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Communication: Spin-boson model with diagonal and off-diagonal coupling to two independent baths: Ground-state phase transition in the deep sub-Ohmic regime

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We investigate a spin-boson model with two boson baths that are coupled to two perpendicular components of the spin by employing the density matrix renormalization group method with an optimized boson basis. It is revealed that in the deep sub-Ohmic regime there exists a novel second-order phase transition between two types of doubly degenerate states, which is reduced to one of the usual types for nonzero tunneling. In addition, it is found that expectation values of the spin components display jumps at the phase boundary in the absence of bias and tunneling. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4873351]

The spin boson model (SBM),[1,2] a two-level system coupled to a bosonic bath represented by a set of harmonic oscillators, describes a molecular dimer in its singly excited state interacting with a large number of slow modes in its environment. It is not surprising that the SBM is a simple, convenient tool for studying environment-induced decoherence and energy transfer phenomena. As an archetype model for quantum dissipation, the SBM has been widely used in fields such as quantum computation,[3–5] amorphous solids,[6] biological molecules,[7,8] as well as studies of thermodynamic properties,[9] spin dynamics,[1,10] and quantum phase transitions.[11,12] The SBM Hamiltonian can be written as

$$\mathrm{H}_{\mathrm{SBM}} = \frac{\varepsilon}{2}\sigma_z - \frac{\Delta}{2}\sigma_x + \sum_l \omega_l b_l^\dagger b_l + \frac{\sigma_z}{2}\sum_l \lambda_l \left(b_l^\dagger + b_l\right), \tag{1}$$

where σ_x and σ_z are the Pauli matrices, ε and Δ are the spin (on-site energy) bias and the tunneling (intermolecular coupling) constant, respectively, ω_l and λ_l are the frequency and coupling constant, respectively, of the lth boson mode, with $b_l(b_l^\dagger)$ being its annihilation (creation) operator. For a quasi-continuous spectral density function $J(\omega) \equiv \sum_l \lambda_l^2 \delta(\omega - \omega_l)$, a power law form can be adopted in the low-frequency regime: $J(\omega) = 2\pi\alpha\omega_c^{1-s}\omega^s$, where ω_c, α, and s are the cut-off frequency, the spin-bath coupling constant, and the spectral exponent that characterizes bath properties, respectively, so that $s = 1$ and $s < 1$ ($s > 1$) are known as the Ohmic and sub-Ohmic (super-Ohmic) regime, respectively. Studies[11,12] have shown that if $\varepsilon = 0$ and $s < 1$, strong spin-bath coupling induces spontaneous symmetry breaking restricting the spin orientation to a specific direction (spin-up or down). Thus, the spin-1/2 will be in a two-fold degenerate state, and the entire system, described by Eq. (1), is said to be in the "localized" phase. For weak coupling, the spin is free to flip between the spin-up and the spin-down states, and the system is in the "delocalized" phase. A critical coupling strength α_c exists for this second order phase transition, which for $s = 1$ emerges as a Kosterlitz-Thouless transition.[1]

In this communication we extend the SBM to a more realistic form by adding to Hamiltonian (1) an off-diagonal coupling term, $\sigma_x/2\sum_l \bar{\lambda}_l(b_l^\dagger + b_l)$. Recent studies[13] reveal that in the sub-Ohmic regime, off-diagonal coupling lifts the degeneracy in the localized phase, hence removing a second order phase transition, while there may exist a first-order phase transition with properly chosen diagonal and off-diagonal coupling strengths. Interplay between localization and delocalization effects, induced by the competition between diagonal and off-diagonal coupling, plays a crucial role in determining energy transfer mechanisms which interpolate between the Forster-Dexter and polaron pictures. Such rivalry manifests itself most clearly at low temperatures, often in form of quantum phase transitions at $T = 0$. For a deeper understanding of the competition, an additional bath coupled to the spin off-diagonally is introduced, resulting in a so-called "two-bath SBM." In the absence of tunneling, the model possesses a high level of symmetry corresponding to a non-abelian group with 8 elements. Our symmetry-based analysis shows that all quantum states of the system are doubly degenerate, and this high symmetry is expected to affect properties such as mechanisms of energy transfer. As a starting step, we study the effects of high symmetry on the low-temperature dynamics, focusing in this communication on the zero-temperature quantum phase transition. We will show that due to high symmetry the system ground state is always doubly degenerate, and the phase transition occurs not between the phases with degenerate and non-degenerate ground states, but rather due to the fact that the ground-state degeneracy does not necessarily imply spontaneous symmetry breaking. Stated differently, a special type of quantum

