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David von Seggern
(vonneg@seismo.unr.edu) University of Nevada
July 2012, page 10
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The article by Thorne Lay and Hiroo Kanamori is an interesting one. It discusses the energy release of the 1964 Chilean earthquake. The authors use the relation for seismic energy release rather than total strain energy release. I believe the authors underestimate the total strain energy release by a factor of about 3, or 10 times. The seismic energy release would increase the earthquake energy number by orders of magnitude. Despite the catastrophic damage potential of nuclear bombs, the forces of nature occasionally unleash much larger energy releases. Although the nuclear bombs are under our control, earthquakes, volcanic eruptions, and extreme weather events are not. However, by judicious preparation and avoidance measures, humans can significantly diminish the damage of natural events. This article does not have any references.

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By the act of hitting a ball with a bat, one calculates the force energy to deliver the ball to its new location, but one must also take into account that the ball extended its energy release to that which became struck by the ball as its momentum ceased and passed energy to the struck item. Therefore the parameters of the damage extend into the future when the received energy to that pushed upon later becomes released in a new event. Perhaps calculations of one added that in while another's calculations did not. E.M.C.
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Dynamics of the sub-Ohmic spin-boson model: A time-dependent variational study

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The Dirac-Frenkel time-dependent variation is employed to probe the dynamics of the zero temperature sub-Ohmic spin-boson model with strong friction utilizing the Davydov D₁ ansatz. It is shown that initial conditions of the phonon bath have considerable influence on the dynamics. Counterintuitively, even in the very strong coupling regime, quantum coherence features still manage to survive under the polarized bath initial condition, while such features are absent under the factorized bath initial condition. In addition, a coherent-incoherent transition is found at a critical coupling strength $\alpha \approx 0.1$ for $s = 0.25$ under the factorized bath initial condition. We quantify how faithfully our ansatz follows the Schrödinger equation, finding that the time-dependent variational approach is robust for strong dissipation and deep sub-Ohmic baths ($s \ll 1$). © 2013 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4792502>]

I. INTRODUCTION

It is of fundamental importance to study macroscopic behavior of open quantum systems under the influence of dissipative baths that they are inevitably in contact with.^{1,2} As an open quantum system and its thermal bath with a finite number of modes together form an isolated system which conserves the energy, according to the Poincaré recurrence theorem,³ the quantum system will eventually return to a state very close to its initial state. To circumvent this recurrence, the bath has to be expanded to contain an infinite number of phonon modes. The simplest model of a quantum system is a two-level system $\hat{H}_S = -\Delta\sigma_x/2$, and Caldeira and Leggett⁴ have shown that a bath of harmonic oscillator, $\hat{H}_B = \sum_l \omega_l b_l^\dagger b_l$, provides a very good approximation to real dissipative systems. Here σ_x is a Pauli matrix, and $b_l^\dagger$ (b_l) is the boson creation (annihilation) operator. In general, it is assumed that the two-level system is linearly coupled to the bath, $\hat{H}_{SB} = \sigma_z \sum_l \lambda_l (b_l^\dagger + b_l)/2$. In the absence of the bath, the quantum two-level system will oscillate between the states $|+\rangle$ and $|-\rangle$ with frequency Δ ($|\pm\rangle$ are the two eigenstates of σ_z), a quantum phenomenon which has no classical analog. Putting together all three Hamiltonian terms,

$$\hat{H} = -\frac{\Delta}{2}\sigma_x + \sum_l \omega_l b_l^\dagger b_l + \frac{\sigma_z}{2} \sum_l \lambda_l (b_l^\dagger + b_l). \quad (1)$$

