalized phase, while in the localized phase both of them become negligible. The vanishing value of the correlation function at any ω_k further supports that bath modes are independent of each other, despite being coupled to two impurities simultaneously. It seems that our multi- D_1 ansatz is capable to capture quantum entanglement prop-

erties built into the Ohmic bath in both the delocalized and localized phase.

To better understand the critical properties of the Ohmic bath, we now turn our attention to the wave function of the ground state. The average coherent-state weights and bosonic displacements are calculated with Eqs. (B10) and (B11). Circles and triangles shown in Fig. 7(a) denote the displacement coefficients $\bar{f}_k$ and $\bar{p}_k$ respectively, for the coupling strengths $\alpha = 0.05, 0.316$, and 0.45 from top to bottom, corresponding to the delocalized phase, transition point, and localized phase, respectively. In the upper panel, the vanishing value of $\bar{f}_k + \bar{p}_k$ marked by the solid line manifests that the anti-symmetry $\bar{f}_k = -\bar{p}_k$ develops naturally in the delocalized phase. At transition point, however, spontaneous symmetry breaking occurs in the low-frequency regime. The good coincidence of circles and triangles presented in the lower panel shows a symmetrical relation $\bar{f}_k = \bar{p}_k$ in the localized phase, contrary to the constrain condition imposed in Silbey-Harris ansatz [52]. Focusing on the 0-th bath mode, we demonstrate $\bar{f}_k + \bar{p}_k$ and $\bar{D}^2 - \bar{A}^2$ as a function of α in Fig. 7(b). The critical point $\alpha_c = 0.316$ is again determined, the same as that obtained in Fig. 4.

For further comparison, the classical displacement $\pm\lambda_k/\omega_k$ estimated by the minimum of the static spin-dependent potential is also plotted in Fig. 7(a) with dashed lines. Distinguishable difference between the average displacement and classical one is found in the delocalized phase, but vanishes at the transition point and in the localized phase, in agreement with the general expectation [38]. Furthermore, an optimal displacement formula is proposed

$$|f_k| = |p_k| = \frac{\lambda_k}{\omega_k + \chi}, \quad (6)$$

where χ denotes an effective energy scale, which was believed to be equal to the renormalized tunneling Δ_r in the unbiased case [27, 42]. Fitting our data to the above equation, χ is obtained as a function of α , as presented in the inset of Fig. 7(b). There are two stages of $\chi(\alpha)$ separated by the dash-dotted line which is located at the transition point. An exponential decay occurs for $\alpha < \alpha_c$, and the slope $27.3(3)$ is consistent with that of Δ_r in Fig. 4. For $\alpha > \alpha_c$, however, it changes to a power-law decrease, quite differ from the abnormal increase of Δ_r in the localized phase, beyond the usual assumption $\chi = \Delta_r$.

C. Phase diagram

Subsequently, we perform comprehensive NVM simulations to identify the influence of the tunneling constant Δ , the bias field ϵ , and the Ising coupling strength K on the ground-state phase transition. The rescaled renormalized tunneling Δ_r/Δ is plotted in Fig. 8(a) for various values of Δ , and the transition points are determined. In a weak tunneling case of $\Delta = 0.01$, an exponential decay

is found in the delocalized phase with a slope of $26.4(3)$, compatible with that of $\Delta = 0.025$ presented in Fig. 4. As Δ increases, Δ_r/Δ is found in the delocalized phase to deviate substantially from the exponential decay. However, data from different values of Δ all collapse onto a single curve in the localized phase, where the tunneling amplitude seems to be irrelevant.

In Fig. 8(b), the behavior of the magnetization $\langle\sigma_z\rangle$ is studied under bias values $\epsilon = 1 \times 10^{-5}, 1 \times 10^{-6}, 1 \times 10^{-7}$, and 1×10^{-10} . Other parameters $\Delta = 0.1, s = 1$, and $\omega_c = 1$ are set. With increasing ϵ , the abrupt jump in $\langle\sigma_z\rangle$ occurring at the transition point is progressively replaced by a smooth behavior. Interestingly, the position where the magnetization falls to $\langle\sigma_z\rangle = -1$ is almost the same, since all the bias values presented here are smaller than the renormalized tunneling strength $\Delta_r \approx 1.9 \times 10^{-5}$ at $\alpha_c = 0.33$. For stronger bias or weaker tunneling, however, there is a suppression of the α bracket with $|\langle\sigma_z\rangle|$ smaller than unity. An example is the case of $\Delta = 0.01$ in Fig. 8(b) wherein $\epsilon = 1 \times 10^{-5}$ is larger than $\Delta_r(\alpha_c) \approx 2.5 \times 10^{-6}$. Dashed lines provide good fits to the numerical data with the form $y = a/[a + \exp(bx)] - 1$, yielding $b = 52.1(5)$ and $45.8(6)$ for $\Delta = 0.01$ and 0.1 , respectively.