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phase transitions is identified, which is confirmed by results of the density matrix renormalization group (DMRG) calculations, a method that has been proven to be robust in numerous studies of quantum phase transitions in the usual SBM.[14]

Previous studies, such as DMRG, numerical renormalization group, and quantum Monte Carlo, have revealed that in the absence of bias $\langle\sigma_z\rangle$ will be zero if α is below some critical value $\alpha_c(\Delta)$, placing the system in a delocalized phase. If $\alpha > \alpha_c$, $\langle\sigma_z\rangle$ acquires a finite value and the system enters a localized phase. This well known delocalized-localized transition is ascribed to the competition between the spin-bath coupling and the tunneling. Off-diagonal spin-bath coupling provides an alternative channel of communications between spin down $|\downarrow\rangle$ and up $|\uparrow\rangle$ states. The single-bath SBM has been investigated via the Davydov D_1 variational ansatz,[13] and a novel first order phase transition was found to arise when the off-diagonal coupling is taken into account along with the diagonal coupling. Motivated by this finding, we expect much richer ground state properties can be uncovered when the diagonal and the off-diagonal coupling is ascribed to two boson baths rather than a common one. The Hamiltonian for the two-bath SBM can be given as

$$\hat{H} = \frac{\varepsilon}{2}\sigma_z - \frac{\Delta}{2}\sigma_x + \sum_{l,i}\omega_l b_{l,i}^{\dagger} b_{l,i} + \frac{\sigma_z}{2}\sum_l \lambda_l\big(b_{l,1}^{\dagger} + b_{l,1}\big) + \frac{\sigma_x}{2}\sum_l \phi_l\big(b_{l,2}^{\dagger} + b_{l,2}\big), \quad (2)$$

where the subscript $i = 1, 2$ is introduced to distinguish the two baths, and λ_l and ϕ_l are the diagonal and off-diagonal coupling strengths, respectively, which can be used to determine spectral densities,

$$J_z(\omega) = \sum_l \lambda_l^2 \delta(\omega - \omega_l) \Rightarrow 2\alpha\omega_c^{1-s}\omega^s, \quad (3)$$

$$J_x(\omega) = \sum_l \phi_l^2 \delta(\omega - \omega_l) \Rightarrow 2\beta\omega_c^{1-\bar{s}}\omega^{\bar{s}}. \quad (4)$$

Here, α and β are dimensionless coupling constants, and ω_c is set to be unity throughout this work. The two baths are characterized by the spectral exponents s and $\bar{s}$.

Equation (1) can be recast into its continuum form

$$\mathrm{H_{SBM}} = \frac{\varepsilon}{2}\sigma_z - \frac{\Delta}{2}\sigma_x + \int_0^{\omega_c} g(\omega) b_\omega^{\dagger} b_\omega + \frac{\sigma_z}{2}\int_0^{\omega_c} h(\omega)\big(b_\omega^{\dagger} + b_\omega\big), \quad (5)$$

where b_ω and $b_\omega^{\dagger}$ are the counterparts of b_l and $b_l^{\dagger}$, $g(\omega)$ is the dispersion relation, and $h(\omega)$ is the coupling function. Starting from Eq. (5), and using the canonical transformation,[15,16] the boson bath can be mapped onto a Wilson chain. Similarly, in order to apply the DMRG algorithm to the two-bath SBM, followed by the standard treatment,[12,15,16] we map the two boson baths in (2) onto two Wilson chains, and Hamiltonian (2) morphs into the form

$$\hat{H} = \frac{\varepsilon}{2}\sigma_z - \frac{\Delta}{2}\sigma_x + \sum_{n=0,i}\left[\omega_{n,i} p_{n,i}^{\dagger} p_{n,i} + t_{n,i}\big(p_{n,i}^{\dagger} p_{n+1,i} + p_{n+1,i}^{\dagger} p_{n,i}\big)\right] + \frac{\sigma_z}{2}\sqrt{\frac{\eta_z}{\pi}}\big(p_{0,1}^{\dagger} + p_{0,1}\big) + \frac{\sigma_x}{2}\sqrt{\frac{\eta_x}{\pi}}\big(p_{0,2}^{\dagger} + p_{0,2}\big), \quad (6)$$