The combined Hamiltonian described by Eq. (1) is called the spin-boson model.¹

Despite its simplicity, the spin-boson model has been widely discussed in condensed phase physics and chemistry, ranging from the process of electron transfer⁵ to quantum entanglement⁶ between a qubit⁷ and its bath. The coupling

between the two-level system and the harmonic bath is completely specified by the spectral function,

$$J(\omega) = \sum_l \lambda_l^2 \delta(\omega - \omega_l) = 2\alpha\omega_c^{1-s} \omega^s e^{-\omega/\omega_c}, \quad (2)$$

with a cutoff frequency ω_c and a dimensionless constant α measuring the strength of the coupling. A bath described by a spectral function with $s = 1$ is referred to as an Ohmic bath. Both static and dynamical properties of the spin-boson model with an Ohmic bath are well understood.^{1,2} It is found that there exist a quantum phase transition from a non-degenerate delocalized phase to a doubly degenerate localized phase, and a turnover from a coherent phase to an incoherent one. The critical coupling for the quantum phase transition is $\alpha_c \approx 1$, and the critical coupling for the turnover to occur is $\alpha_{CI} \approx 0.5$. In the Ohmic regime, the spin-boson model can be readily mapped onto the anisotropic Kondo model using bosonization techniques,¹ and known results can be borrowed from the Kondo model. However, success still eludes us in arriving at a correct description of the spin-boson physics in the sub-Ohmic regime ($0 < s < 1$).

Several sophisticated numerical methods have been used to study the sub-Ohmic spin-boson model. An incomplete list includes: the numerical renormalization group method developed by Wilson,⁸ which reveals a continuous quantum phase transition for $0 < s < 1$ and weakly damped coherent oscillations on short time scales in the localized phase;⁹ numerically exact real-time path integral method with quasia-diabatic propagator revealing effective dynamic asymmetry in the presence of a sub-Ohmic bath;^{10,11} quantum Monte Carlo method which determines the critical exponents for $s < 1/2$;¹² the sparse polynomial space representation method which is based on the exact diagonalization to obtain numerical results;¹³ the real-time path integral Monte Carlo techniques which show that the coherent phase exists even in the

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presence of strong dissipation for $s < 1/2$,^{14,15} and the numerically exact multilayer multi-configuration time-dependent Hartree method (ML-MCTDH) which shows that the transition of the dynamics from weakly damped coherent motion to localization upon increase of the system-bath coupling strength.^{16,17}

Unlike in the Ohmic regime, dynamics of sub-Ohmic spin-boson model is very sensitive to the initial conditions. There are two initial conditions of interest: one is the factorized initial condition with the bath in its vacuum state initially and the other is the polarized initial condition consistent with typical experimental scenarios,² under which the system is prepared in the ground state of $H_B + H_{SB}|_{\sigma_z=1}$. Many recent studies use the polarized initial condition.^{11–13,15} The typical time scale of the spin dynamics is $1/\Delta$, the time it takes to hop from a spin state to another. On the other hand, the reorganization energy,¹⁸ which describes the change in population disparity between the two states $|+\rangle$ and $|-\rangle$, as one goes from one initial condition to the other, is given as $\int_0^\infty d\omega J(\omega)/\omega = 2\alpha\omega_c\Gamma(s)$, where $\Gamma(s)$ is the gamma function of s . Lucke *et al.*,¹⁸ showed that the difference in spin dynamics under the two initial conditions is negligible for the Ohmic bath in the scaling limit $\Delta \ll \omega_c$. However, reorganization energies in the sub-Ohmic regime are larger than those in the Ohmic regime. It implies that much more time is needed for a sub-Ohmic bath to return to thermal equilibrium, and therefore, the spin dynamics corresponding to the two initial conditions will display sizeable differences for certain parameter space $(\Delta/\omega_c, s)$. Nalbach and Thorwart¹¹ have confirmed such a physical picture. It is commonly accepted that an increase in the strength of the spin-bath coupling will eventually turn quantum coherent oscillations into classical-like damping, a picture supported by the aforementioned numerical approaches for $1/2 < s < 1$. However, Kast and Ankerhold¹⁵ have recently claimed that such a picture may not always hold. Numerical data in the strong coupling regime, for example, with $\alpha = 30\alpha_c$, show that the coherent phase exists for exponents up to $s = 0.49$. Such an “anomalous” result warrants further investigations.