We then demonstrate the phase diagram of the two-impurity model with Ohmic dissipation in Fig. 9, in comparison with QMC and NRG results estimated from Res. [36, 39]. In the inset, the transition boundary of NVM shows weak Δ -dependent behavior, and locates at $\alpha_c \approx 0.31 + \mathcal{O}(\Delta/\omega_c)$, much greater than $\alpha_c \approx 0.22$ and 0.18 in the presence of $\Delta = 0.025$ for QMC and NRG, respectively, which could not be ruled out by numerical errors. The underestimation of the transition point in NRG and QMC results may be due to the trapping in the metastable state. Besides, the phase diagram in the α - ϵ plane is also investigated (not shown), which exhibits the same qualitative features as that in the α - Δ plane when the bias is small.

The contribution of the spin-spin coupling K to the quantum transition is also presented in Fig. 9. For ferromagnetic case ($K < 0$), the phase boundary depends on K very weakly, while for the antiferromagnetic one ($K > 0$), α_c increases rapidly with K following the asymptotic line of $\alpha_c = 0.25K$, a result consistent with that given by the vanishing renormalized Ising coupling, $K_r = K - 4\alpha\omega_c^s/s = 0$, as marked by the dashed line in Fig. 9 [36, 41]. The NRG and NVM results for $K \geq 1.5$ concur within the error bars, but the two differ in the ferromagnetic regime where the critical coupling α_c is found to be $0.31(1)$ for NVM and $0.17(1)$ for NRG. It follows that that metastable states seem to be suppressed at a large K , and the phase transition is governed by the interplay between the spin-spin coupling and environment dissipation.

Furthermore, we focus on the ground-state properties of the two-impurity model at strong antiferromagnetic coupling, taking $K = 3.0$ as an example. The discontinuity in the magnetization $\langle\sigma_z\rangle$ is shown in Fig. 10(a),

Figure 7. (a) Average displacement coefficients $\bar{f}_k$ (circles) and $\bar{p}_k$ (triangles) for three coupling strengthes $\alpha = 0.05, 0.316$ and 0.45 , corresponding to the delocalized phase, transition point, and localized phase, respectively. Solid lines represent the summations of $\bar{f}_k$ and $\bar{p}_k$, and dashed lines stand for the classical displacements λ_k/ω_k . (b) The average displacements function $\bar{f}_k + \bar{p}_k$ and average weights function $\bar{D}^2 - \bar{A}^2$ for the 0-th bath mode. Inset shows the effective energy scale χ estimated from Eq. (6). The dashed and dash-dotted lines indicate a two-stage fit and critical coupling α_c , respectively.

Figure 8. (a) The rescaled renormalized tunneling Δ_r/Δ for different tunneling constants $\Delta = 0.01, 0.025, 0.05, 0.1$, and 0.2 at $\epsilon = K = 0, s = 1$, and $\omega_c = 1$. The dashed line shows an exponential fit. (b) The magnetization $\langle \sigma_z \rangle$ as a function of α for different values of the bias $\epsilon = 10^{-5}, 10^{-6}, 10^{-7}$, and 10^{-10} at $\epsilon = K = 0, s = 1$, and $\Delta = 0.1$. In addition, the case of $\Delta = 0.01$ is shown with circles, and exponential-like fits are presented with dashed lines.

similar with that in Fig. 1(b). However, two different slopes of E_g from linear fittings, i.e., 0.00 and 2.00, indicate that the derivative of the free energy with respect to α , $\partial E_g/\partial \alpha$, is discontinuous at the transition point, suggesting that the transition is of first order, instead

of the Kosterlitz-Thouless type. In Fig. 10(b), both the rescaled, renormalized tunneling Δ_r/Δ and the correlation function Cor_χ are symmetric about the transition point. This points to the same properties of the Ohmic bath in the delocalized and localized phases, therefore

Figure 9. Phase diagram of the Ohmic two-impurity SBM in the plane of the dissipation α and spin-spin coupling strength K . The dashed line represents the renormalized coupling $K_r = K - 4\alpha\omega_c^s/s = 0$. In the inset, transition boundary α_c obtained from NVM is plotted as a function of the tunneling amplitude Δ , in comparison with those of QMC and NRG in Refs.[36, 39].

Figure 10. Ground-state properties including E_g , $\langle\sigma_z\rangle$, Δ_r/Δ , and Cor_X are presented as a function of α for the antiferromagnetic case with $K = 3.0$. The dashed lines in (a) are guides to the eye for linear fits.

lending further support to the first-order transition.