where $i = 1, 2$ label the baths, $\omega_{n,i}$ is the on site energy of site n in the ith bath, $p_{n,i}^{\dagger}$ ($p_{n,i}$) is corresponding boson creation (annihilation) operator, $t_{n,i}$ is the hopping amplitude between sites n and $n + 1$, and η_z (η_x) is a coupling constant proportional to α (β). One has

$$\eta_x = \int_0^{\omega_c} J_x(\omega)d\omega = \frac{2\pi\beta}{1+\bar{s}}\omega_c^2, \quad (7)$$

$$\eta_z = \int_0^{\omega_c} J_z(\omega)d\omega = \frac{2\pi\alpha}{1+s}\omega_c^2, \quad (8)$$

$$\omega_{n,1} = \zeta_s(A_n + C_n), \qquad t_{n,1} = -\zeta_s\left(\frac{N_{n+1}}{N_n}\right)A_n, \quad (9)$$

$$\zeta_s = \frac{s+1}{s+2}\frac{1-\lambda^{-(s+2)}}{1-\lambda^{-(s+1)}}\omega_c,$$

$$A_n = \lambda^{-n}\frac{(1-\lambda^{-(n+1+s)})^2}{(1-\lambda^{-(2n+1+s)})(1-\lambda^{-(2n+2+s)})},$$

$$C_n = \lambda^{-n+s}\frac{(1-\lambda^{-n})^2}{(1-\lambda^{-(2n+s)})(1-\lambda^{-(2n+1+s)})},$$

$$N_n^2 = \lambda^{-n(1+s)}\frac{(\lambda^{-1};\lambda^{-1})_n^2}{(\lambda^{-(s+1)};\lambda^{-1})_n^2(1-\lambda^{-(2n+1+s)})},$$

with $(a; b)_n = (1 - a)(1 - ab)(1 - ab^2)\cdots(1 - ab^{(n-1)})$. Here $\lambda > 1$ is the discretization parameter. In the Fock representation, the ground state wave function of Hamiltonian (6) characterizing a single chain system can be written in the form of matrix-product states (MPS) as

$$|\psi\rangle = \sum_{i_0=\uparrow,\downarrow;j} X^{i_0}X^{j_1}X^{j_2}\cdots X^{j_{L-1}}|i_0, \vec{j}\rangle, \quad (10)$$

where i_0 is the spin index, $\vec{j} = (j_1, j_2, \ldots j_{L-1})$, with $0 \leq j_i \leq d_p$, represents the quantum numbers for the boson basis, L is the length of the chain (chosen as 51), and d_p is the number of boson modes allocated on each site. X^j are single matrices whose dimensions are restricted by a cutoff $D_c = 50$. Subsequently, performing an iterative optimization procedure,[17] each matrix X can be optimized to a truncation error less than 10^{-7}. Furthermore, if a DMRG algorithm with an optimized boson basis[14] is used, the boson number d_p on each site of the Wilson chain can be kept up to 100. Therefore, a total of 10^2L phonons are included in our calculations. A minimum of $d_p = 20$ phonons need to be kept to arrive at a clear conclusion about the phase transition, which points to the difficulty in dealing with off-diagonal coupling. Using the obtained MPS wave functions, we can extract $\langle\sigma_x\rangle$ (i.e., excitonic coherence between the two levels), $\langle\sigma_z\rangle$ (i.e., exciton population difference), and the von-Neumann entropy $S_{v-N} \equiv -\mathrm{Tr}\rho_s\log\rho_s$, where ρ_s is the reduced density matrix of the spin.

The sub-Ohmic SBM with $\beta = 0$ and the spectral density (3) may exhibit a second order transition from a delocalized phase ($\langle\sigma_z\rangle = 0$) to a localized one ($\langle\sigma_z\rangle \neq 0$), if $\alpha > \alpha_c$ ($0 < \alpha_c < 1$).[12] Especially, if $s < 1/2$, critical exponents of the phase transition, e.g., $\langle\sigma_z\rangle = (\alpha - \alpha_c)^{\beta_{\mathrm{MF}}}$ where $\beta_{\mathrm{MF}} = 1/2$, can be obtained via quantum-to-classical correspondence as demonstrated by a variety of numerical techniques.[11,12] In the two-bath SBM of Eq. (6), competition between the baths poses a significant challenge to the numerical simulations due to an increased total boson number that must be kept. DMRG calculations[14] have so far revealed that if $s = \bar{s} < 1/2$ and σ_x and σ_z coupled to two boson baths with equivalent coupling strengths ($\alpha = \beta$), the spin is situated in a localized state. Furthermore, to obtain a deeper insight into the properties of the two-bath SBM, it is interesting to investigate the deep sub-Ohmic regime of the two-bath SBM with differing α and β, for a general scenario of $s = \bar{s}$ and $s \neq \bar{s}$. At last, we will discuss the situations with finite ε or Δ.