In this work, we adopt a variational framework to study the zero temperature dynamical properties of the sub-Ohmic spin-boson model. This is motivated by two facts: (i) The spin-bath interactions are formally identical to the exciton-phonon coupling in a quasiparticle named a polaron, which is generally described by the Holstein model,¹⁹

$$\hat{H}_{\text{Holstein}} = \sum_m \epsilon_m a_m^\dagger a_m + \sum_{m \neq n} J_{mn} (a_m^\dagger a_n + a_n^\dagger a_m) + \sum_{qm} g_q a_m^\dagger a_m (b_q + b_q^\dagger) + \sum_q \omega_q b_q^\dagger b_q, \quad (3)$$

where $a_m^\dagger$ (a_m) is the exciton creation (annihilation) operator, J_{mn} is the hopping integral, and g_q labels the exciton-phonon coupling strength; and (ii) A time-dependent variational approach based on the Davydov *Ansätze* has been widely used for describing the dynamics of Holstein systems. As a semi-classical approach for studying energy transport in deformable molecular chains, those *Ansätze*²⁰ were put forward by Davydov and co-workers as two trial wave func-

tions, namely, the Davydov D_1 and D_2 *Ansätze*. The first of the Davydov *Ansätze* has the form,

$$|D_1(t)\rangle = \sum_n \alpha_n(t) a_n^\dagger |0\rangle_{\text{ex}} \exp \left[\sum_q (\lambda_{nq}(t) b_q^\dagger - h.c.) \right] |0\rangle_{\text{ph}}, \quad (4)$$

where $\alpha_n(t)$ and $\lambda_{nq}(t)$ are the variational parameters representing the exciton amplitude and the phonon displacements at the n th site, respectively, and $|0\rangle_{\text{ex}}$ and $|0\rangle_{\text{ph}}$ denote the exciton and the phonon vacuum states, respectively. The second of the Davydov *Ansätze* is given by

$$|D_2(t)\rangle = \sum_n \alpha_n(t) a_n^\dagger |0\rangle_{\text{ex}} \exp \left[\sum_q (\beta_q(t) b_q^\dagger - h.c.) \right] |0\rangle_{\text{ph}}. \quad (5)$$

Note that the phonon-displacement parameter in the much simplified $|D_2(t)\rangle$, $\beta_q(t)$, is independent of the site index n . The Davydov *Ansätze* and their variants have been applied successfully to study the one-dimensional Holstein polaron by Zhao and co-workers.^{21–24} To probe polaron dynamics of the Holstein system using Davydov's *Ansätze*,^{22,23} we have employed the Dirac-Frenkel time-dependent variational principle, a powerful technique to obtain approximate dynamics for quantum systems for which exact solutions are elusive.²⁵

By exploiting the analogy between the spin-boson model and the Holstein molecular crystal model, we propose a time-dependent trial wave function very similar to the Davydov D_1 ansatz, and seek to develop an accurate description for dynamical properties of the sub-Ohmic spin-boson model with $0 < s < 1/2$ under both the polarized and factorized initial conditions. It was pointed out earlier²⁶ that the Davydov *Ansätze* bear close resemblance to a multi-configurational ansatz, which contains more than one Slater determinant. We note that the ansatz employed in this work shares many characteristics with the multi-configurational Gaussian wave packets,^{27–31} used in a variant of the powerful multi-configuration time-dependent Hartree technique (MCTDH),³² also known as the G-MCTDH method. Proposed in Ref. 27 and developed further in Refs. 28, 33, the G-MCTDH method extends MCTDH to higher-dimensional systems by including a moving basis of Gaussian functions while restricted to an optimally chosen subset of the bath modes. It has been successfully applied to describe dynamics of the Henon-Heiles potential model³³ and the oscillator-bath model.²⁸