IV. DISCUSSION AND CONCLUSIONS

As demonstrated by the NVM results in Figs. 1-7, we have accurately determined the transition point $\alpha_c = 0.316(1)$ for the two-impurity Ohmic SBM with a tun-

neling constant of $\Delta = 0.025$ in the absence of spin-spin coupling and the bias. Our result is closely supported by the ED result of $\alpha_c \approx 0.26$, but is clearly much greater than the NRG result of $\alpha_c \approx 0.18$ [36]. The NRG deviation is likely caused by the minute bias field $10^{-8}\omega_c$ imposed on the NRG calculations. As a consequence, the jump in the magnetization is now replaced by the smooth decay towards $\langle\sigma_z\rangle = -1$ as α is increased to

α_c [cf. Fig. 8(b)]. It follows that in such a situation the transition point should be located by the emergence of $|\langle\sigma_z\rangle| = 1$ instead of a nonzero $|\langle\sigma_z\rangle|$. With this criterion, $\alpha_c \approx 0.3$ can be obtained according to the NRG results in Fig. 4 of Ref. [36], in good agreement with our NVM result here. Similarly, the underestimated result of $\alpha_c = 0.125$ reported in Ref. [41] can also be attributed to a bias of $10^{-5}\omega_c$. Considering the notorious difficulty associated with numerical studies of the Kosterlitz-Thouless transition thanks to the existence of numerous metastable states in the vicinity of the ground state, the results of $\alpha_c = 0.22$ and 0.16 from QMC and quantum dynamics simulations in Refs. [39, 40], respectively, may be unreliable, let alone that of $\alpha_c = 0.5$ obtained by the variational treatment based on Silbey-Harris ansatz and simple approximations [38].

In addition, the quantum criticality of the Ohmic bath has also been investigated. For $\alpha \leq \alpha_c$, perfect power-law behaviors of the correlation function Cor_X and the coordinate variance function of $2\Delta X_b - 1$ with respect to the frequency ω_k have been revealed, as shown in Figs. 5(a) and 6(a), pointing to a divergent correlation length both in the delocalized phase and at the critical point. Similarity can be drawn with the classical two-dimensional XY model in which the low-temperature phase exhibiting quasi-long-range order is characterized by a power-law behavior of the spin-spin correlations decaying with the distance [53]. Analogous to the universal jump of the superfluid density in the XY model [54], abrupt changes at the critical coupling take place in the magnetization $\langle\sigma_z\rangle$, correlation function Cor_X between the two bath modes at $l = 0$ and $k = 1$, and departure from the uncertainty relation of $\Delta X_b \Delta P_b = 1/4$ for the 0-th bath mode. Combining with the continuous character in derivatives of E_g of any order, it can be concluded that the quantum phase transition of the two-impurity Ohmic SBM belongs to the Kosterlitz-Thouless universality class, similar to that of the two-dimensional XY model.

Let us turn to the influence of the spin-spin coupling. For the antiferromagnetic regime ($K > 0$), the absence of the Kosterlitz-Thouless transition is triggered by the emergence of the antiparallel spin configuration $\langle\sigma_1^z \sigma_2^z\rangle \approx -1$ in the delocalized phase. The dominating spin-spin coupling term $K\sigma_1^z \sigma_2^z/4$ then leads to an α -independent ground-state energy of $E_g \approx -K/4$ and the vanishing of the quantum correlation between bath modes, quite different from that at $K = 0$. In the localized phase, however, one obtains the parallel state with $\langle\sigma_1^z \sigma_2^z\rangle \approx 1$ instead.

Hence, the energy shift induced by the spin-spin coupling term is $\delta_1 = K/4 - (-K/4) = K/2$ after the spin-bath coupling strength crosses α_c . Substituting the classical displacement coefficients $f_k \approx \lambda_k/\omega_k$, the environment dissipation term can be simplified as $(\sigma_1^z + \sigma_2^z) \int J(\omega) d\omega/\omega \propto \alpha(\sigma_1^z + \sigma_2^z)$. According to the jump of the magnetization from $\langle\sigma_z\rangle = 0$ to -1 at α_c as presented in Fig. 10(a), and the relation $\sigma_1^z = \sigma_z^2 = \sigma_z$, the energy shift is calculated as $\delta_2 = -2\alpha$, which should be

equal to $-\delta_1$ since the ground-state energy E_g and the spin coherence $\langle\sigma\rangle$ are continuous at the transition point. Thus, the transition point $\alpha_c = K/4$ is estimated, consistent with our numerical results in Fig. 9 for a large antiferromagnetic coupling strength K . Moreover, the ground-state energy is predicted to be $E_g \approx -2\alpha + K/4$ in the localized phase and $-K/4$ in the delocalized phase, in excellent agreement with that in Fig. 10(a). The transition is then inferred to be of first order according to the discontinuity in the derivative of the ground-state energy and the few-body nature induced by the independence of bath modes in the two phases. In contrast, the transition is of the Kosterlitz-Thouless type in the ferromagnetic regime ($K < 0$), and both the transition point and the critical exponents are almost the same as those in the absence of spin-spin coupling.

