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<td>Citation</td>
<td>Zhao, Y., Yao, Y., Chernyak, V., &amp; Zhao, Y. (2014). Communication: Spin-boson model with diagonal and off-diagonal coupling to two independent baths: Ground-state phase transition in the deep sub-Ohmic regime. The Journal of Chemical Physics, 140(16), 161105-.</td>
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<td>Date</td>
<td>2014</td>
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<td><a href="http://hdl.handle.net/10220/19601">http://hdl.handle.net/10220/19601</a></td>
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Citation: The Journal of Chemical Physics 140, 161105 (2014); doi: 10.1063/1.4873351
View online: http://dx.doi.org/10.1063/1.4873351
View Table of Contents: http://scitation.aip.org/content/aip/journal/jcp/140/16?ver=pdfcov
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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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(Received 16 February 2014; accepted 15 April 2014; published online 25 April 2014)

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 ground 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 transitions11,12. The SBM Hamiltonian can be written as

$$H_{SBM} = \frac{\epsilon}{2} \sigma_z - \frac{\Delta}{2} \sigma_x + \sum_l \omega_l b_l^\dagger b_l + \frac{\sigma_z}{2} \sum_l \lambda_l (b_l^\dagger + b_l),$$  \hspace{0.5cm} (1)

where $\sigma_x$ and $\sigma_z$ are the Pauli matrices, $\epsilon$ and $\Delta$ are the spin (on-site energy) bias and the tunneling (intramolecular coupling) constant, respectively, $\omega_l$ and $\lambda_l$ are the frequency and coupling constant, respectively, of the $l$th boson mode, with $b_l^\dagger (b_l)$ 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: $J(\omega) = 2\pi \alpha \omega^{s-1} \omega^s$, where $\omega_c$, $\alpha$, and $s$ are the cutoff 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 (super-Ohmic) regime, respectively. Studies11,12 have shown that if $\epsilon = 0$ 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 “de-localized” phase. A critical coupling strength $\alpha_c$ exists for this second order phase transition, which for $s = 1$ emerges as a Kosterlitz-Thouless transition.3

In this communication we extend the SBM to a more realistic form by adding to Hamiltonian (1) an off-diagonal coupling term, $\frac{\alpha}{2} \sum_l \lambda_l (b_l^\dagger + b_l)$. Recent studies13 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 de-localization effects, induced by the competition between diagonal and off-diagonal coupling, plays a crucial role in determining energy transfer mechanisms which interpolate between the Förster-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
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 \((\sigma_z)\) will be zero if \(\alpha\) is below some critical value \(\alpha_c(\Delta)\), placing the system in a delocalized phase. If \(\alpha > \alpha_c, (\sigma_z)\) 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 (\(\downarrow\)) and up (\(\uparrow\)) 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

\[
\hat{H} = \frac{\varepsilon}{2} \sigma_z - \frac{\Delta}{2} \sigma_x + \sum_{i,l} \omega_{b_l} b^\dagger_{l,i} b_{l,i} + \sum_{i,l} \lambda_l (b^\dagger_{l,1} + b_{l,1}) + \frac{\sigma_z}{2} \sum_{i,l} \phi_l (b^\dagger_{l,2} + b_{l,2}),
\]

where the subscript \(i = 1, 2\) is introduced to distinguish the two baths, and \(\lambda_l\) and \(\phi_l\) are the diagonal and off-diagonal coupling strengths, respectively, which can be used to determine spectral densities,

\[
J_x(\omega) = \sum_l \phi_l^2 \delta(\omega - \omega_l) \Rightarrow 2\beta \omega_A^2 \delta^s(\omega),
\]

\[
J_y(\omega) = \sum_l \phi_l \delta(\omega - \omega_l) \Rightarrow 2\beta \omega_A \delta^s(\omega),
\]

Here, \(\alpha\) and \(\beta\) are dimensionless coupling constants, and \(\omega_c\) is set to be unity throughout this work. The two baths are characterized by the spectral exponents \(s\) and \(\tilde{s}\).