We first explore the case of $\varepsilon = \Delta = 0$ and $s = \bar{s} = 0.25$ for which Hamiltonian (6) is invariant under operation

$$\mathcal{P} = \sigma_y e^{i\sum_n (b_{n,1}^\dagger b_{n,1} + b_{n,2}^\dagger b_{n,2})}, \quad (11)$$

indicating a two-fold degeneracy of the ground state. A tiny symmetry-breaking perturbation is often applied to a state with two-fold degeneracy in the DMRG calculations. Due to diagonal coupling, the spin will be trapped with a finite $\langle\sigma_z\rangle$, forming a localized phase. The coupling with σ_x, however, induces a spin flip between $|\uparrow\rangle$ and $|\downarrow\rangle$, thereby hindering the self-trapping process. Fig. 1(a) shows calculated $\langle\sigma_x\rangle$ and $\langle\sigma_z\rangle$ for $\alpha = 0.02$ and a range of β values from 0.0 to 0.05. It is clear that when the off-diagonal coupling is dominant, i.e., $\beta \gg \alpha$, $\langle\sigma_x\rangle$ is finite so that the spin is in the superposition state of $|\uparrow\rangle$ and $|\downarrow\rangle$. We ascribe this phase as "phase I." Similar arguments remain valid for the case of $\beta \ll \alpha$, when $\langle\sigma_z\rangle$ assumes a finite value and we term this phase as "localized phase II," abbreviated as "phase II." As shown in Fig. 1(b), S_{v-N} also shows a sharp peak at the critical point, $\beta \sim 0.0204$. In addition, we have also calculated the fidelity near the critical point reaching the same conclusion. As shown in Fig. 1(a), $\langle\sigma_z\rangle$ and $\langle\sigma_x\rangle$ are sensitive to the boson number d_p being kept in DMRG calculation. Evidently, to obtain reliable data at the critical point, it is necessary to choose a sufficiently large d_p (over 20).

Next, we study the case of $s \neq \bar{s}$. According to Eq. (7) [Eq. (8)], if $\omega < \omega_c = 1$, the strength of η_x (η_y) is inversely proportional to $1 + s$ ($1 + \bar{s}$). Therefore, as opposed to the case of $s = \bar{s}$, where the spin-bath interactions are governed solely by α and β, if $s \neq \bar{s}$, the effective spin-bath interactions are modified, leading to a shift of the two critical points as shown in Fig. 1. In Fig. 2, we present calculated $\langle\sigma_z\rangle$ and $\langle\sigma_x\rangle$ for the case of $s = 0.3$, $\bar{s} = 0.2$. Similarly, the properties of the transition from I to II are analogous to those exhibited in Fig. 1(a), and the critical point moves from 0.0204 to 0.0115, as indicated by the peak of the entanglement entropy in Fig. 2. It is convenient to renormalize α and β by the factors $1/(1 + s)$ and $1/(1 + \bar{s})$, respectively. Here, s ($\bar{s}$) increases (decreases) from 0.25 to 0.3 (0.2), and therefore, the effective diagonal (off diagonal) coupling will become smaller (larger). In order to reproduce the phase transition in Fig. 1, the critical value of