In summary, the ground-state phase transitions in the two-impurity SBM coupled to a common Ohmic bath have been studied comprehensively by variational calculations using the multi- D_1 ansatz. With more than ten thousand variational parameters, the ground-state energy E_g , spin magnetization $\langle\sigma_z\rangle$, and spin coherence $\langle\sigma_x\rangle$ as well as observables related to the Ohmic bath have been investigated, and the results show superior accuracy in comparison with those from ED and earlier variational calculations. A critical coupling strength of $\alpha_c \approx 0.31(1)$ is determined in the weak tunneling limit, which is comparable to the ED result $\alpha_c \approx 0.26$, but very different from results previously obtained by NRG (0.18), QMC (0.22), and other numerical studies (0.5, 0.16, and 0.125) [36, 38–41]. The inaccuracies of the latter may be caused by the incorrect criteria of the transition point, the influence of an imposed bias, and the existence of the metastable states. In the ferromagnetic coupling regime $K < 0$ and in the absence of spin-spin coupling ($K = 0$), the transitions are found to belong to the Kosterlitz-Thouless universality class. In the antiferromagnetic regime ($K > 0$), however, the transition is inferred to be of first order. Furthermore, we have also examined the influences of the tunneling constant Δ and the bias field ε , and have established the phase diagram.

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Appendix A: numerical variational method (NVM)

Using the “multi- D_1 ” ansatz defined in Eq. (4) as trial wave function, the system energy can be calculated as $E = \mathcal{H}/N$, where $\mathcal{H}$ is the Hamiltonian expectation, and

$\mathcal{N}$ is the normal of the wave function.

$$\begin{aligned} \mathcal{H} = & -\Delta \sum_{m,n} \left(A_m C_n S_{mn}^{fh} + B_m D_n S_{mn}^{gp} + A_m B_n S_{mn}^{fg} + C_m D_n S_{mn}^{hp} \right) \\ & + \frac{K}{4} \sum_{m,n} (A_m A_n F_{mn} - B_m B_n G_{mn} - C_m C_n H_{mn} + D_m D_n P_{mn}) \\ & + \varepsilon \sum_{m,n} (A_m A_n F_{mn} - D_m D_n P_{mn}) \\ & + \sum_{m,n} \left[A_m A_n F_{mn} \left(\sum_k \omega_k f_{m,k} f_{n,k} \right) + B_m B_n G_{mn} \left(\sum_k \omega_k g_{m,k} g_{n,k} \right) \right] \\ & + \sum_{m,n} \left[C_m C_n H_{mn} \left(\sum_k \omega_k h_{m,k} h_{n,k} \right) + D_m D_n P_{mn} \left(\sum_k \omega_k p_{m,k} p_{n,k} \right) \right] \\ & + \sum_{m,n} \left[A_m A_n F_{mn} \sum_k \lambda_k (f_{m,k} + f_{n,k}) - D_m D_n P_{mn} \sum_k \lambda_k (p_{m,k} + p_{n,k}) \right], \end{aligned} \quad \text{and}$$

and

$$\begin{aligned} \mathcal{N} &= \langle \psi | \psi \rangle \\ &= \sum_{m,n} (A_m A_n F_{mn} + B_m B_n G_{mn} + C_m C_n H_{mn} + D_m D_n P_{mn}), \end{aligned} \quad (\text{A2})$$

where Debye Walyer factors S_{mn}^{fh} , S_{mn}^{gp} , S_{mn}^{fg} , and S_{mn}^{hp} are defined as

$$\begin{aligned} S_{mn}^{fh} &= \exp \left[-\frac{1}{2} \sum_k (f_{m,k} - h_{n,k})^2 \right], \\ S_{mn}^{gp} &= \exp \left[-\frac{1}{2} \sum_k (g_{m,k} - p_{n,k})^2 \right], \\ S_{mn}^{fg} &= \exp \left[-\frac{1}{2} \sum_k (f_{m,k} - g_{n,k})^2 \right], \\ S_{mn}^{hp} &= \exp \left[-\frac{1}{2} \sum_k (h_{m,k} - p_{n,k})^2 \right], \end{aligned} \quad (\text{A3})$$

and F_{mn} , G_{mn} , H_{mn} , and P_{mn} are defined as

$$\begin{aligned} F_{mn} &= \exp \left[-\frac{1}{2} \sum_k (f_{m,k} - f_{n,k})^2 \right], \\ G_{mn} &= \exp \left[-\frac{1}{2} \sum_k (g_{m,k} - g_{n,k})^2 \right], \\ H_{mn} &= \exp \left[-\frac{1}{2} \sum_k (h_{m,k} - h_{n,k})^2 \right], \\ P_{mn} &= \exp \left[-\frac{1}{2} \sum_k (p_{m,k} - p_{n,k})^2 \right]. \end{aligned} \quad (\text{A4})$$