Equation (1) can be recast into its continuum form

\[
\hat{H}_{\text{SBM}} = \frac{\varepsilon}{2} \sigma_z - \frac{\Delta}{2} \sigma_x + \int_0^{\omega_c} g(\omega) b^\dagger_{\omega} b_{\omega}
\]

\[
+ \frac{\sigma_z}{2} \int_0^{\omega_c} h(\omega) (b^\dagger_{\omega} + b_{\omega}),
\]

where \(b_{\omega}\) and \(b^\dagger_{\omega}\) are the counterparts of \(b_l\) and \(b^\dagger_l\), \(g(\omega)\) 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

\[
\hat{H} = \frac{\varepsilon}{2} \sigma_z - \frac{\Delta}{2} \sigma_x
\]

\[
+ \sum_{n=0,i} \left[ \omega_{n,i} b^\dagger_{n,i} b_{n,i} + \lambda_{n,i} (b^\dagger_{n,i} b_{n,i+1} + b^\dagger_{n,i+1} b_{n,i}) \right]
\]

\[
+ \frac{\sigma_z}{2} \sqrt{\eta_{n,i}} (p_{0,1} + p_{0,1}^\dagger) + \frac{\sigma_z}{2} \sqrt{\eta_{n,i}} (p_{0,2} + p_{0,2}^\dagger),
\]

where \(i = 1, 2\) label the baths, \(\omega_{n,i}\) is the on site energy of site \(n\) in the \(i\)th bath, \(p^\dagger_{n,i} (p_{n,i})\) is corresponding boson creation (annihilation) operator, \(\lambda_{n,i}\) is the hopping amplitude between sites \(n\) and \(n + 1\), and \(\eta_{n,i}\) is a coupling constant proportional to \(\alpha (\beta)\). One has

\[
\eta_x = \int_0^{\omega_c} J_x(\omega) d\omega = \frac{2\pi \beta}{1 + \delta} \omega_A^{\delta},
\]

\[
\eta_z = \int_0^{\omega_c} J_y(\omega) d\omega = \frac{2\pi \alpha}{1 + \delta} \omega_A^{\delta},
\]

\[
\omega_{n,1} = \xi_s (A_n + C_n), \quad \xi_{n,1} = -\xi_s \left( \frac{N_{n+1}}{N_n} \right) A_n,
\]

\[
\xi_s = \frac{s + 1}{s + 2} - \frac{\lambda_s^{(-s+2)}}{\lambda_s^{(-s+2)}},
\]

\[
A_n = \lambda^{\alpha - n} (1 - \lambda^{(n+1)(2s)}) (1 - \lambda^{(2n+2s)}),
\]

\[
C_n = \lambda^{\alpha - s} (1 - \lambda^{n(2s+1)} (1 - \lambda^{(2n+2s)})),
\]

\[
N_n^2 = \lambda^{\alpha - s(2s+1)} (\lambda^{(s-1)(2s)} (1 - \lambda^{(2n+2s)})),
\]

with \((\alpha; b_{\omega})\) \(= 1 - (1 - ab)(1 - ab^2)\cdots(1 - ab^{\alpha - 1})\). 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

\[
|\psi\rangle = \sum_{i_0 = 1, 2, \cdots, j} \sum_{i_0} X^{i_0} X^{i_1} X^{i_2} \cdots X^{i_{L-1}} |i_0, \tilde{j}\rangle,
\]