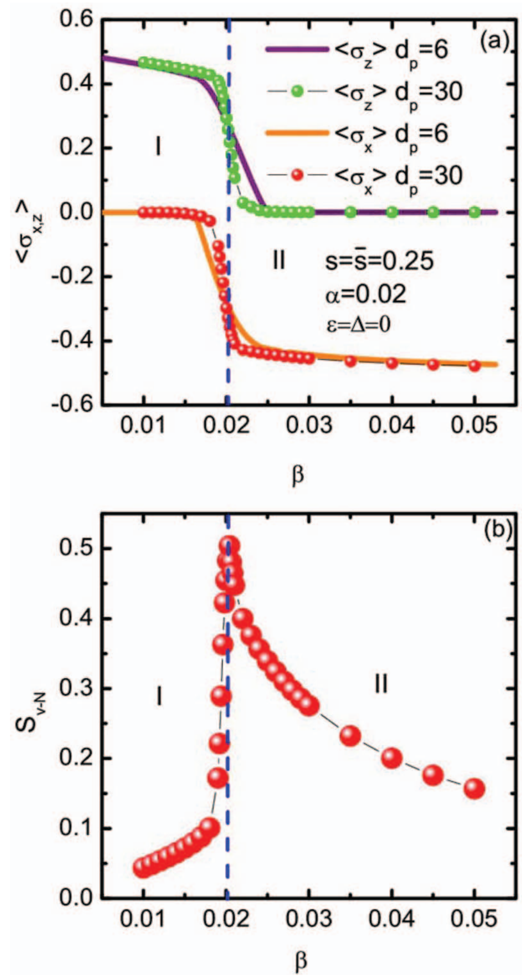

FIG. 1. (a) $\langle\sigma_x\rangle$ and $\langle\sigma_z\rangle$ as a function of β using two on-site boson numbers, $d_p = 6$ and 30; (b) the von-Neumann entropy S_{v-N} as a function of β. The critical point is labeled by the dashed lines, and we set $s = \bar{s} = 0.25$ and $\alpha = 0.02$.

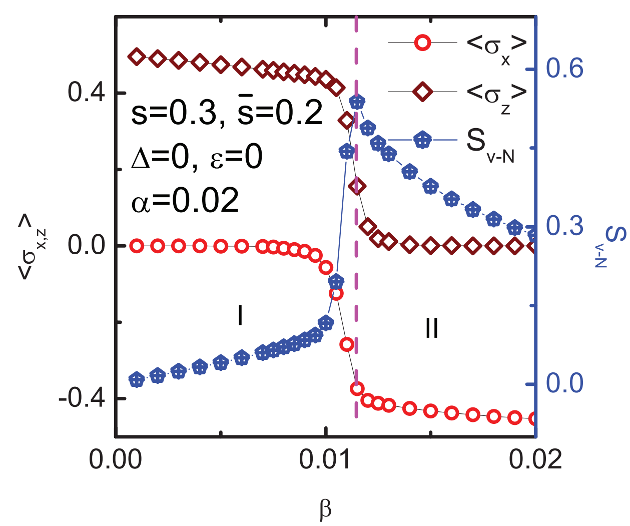

FIG. 2. $\langle\sigma_x\rangle$ and $\langle\sigma_z\rangle$ as a function of β with $s = 0.3$, $\bar{s} = 0.2$, and $\alpha = 0.02$. The transition points are marked by the dashed line. Also shown is the von-Neumann entropy (S_{v-N}) with a remarkably sharp peak at the critical point (at about 0.0115) where phase I goes into II.

β will have to shift to the left, which is just the result shown in Fig. 2.

It is now clear that due to the competition of the two baths a second order phase transition exists in the two-bath SBM. In the absence of ε and Δ, σ_x and σ_z swap their roles through a rotation along the y axis. This results in a similar swap of $\langle\sigma_x\rangle$ and $\langle\sigma_z\rangle$ near the critical point, where $\langle\sigma_x\rangle$ displays a kink when $\Delta \neq 0$. In contrast to the single-bath SBM, $\langle\sigma_x\rangle$ vanishes due to the full $SU(2)$ symmetry of the spin and the absence of a confining potential for σ_x. It should be stressed that both phases, phases I and II, are doubly degenerate, in agreement with the parity symmetry of Hamiltonian (6). The degeneracy of phase I (II) is characterized by the eigenstates of σ_z (σ_x), $|\uparrow\rangle$ and $|\downarrow\rangle$ ($|\leftarrow\rangle$ and $|\rightarrow\rangle$). This is a novel feature of a second order phase transition between states with two-fold degeneracy as a result of bath competition.