A set of self-consistency equations with the form of Eq. (5) are deduced by minimizing the energy E with respect to variational parameters, i.e., the displacements $f_{n,k}$, $g_{n,k}$, $h_{n,k}$, and $p_{n,k}$, and coherent-state weights A_n , B_n , C_n , and D_n . The iterative equations are thus

obtained

$$\begin{aligned} A_n^* &= \frac{-\Delta \sum_m (B_m S_{nm}^{fg} + C_m S_{nm}^{fh}) + 2 \sum_m^{m \neq n} A_m F_{mn} (aa_{mn} - E)}{2(E - aa_{nn})}, \\ B_n^* &= \frac{-\Delta \sum_m (D_m S_{nm}^{gp} + A_m S_{nm}^{fg}) + 2 \sum_m^{m \neq n} B_m G_{mn} (bb_{mn} - E)}{2(E - bb_{nn})}, \\ C_n^* &= \frac{-\Delta \sum_m (A_m S_{nm}^{fh} + D_m S_{nm}^{hp}) + 2 \sum_m^{m \neq n} C_m H_{mn} (cc_{mn} - E)}{2(E - cc_{nn})}, \\ D_n^* &= \frac{-\Delta \sum_m (B_m S_{nm}^{gp} + C_m S_{nm}^{hp}) + 2 \sum_m^{m \neq n} D_m P_{mn} (dd_{mn} - E)}{2(E - dd_{nn})}, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} f_{n,k}^* &= \frac{2 \sum_m^{m \neq n} A_m F_{mn} [f_{m,k} aa_{mn} + \omega_k f_{m,k} + \lambda_k - f_{m,k} E]}{2A_n (E - aa_{nn} - \omega_k)} \\ &+ \frac{2\lambda_k A_n - \Delta \sum_m [C_m S_{nm}^{fh} h_{m,k} + B_m S_{nm}^{fg} g_{m,k}]}{2A_n (E - aa_{nn} - \omega_k)}, \\ g_{n,k}^* &= \frac{2 \sum_m^{m \neq n} B_m G_{mn} [g_{m,k} bb_{mn} + \omega_k g_{m,k} - g_{m,k} E]}{2B_n (E - bb_{nn} - \omega_k)} \\ &+ \frac{-\Delta \sum_m [D_m S_{nm}^{gp} p_{m,k} + A_m S_{nm}^{fg} f_{m,k}]}{2B_n (E - bb_{nn} - \omega_k)}, \\ h_{n,k}^* &= \frac{2 \sum_m^{m \neq n} C_m H_{mn} [h_{m,k} cc_{mn} + \omega_k h_{m,k} - h_{m,k} E]}{2C_n (E - cc_{nn} - \omega_k)} \\ &+ \frac{-\Delta \sum_m [A_m S_{nm}^{fh} f_{m,k} + D_m S_{nm}^{hp} p_{m,k}]}{2C_n (E - cc_{nn} - \omega_k)}, \\ p_{n,k}^* &= \frac{2 \sum_m^{m \neq n} D_m P_{mn} [p_{m,k} dd_{mn} + \omega_k p_{m,k} - \lambda_k - p_{m,k} E]}{2D_n (E - dd_{nn} - \omega_k)} \\ &+ \frac{-2\lambda_k D_n - \Delta \sum_m [B_m S_{nm}^{gp} g_{m,k} + C_m S_{nm}^{hp} h_{m,k}]}{2D_n (E - dd_{nn} - \omega_k)}, \end{aligned} \quad (\text{A6})$$

where * denotes the renewal of variational parameters, and aa_{mn} , bb_{mn} , cc_{mn} , and dd_{mn} are defined as

$$\begin{aligned} aa_{mn} &= \sum_k \omega_k f_{m,k} f_{n,k} + \sum_k \lambda_k (f_{m,k} + f_{n,k}) + \frac{K}{4} + \varepsilon, \\ bb_{mn} &= \sum_k \omega_k g_{m,k} g_{n,k} - \frac{K}{4}, \\ cc_{mn} &= \sum_k \omega_k h_{m,k} h_{n,k} - \frac{K}{4}, \\ dd_{mn} &= \sum_k \omega_k p_{m,k} p_{n,k} - \sum_k \lambda_k (p_{m,k} + p_{n,k}) + \frac{K}{4} - \varepsilon. \end{aligned} \quad (\text{A7})$$

With the relaxation iteration technique, variation parameters are updated based on the rule $x'_i = x_i + t(x_i^* - x_i)$, where x_i^* is calculated with Eqs. (A5) and (A6), and the relaxation factor $t = 0.1$ is set. In the variational procedure with simulated annealing algorithm, however, t gradually decreases to 0.001.