In the Holstein molecular crystal model, a similar reorganization energy²² can be calculated from the phonon spectral density function using $\int_0^\infty d\omega J(\omega)/\omega$, and is known to be proportional to the Huang-Rhys factor,³⁴ which measures the exciton-phonon coupling strength. For the factorized initial conditions, our previous studies on the Holstein model reveal that the Davydov *Ansätze* are especially accurate in the strong exciton-phonon coupling regime,²¹ a fact that will also be confirmed by calculating the relative deviation for the sub-Ohmic spin-boson model studied here.²² Furthermore, for a given spin-bath coupling strength, a smaller s yields a smaller relative deviation, inferring the highest accuracy of our ansatz in the deep sub-Ohmic regime $s \ll 1$. A similar trend is believed for the polarized initial conditions.

This paper is organized as follows. In Sec. II, we propose a Davydov-like ansatz, and use the Dirac-Frenkel variational method to obtain the equations of motion for its parameters. In Sec. III, we present the numerical results, which also reveal the time evolution of quantum coherence and entanglement for the spin-boson model. The effect of different initial conditions is discussed in this section. In Sec. IV, conclusions are drawn.

II. METHODOLOGY

Note that the spin-boson model can be viewed as a two-site Holstein model with an infinite number of phonon modes in the one-exciton subspace. This equivalence between the exciton-phonon coupling and the spin-boson interaction naturally leads to a trial wave function similar to Davydov D₁ ansatz for the spin-boson model,

$$|D_s(t)\rangle = A(t)|+\rangle \exp\left[\sum_l (f_l(t)b_l^\dagger - h.c.)\right] |0\rangle_{\text{ph}} + B(t)|-\rangle \exp\left[\sum_l (g_l(t)b_l^\dagger - h.c.)\right] |0\rangle_{\text{ph}}, \quad (6)$$

where $A(t)$ and $B(t)$ are complex variational parameters representing occupation amplitudes in states $|+\rangle$ and $|-\rangle$, respectively, and $f_l(t)$ and $g_l(t)$ label the corresponding complex phonon displacements of the l th phonon mode. In this work, we choose the Lagrangian formalism of the Dirac-Frenkel time-dependent variational principle to obtain equations of motion for the variational parameters. The Lagrangian associated with the trial state $|D_s(t)\rangle$ is given as

$$L = \langle D_s(t) | \frac{i}{2} \frac{\overleftrightarrow{\partial}}{\partial t} - \hat{H} | D_s(t) \rangle. \quad (7)$$

Substituting the trial state $|D_s(t)\rangle$ into the Lagrangian (7), we arrive at the Lagrangian for the spin-boson model,

$$L = \frac{i}{2} (A^* \dot{A} - \dot{A}^* A + B^* \dot{B} - \dot{B}^* B) + \frac{i}{2} \sum_l [|A|^2 (\dot{f}_l^* \dot{f}_l - \dot{f}_l^* \dot{f}_l) + |B|^2 (\dot{g}_l^* \dot{g}_l - \dot{g}_l^* \dot{g}_l)] - \langle D_s(t) | \hat{H} | D_s(t) \rangle, \quad (8)$$

where

$$\begin{aligned} \langle D_s(t) | \hat{H} | D_s(t) \rangle &= \sum_l \omega_l (|A|^2 |f_l|^2 + |B|^2 |g_l|^2) \\ &- \frac{\Delta}{2} (A^* B e^{\sum_l f_l^* g_l} + A B^* e^{\sum_l f_l g_l^*}) e^{-\frac{1}{2} \sum_l (|f_l|^2 + |g_l|^2)} \\ &+ \frac{1}{2} \sum_l \lambda_l [|A|^2 (f_l + f_l^*) - |B|^2 (g_l + g_l^*)]. \end{aligned} \quad (9)$$