As pointed out in Ref. 13, finite ε or Δ can break the symmetry of the ground-state free energy and thus prevent the occurrence of a second order phase transition. For $s = 0.3$, $\bar{s} = 0.2$, Fig. 3 shows $\langle\sigma_z\rangle$ as a function of α and β, where a finite tunneling constant of $\Delta = 0.1$ is imposed on the x spin component. A phase boundary in the α-β plane is clearly visible judging from a sudden disappearance of the expectation value of the z component. Fig. 4, which displays $\langle\sigma_z\rangle$, $\langle\sigma_x\rangle$, and S_{v-N} as a function of α for the case of $\beta = 0.03$, further confirms the phase boundary in Fig. 3. Unlike the large spike at the critical point shown in Fig. 1, only a much less pronounced kink is found in $\langle\sigma_x\rangle$. It is argued that the occurrence of the kink is ascribed to a sufficiently large value of Δ. Similar results can be obtained under a spin bias in the z component after rotating along the y axis. Moreover, through intensive DMRG calculations, we find that $\langle\sigma_z\rangle$ can be reduced to zero by increasing Δ in the localized phase, while $\langle\sigma_x\rangle$ reaches a saturation value.

To summarize, in the deep sub-Ohmic regime, for an extended SBM with two independent baths coupled to two perpendicular spin components, there exists a second order phase transition, from the doubly degenerated "coherent phase I" to another doubly degenerated "localized phase II." This phase transition, which survives the introduction of finite Δ or ε, offers a notable difference between the single-bath SBM and the two-bath SBM. Varying bath spectral densities ($s \neq \bar{s}$) shifts the critical point, and for $\varepsilon = 0$ and $\Delta = 0$, $\langle\sigma_z\rangle$ and $\langle\sigma_x\rangle$ display jumps near the critical point, a feature that is absent from the single-bath SBM. It is found that the DMRG algorithm combined with an optimized phonon basis is a robust approach to deal with SBM with off-diagonal coupling, despite that further improvement is in need to give accurate estimates of the critical exponents and other quantities of importance.

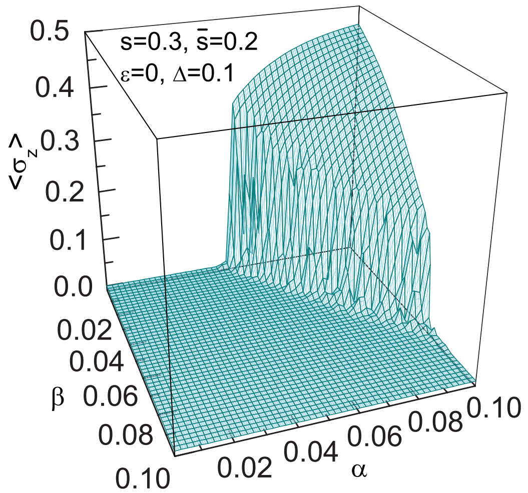

FIG. 3. $\langle\sigma_z\rangle$ as a function of α and β, wherein $s = 0.3$, $\bar{s} = 0.2$, and $\Delta = 0.1$. The spin bias ε is set to zero.

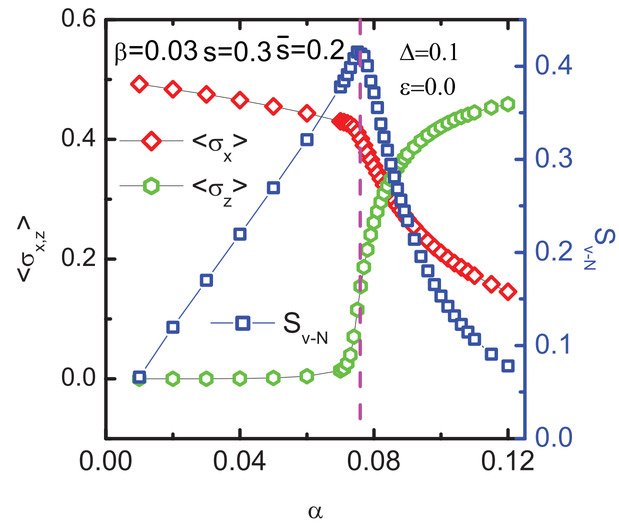

FIG. 4. $\langle\sigma_z\rangle$, $\langle\sigma_x\rangle$, and entanglement entropy S_{v-N} as a function of α near the critical point, pointing to a second order phase transition. The off-diagonal coupling strength β is set to 0.03, and the same spectral densities are used for the two baths as in Fig. 3. The tunneling strength Δ and the spin bias ε also remain the same as in Fig. 3. $\langle\sigma_x\rangle$ shows a small kink at the critical point.

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