With the ground state $|\Psi_g\rangle$ at hand, the magnetization $\langle \sigma_1^z \rangle$ and $\langle \sigma_2^z \rangle$ as well as the spin coherence $\langle \sigma_1^x \rangle$ and $\langle \sigma_2^x \rangle$

can be calculated with

$$\begin{aligned}
\langle \sigma_1^z \rangle &= \frac{\sum_{m,n} A_m A_n F_{mn} + B_m B_n G_{mn} - C_m C_n H_{mn} - D_m D_n P_{mn}}{\sum_{m,n} A_m A_n F_{mn} + B_m B_n G_{mn} + C_m C_n H_{mn} + D_m D_n P_{mn}}, \\
\langle \sigma_2^z \rangle &= \frac{\sum_{m,n} A_m A_n F_{mn} - B_m B_n G_{mn} + C_m C_n H_{mn} - D_m D_n P_{mn}}{\sum_{m,n} A_m A_n F_{mn} + B_m B_n G_{mn} + C_m C_n H_{mn} + D_m D_n P_{mn}}, \\
\langle \sigma_1^x \rangle &= \frac{\sum_{m,n} 2A_m C_n S_{mn}^{fh} + \sum_{m,n} 2B_m D_n S_{mn}^{gp}}{\sum_{m,n} A_m A_n F_{mn} + B_m B_n G_{mn} + C_m C_n H_{mn} + D_m D_n P_{mn}}, \\
\langle \sigma_2^x \rangle &= \frac{\sum_{m,n} 2A_m B_n S_{mn}^{fg} + \sum_{m,n} 2C_m D_n S_{mn}^{hp}}{\sum_{m,n} A_m A_n F_{mn} + B_m B_n G_{mn} + C_m C_n H_{mn} + D_m D_n P_{mn}}. \tag{A8}
\end{aligned}$$

The ground-state energy $E_g = \mathcal{H}/\mathcal{N}$ is obtained with Eqs. (A1) and (A2). Since the relations $\langle \sigma_1^z \rangle \approx \langle \sigma_2^z \rangle$ and $\langle \sigma_1^x \rangle \approx \langle \sigma_2^x \rangle$ hold due to the homogeneity of the two spins, the magnetization and spin coherence are estimated with $\langle \sigma_z \rangle = (\langle \sigma_1^z \rangle + \langle \sigma_2^z \rangle)/2$ and $\langle \sigma_x \rangle = (\langle \sigma_1^x \rangle + \langle \sigma_2^x \rangle)/2$, respectively.

Appendix B: Observables related to the Ohmic bath

To depict the properties of the Ohmic bath, two phase space variables x_k and p_k are introduced as position and momentum of the k -th bath mode, where the corresponding quadrature phase operators $\hat{x}_k$ and $\hat{p}_k$ are defined as

$$\hat{x}_k = (b_k + b_k^\dagger)/\sqrt{2}, \quad \hat{p}_k = i(b_k^\dagger - b_k)/\sqrt{2}. \tag{B1}$$

Thus, the position variance $\Delta X_b = \langle \Psi_g | (\hat{x}_k)^2 | \Psi_g \rangle - \langle \Psi_g | \hat{x}_k | \Psi_g \rangle^2$ is calculated for k -th bath mode with

$$\begin{aligned}
\langle \Psi_g | \hat{x}_k | \Psi_g \rangle &= \frac{\sqrt{2}}{2} \langle \Psi_g | b_k^\dagger + b_k | \Psi_g \rangle \\
&= \frac{\sqrt{2}}{2\mathcal{N}} \sum_{m,n} [A_m A_n F_{mn} (f_{m,k} + f_{n,k}) + B_m B_n G_{mn} (g_{m,k} + g_{n,k})] \\
&+ \frac{\sqrt{2}}{2\mathcal{N}} \sum_{m,n} [C_m C_n H_{mn} (h_{m,k} + h_{n,k}) + D_m D_n P_{mn} (p_{m,k} + p_{n,k})], \tag{B2}
\end{aligned}$$

and

$$\begin{aligned}
\langle \Psi_g | (\hat{x}_k)^2 | \Psi_g \rangle &= \frac{1}{2} \langle \Psi_g | (b_k^\dagger + b_k)^2 | \Psi_g \rangle \\
&= \frac{1}{2\mathcal{N}} \sum_{m,n} [A_m A_n F_{mn} (f_{m,k} + f_{n,k})^2 + B_m B_n G_{mn} (g_{m,k} + g_{n,k})^2] \\
&+ \frac{1}{2\mathcal{N}} \sum_{m,n} [C_m C_n H_{mn} (h_{m,k} + h_{n,k})^2 + D_m D_n P_{mn} (p_{m,k} + p_{n,k})^2] \\
&+ \frac{1}{2}. \tag{B3}
\end{aligned}$$