The Dirac-Frenkel time-dependent variational principle yields the equations of motion for A , B , f_l , and g_l ,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{u}_n^*} \right) - \frac{\partial L}{\partial u_n^*} = 0, \quad (10)$$

where u_n^* denotes the complex conjugate of variational parameters u_n , which can be A , B , f_l , or g_l . From Eq. (10), one arrives at the equations of motion for $A(t)$ and $B(t)$,

$$0 = i \dot{A} + i \frac{A}{2} \sum_l (\dot{f}_l f_l^* - \dot{f}_l^* f_l) - \frac{A}{2} \sum_l \lambda_l (f_l + f_l^*) + \frac{\Delta B}{2} e^{\sum_l [f_l^* g_l - \frac{1}{2} (|f_l|^2 + |g_l|^2)]} - A \sum_l \omega_l |f_l|^2, \quad (11)$$

$$0 = i \dot{B} + i \frac{B}{2} \sum_l (\dot{g}_l g_l^* - \dot{g}_l^* g_l) + \frac{B}{2} \sum_l \lambda_l (g_l + g_l^*) + \frac{\Delta A}{2} e^{\sum_l [g_l^* f_l - \frac{1}{2} (|f_l|^2 + |g_l|^2)]} - B \sum_l \omega_l |g_l|^2. \quad (12)$$

Similarly, the equations of motion for $f_l(t)$ and $g_l(t)$ are given as

$$i A \dot{f}_l - A \frac{\lambda_l}{2} - A \omega_l f_l = \frac{\Delta B}{2} (f_l - g_l) e^{\sum_l [f_l^* g_l - \frac{1}{2} (|f_l|^2 + |g_l|^2)]}, \quad (13)$$

$$i B \dot{g}_l + B \frac{\lambda_l}{2} - B \omega_l g_l = \frac{\Delta A}{2} (g_l - f_l) e^{\sum_l [g_l^* f_l - \frac{1}{2} (|f_l|^2 + |g_l|^2)]}. \quad (14)$$

Equations (11) and (12) have been used to deduce the equations of motion for $f_l(t)$ and $g_l(t)$. It is found from Eqs. (11) and (12) that

$$\frac{d}{dt} (|A|^2 + |B|^2) = \frac{d}{dt} \langle D_s(t) | D_s(t) \rangle = 0. \quad (15)$$

That the sum of $|A|^2$ and $|B|^2$ is conserved follows from early assignments of $A(t)$ and $B(t)$ in Eq. (6). Therefore, $|A|^2 + |B|^2$, which is the norm of $|D_s(t)\rangle$, can be set to unity,

$$|A|^2 + |B|^2 = 1. \quad (16)$$

The equations of motion (11)–(14) give a complete description of the time evolution of $|D_s(t)\rangle$, and therefore, the dynamics of the spin-boson model. In the spin-boson model, physical observables of interest are

$$P_i(t) \equiv \langle \sigma_i \rangle = \langle D_s(t) | \sigma_i | D_s(t) \rangle, \quad i = x, y, z. \quad (17)$$

Here $P_x(t)$ describes the coherence between the $|+\rangle$ and $|-\rangle$ states, and $P_z(t)$, the population difference. Upon substitution of the trial wave function (6) into Eq. (17), we obtain

$$P_z(t) = |A|^2 - |B|^2, \quad (18)$$

$$P_x(t) = A^* B e^{\sum_l [f_l^* g_l - \frac{1}{2} (|f_l|^2 + |g_l|^2)]} + A B^* e^{\sum_l [g_l^* f_l - \frac{1}{2} (|f_l|^2 + |g_l|^2)]}, \quad (19)$$

$$P_y(t) = -i A^* B e^{\sum_l [f_l^* g_l - \frac{1}{2} (|f_l|^2 + |g_l|^2)]} + i A B^* e^{\sum_l [g_l^* f_l - \frac{1}{2} (|f_l|^2 + |g_l|^2)]}. \quad (20)$$

Due to the invariance of $\hat{H}$ under $\sigma_y \rightarrow -\sigma_y$, one usually has $P_y = 0$ for the ground state or thermal averages. However, the time-dependent observable $P_y(t)$ is in general nonzero.