where \(i_0\) is the spin index, \(\tilde{j} = (j_1, j_2, \cdots, j_{L-1})\), with \(0 \leq j_i \leq d_{\rho}\), represents the quantum numbers for the boson basis, \(L\) is the length of the chain (chosen as 51), and \(d_{\rho}\) is the number of boson modes allocated on each site. Each matrix \(X\) is single matrices whose dimensions are restricted by a cutoff \(D_f = 50\). Subsequently, performing an iterative optimization procedure, 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 \(d_{\rho}\) on each site of the Wilson chain can be kept up to 100. Therefore, a total of \(10^2 L\) phonons are included in our calculations. A minimum of \(d_{\rho} = 20\) 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 \((\sigma_z)\) \((i.e., \text{excitonic coherence between the two levels}), \langle \sigma_z \rangle\) \((\text{i.e., exciton population difference})\), and the von-Neumann entropy \(S_\sigma = -\text{Tr} \rho_s \log \rho_s\), where \(\rho_s\) 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 $\alpha > \alpha_c$ ($0 < \alpha_c < 1$).\footnote{In this case, the transition takes place at a critical point where $\beta_{MF} = 1/2$, and the properties of the two-bath SBM are sensitive to the interplay between the baths.} Especially, if $s < 1/2$, critical exponents of the phase transition, e.g., $\langle \sigma_z \rangle = (\alpha - \alpha_c)^\beta$ where $\beta_{MF} = 1/2$, can be obtained via quantum-to-classical correspondence as demonstrated by a variety of numerical techniques.\footnote{In this case, the transition takes place at a critical point where $\beta_{MF} = 1/2$, and the properties of the two-bath SBM are sensitive to the interplay between the baths.} 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\footnote{In this case, the transition takes place at a critical point where $\beta_{MF} = 1/2$, and the properties of the two-bath SBM are sensitive to the interplay between the baths.} have so far revealed that if $s = \bar{s} < 1/2$ and $\sigma_x$ and $\sigma_z$ 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 $\alpha$ and $\beta$, for a general scenario of $s = \bar{s}$ and $s \neq \bar{s}$. At last, we will discuss the situations with finite $\varepsilon$ or $\Delta$.

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

$$P = \sigma_z e^{\sum_a (\eta_a \eta_{a+1} + \eta_{a+1} \eta_{a})},$$

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 $\sigma_x$, however, induces a spin flip between $|\uparrow\rangle$ and $|\downarrow\rangle$, thereby hindering the self-trapping process. Fig. 1(a) shows calculated $\langle \sigma_z \rangle$ and $\langle \sigma_x \rangle$ for $\alpha = 0.02$ and a range of $\beta$ 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 $\eta_k$ ($\eta_n$) 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 $\alpha$ and $\beta$, 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 $\alpha$ and $\beta$ 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) $\langle \sigma_z \rangle$ and $\langle \sigma_x \rangle$ as a function of $\beta$ using two on-site boson numbers, $d_p = 6$ and 30; (b) the von-Neumann entropy $S_{v-N}$ as a function of $\beta$. 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 $\beta$ 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.*
$\beta$ 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 $\varepsilon$ and $\Delta$, $\sigma_x$ and $\sigma_z$ 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 $\langle \sigma_z \rangle$ displays a kink when $\Delta \neq 0$. In contrast to the single-bath SBM, $\langle \sigma_z \rangle$ vanishes due to the full $SU(2)$ symmetry of the spin and the absence of a confining potential for $\sigma_z$. 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 $| \cdots \rangle$ and $| \uparrow \rangle$ (| $\leftarrow \rangle$ 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 $\varepsilon$ or $\Delta$ can break the symmetry of the ground-state free energy and thus prevent the occurrence of a second order phase transition. For $s=0.3$, $\delta=0.2$, Fig. 3 shows $\langle \sigma_x \rangle$ as a function of $\alpha$ and $\beta$, where a finite tunneling constant of $\Delta=0.1$ is imposed on the $x$ spin component. A phase boundary in the $\alpha$-$\beta$ plane is clearly visible judging from a sudden disappearance of the expectation value of the $z$ component. Fig. 4, which displays $\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$, and $S_{v-N}$ as a function of $\alpha$ 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 $\Delta$. 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 $\langle \sigma_x \rangle$ can be reduced to zero by increasing $\delta$ in the localized phase, while $\langle \sigma_z \rangle$ 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 $\Delta$ or $\varepsilon$, offers a notable difference between the single-bath SBM and the two-bath SBM. Varying bath spectral densities ($s \neq \delta$) 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.

This work is supported by the Singapore National Research Foundation under Project No. NRF-CRP5-2009-04 and the U.S. National Science Foundation under Grant No. CHE-1111350.

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