Since the expected value of the momentum $\langle \Psi_g | \hat{p}_k | \Psi_g \rangle = i \langle \Psi_g | (b_k^\dagger - b_k) | \Psi_g \rangle / \sqrt{2}$ vanishes in the ground state, the variance of the momentum $\Delta P_b = \langle \Psi_g | (\hat{p}_k)^2 | \Psi_g \rangle$ is then

obtained for the k -th bath mode with

$$\begin{aligned}
\langle \Psi_g | (\hat{p}_k)^2 | \Psi_g \rangle &= -\frac{1}{2} \langle \Psi_g | (b_k^\dagger - b_k)^2 | \Psi_g \rangle \\
&= \frac{-1}{2\mathcal{N}} \sum_{m,n} [A_m A_n F_{mn} (f_{m,k} - f_{n,k})^2 + B_m B_n G_{mn} (g_{m,k} - g_{n,k})^2] \\
&- \frac{1}{2\mathcal{N}} \sum_{m,n} [C_m C_n H_{mn} (h_{m,k} - h_{n,k})^2 + D_m D_n P_{mn} (p_{m,k} - p_{n,k})^2] \\
&+ \frac{1}{2}. \tag{B4}
\end{aligned}$$

Besides, the correlation functions Cor_X and Cor_P between k -th and l -th bath modes are also investigated,

$$\begin{aligned}
\text{Cor}_X &= \langle \Psi_g | \hat{x}_k \hat{x}_l | \Psi_g \rangle - \langle \Psi_g | \hat{x}_k | \Psi_g \rangle \langle \Psi_g | \hat{x}_l | \Psi_g \rangle \\
&= \frac{1}{2\mathcal{N}} \sum_{m,n} A_m A_n F_{mn} (f_{m,k} + f_{n,k})(f_{m,l} + f_{n,l}) \\
&+ \frac{1}{2\mathcal{N}} \sum_{m,n} B_m B_n G_{mn} (g_{m,k} + g_{n,k})(g_{m,l} + g_{n,l}) \\
&+ \frac{1}{2\mathcal{N}} \sum_{m,n} C_m C_n H_{mn} (h_{m,k} + h_{n,k})(h_{m,l} + h_{n,l}) \\
&+ \frac{1}{2\mathcal{N}} \sum_{m,n} D_m D_n P_{mn} (p_{m,k} + p_{n,k})(p_{m,l} + p_{n,l}) \\
&- \frac{1}{2} \langle \Psi_g | b_k^\dagger + b_k | \Psi_g \rangle \langle \Psi_g | b_l^\dagger + b_l | \Psi_g \rangle, \tag{B5}
\end{aligned}$$

and

$$\begin{aligned}
\text{Cor}_P &= \langle \Psi_g | \hat{p}_k \hat{p}_l | \Psi_g \rangle \\
&= \frac{-1}{2\mathcal{N}} \sum_{m,n} A_m A_n F_{mn} (f_{m,k} - f_{n,k})(f_{m,l} - f_{n,l}) \\
&- \frac{1}{2\mathcal{N}} \sum_{m,n} B_m B_n G_{mn} (g_{m,k} - g_{n,k})(g_{m,l} - g_{n,l}) \\
&- \frac{1}{2\mathcal{N}} \sum_{m,n} C_m C_n H_{mn} (h_{m,k} - h_{n,k})(h_{m,l} - h_{n,l}) \\
&- \frac{1}{2\mathcal{N}} \sum_{m,n} D_m D_n P_{mn} (p_{m,k} - p_{n,k})(p_{m,l} - p_{n,l}), \tag{B6}
\end{aligned}$$

where $\langle \Psi_g | b_k^\dagger + b_k | \Psi_g \rangle$ defined in Eq. (B2) represents the average displacement of the k -th bath mode.

Due to system-bath interactions, the tunneling term Δ is renormalized such that $\Delta_r = \Delta \langle B_{\uparrow\uparrow} | B_{\downarrow\downarrow} \rangle$, where $|B_{\uparrow\uparrow}\rangle$ and $|B_{\downarrow\downarrow}\rangle$ denote two basis of the bath in the “multi- D_1 ” ansatz, corresponding to the spin states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, respectively,

$$\begin{aligned}
|B_{\uparrow\uparrow}\rangle &= \sum_{n=1}^N A_n \exp \left[\sum_k f_{n,k} (b_k^\dagger - b_k) \right] |0\rangle_b, \\
|B_{\downarrow\downarrow}\rangle &= \sum_{n=1}^N D_n \exp \left[\sum_k p_{n,k} (b_k^\dagger - b_k) \right] |0\rangle_b. \tag{B7}
\end{aligned}$$

Thus, the rescaled renormalized tunneling Δ_r/Δ is measured by

$$\Delta_r/\Delta = \sum_{mn} A_m D_n \exp \left[-\frac{1}{2} \sum_k (f_{m,k} - p_{n,k})^2 \right]. \tag{B8}$$

To further understand the ground-state properties, $|\Psi_{\text{single}}\rangle$ is introduced as an equivalent single-coherent

version of the “multi-D₁” ansatz, which is defined as

$$\begin{aligned}
|\Psi_{\text{single}}\rangle = & \bar{A} |\uparrow\uparrow\rangle \exp \left[\sum_k \bar{f}_k (b_k^\dagger - b_k) \right] |0\rangle_b \\
& + \bar{B} |\uparrow\downarrow\rangle \exp \left[\sum_k \bar{g}_k (b_k^\dagger - b_k) \right] |0\rangle_b \\
& + \bar{C} |\downarrow\uparrow\rangle \exp \left[\sum_k \bar{h}_k (b_k^\dagger - b_k) \right] |0\rangle_b \\
& + \bar{D} |\downarrow\downarrow\rangle \exp \left[\sum_k \bar{p}_k (b_k^\dagger - b_k) \right] |0\rangle_b,
\end{aligned} \tag{B9}$$

with the average coherent-state weights

$$\begin{aligned}
\bar{A} &= \sqrt{\sum_{mn} A_m A_n F_{mn}}, \\
\bar{B} &= \sqrt{\sum_{mn} B_m B_n G_{mn}}, \\
\bar{C} &= \sqrt{\sum_{mn} C_m C_n H_{mn}}, \\
\bar{D} &= \sqrt{\sum_{mn} D_m D_n P_{mn}},
\end{aligned} \tag{B10}$$

and the average displacements coefficients

$$\begin{aligned}
\bar{f}_k &= \sum_{mn} \frac{A_m A_n F_{mn} (f_{m,k} + f_{n,k})}{2\bar{A}^2}, \\
\bar{g}_k &= \sum_{mn} \frac{B_m B_n G_{mn} (g_{m,k} + g_{n,k})}{2\bar{B}^2}, \\
\bar{h}_k &= \sum_{mn} \frac{C_m C_n H_{mn} (h_{m,k} + h_{n,k})}{2\bar{C}^2}, \\
\bar{p}_k &= \sum_{mn} \frac{D_m D_n P_{mn} (p_{m,k} + p_{n,k})}{2\bar{D}^2}.
\end{aligned} \tag{B11}$$

Appendix C: Convergence test

The convergence of variational results is carefully examined for NMV results in this section. As mentioned before, a linear coarse-grain procedure is adopted for the continuous spectral density $J(\omega)$, where M is the number of effective bath modes. In Fig. 11(a), the ground-state energy E_g is displayed as a function of M in the case of $s = 1$, $\alpha = 0.1$, $\Delta = 0.1$, and $K = \epsilon = 0$. A monotonic decay with the form $E_g(M) = aM^{-b} + E_{g,\infty}$ is derived with the dashed line providing a good fitting to the numerical data, which yields the asymptotic value $E_{g,\infty} = -0.22306$. In the inset, the exponent value $b = 1.58(2)$ is measured from the slope of the log-log plot of $E_g - E_{g,\infty}$. Besides, the spin coherence $\langle\sigma_x\rangle$ is also investigated in Fig. 11(b) with respect to M . A similar power-law decay is observed with the exponent $b = 1.30(2)$ and the asymptotic value $\langle\sigma_x\rangle_\infty = -0.4797$. We have found that $M = 500$ is sufficient in obtaining reliable results, as simulations with $M = 1000$ show no appreciable difference from that with 500.

In Fig. 12, the convergence of E_g and $\langle\sigma_x\rangle$ are also examined with the number of the coherent superposition states N defined in Eq. (4). The ground-state energy E_g exhibits a power-law decay with N , and the slope $b = 4.9(1)$ of the log-log plot in the inset is significantly larger than that of $E_g(M)$ in Fig. 11(a). Interestingly, the spin coherence obtained from multi-D₁ ansatz ($N > 1$) is visibly increased compared to that of the usual Davydov D₁ ansatz ($N = 1$), pointing to the superiority of the refined trail wavefunction. According to the results in both (a) and (b), the number of coherent-superposition states $N = 6$ has been believed to be sufficient for convergence.

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Figure 11. The ground-state energy E_g in (a) and spin coherence $\langle \sigma_x \rangle$ in (b) as a function of bath-mode number M in a case of $s = 1$, $\alpha = 0.1$, $\Delta = 0.1$ and $K = \epsilon = 0$. The superposition number $N = 4$ is set. In the inset, $E_g(M) - E_{g,\infty}$ is shown on a log-log scale. The dashed lines represent the fits with the form $y = ax^{-b} + c$, and dash-dotted line shows a power-law fit.

Figure 12. The ground-state energy E_g in (a) and spin coherence $\langle \sigma_x \rangle$ in (b) against the superposition number N . The model parameters $s = 1$, $\alpha = 0.1$, $\Delta = 0.1$, and $K = \epsilon = 0$ are set, and the number of the bath modes $M = 50$ is used. In the inset of (a), $E_g(N) - E_{g,\infty}$ is given on a log-log scale. The dashed lines represent the fits with the form $y = ax^{-b} + c$, and the dash-dotted line shows a power-law fit.

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