As mentioned in the Introduction, the initial condition has a vital influence on the dynamics of the spin-boson model with the sub-Ohmic bath. We assume that the spin is prepared in state $|+\rangle$ at $t = 0$, or $A(0) = 1$ and $B(0) = 0$. At zero temperature, the factorized bath initial condition corresponds to a phonon vacuum state with $f_l(0) = g_l(0) = 0$, while the polarized bath initial condition is one in which the bath phonons are in a displaced-oscillator state with $f_l(0) = g_l(0) = -\lambda_l/2\omega_l$.

When the phonon bath is absent, the dynamics of $P_z(t)$ will be fully coherent and has no classical component. The bath will induce decoherence, and for a quantum dissipative system such as the spin-boson model, its population difference has the form that $P_z(t) \sim \cos(\Omega t)e^{-\gamma t}$ ^{1,2} on certain time scales. The oscillation $\cos(\Omega t)$ represents the quantum coherence. The exponential decay is classical friction effect that is induced by the bath. The dynamics is said to be coherent if $\Omega \neq 0$, otherwise it is incoherent. On the other hand, the steady state is said to be localized if $P_z(t \rightarrow \infty) \neq 0$, otherwise it is delocalized $P_z(t \rightarrow \infty) = 0$.^{9,12,15,35,36}

Another physical quantity of interest is the entanglement between the spin and the surrounding bath described by the von Neumann entropy S , also known as the entanglement entropy.^{37,38} In the spin-boson model, it is given as^{6,39}

$$S = -\omega_+ \ln \omega_+ - \omega_- \ln \omega_-, \quad (21)$$

where

$$\begin{aligned} \omega_{\pm} &= \left(1 \pm \sqrt{P_x^2 + P_y^2 + P_z^2}\right) / 2 \\ &= \frac{1}{2} \pm \frac{1}{2} \sqrt{1 + 4|A|^2|B|^2(e^{-\sum_l |f_l - g_l|^2} - 1)}. \end{aligned} \quad (22)$$

From Eq. (20), it is clear that $P_y(t) = 0$ if and only if $A^* B e^{\sum_l f_l^* g_l}$ is a real number, a condition that is satisfied in the ground state (or ensemble averages) due to Hamiltonian invariance under the transformation $\sigma_y \rightarrow -\sigma_y$.⁶

III. NUMERICAL RESULTS

The spectral function (2) gives full information for the spin-bath coupling λ_l . Together with equations of motion (11)–(14), the dynamics of spin-boson model could be deduced for given specific initial conditions. The $|+\rangle$ state is usually populated at $t = 0$, i.e., $A(0) = 1$ and $B(0) = 0$. The initial conditions of the phonon bath are $f_l(0) = g_l(0) = 0$ and $f_l(0) = g_l(0) = -\lambda_l/2\omega_l$ for factorized and polarized initial conditions, respectively. We have to solve the $2N_b + 2$ equations of motion, Eqs. (11)–(14), together with the $2N_b + 2$ initial conditions mentioned above, where N_b is the number of the phonon modes considered.

We will adopt the homogeneous discretization procedure used in Ref. 40. The frequencies of the N_b harmonic modes are equally distributed in the frequency range $\omega \in [\omega_{\min}, \omega_{\max}]$ with spacing $\Delta\omega = \omega_{\max}/N_b$, so that $\omega_{\min} = \omega_1 = \Delta\omega$ and $\omega_l = l\Delta\omega$. The frequency spacing $\Delta\omega$ determines the Poincaré recurrence time $T_p = 2\pi/\Delta\omega$, which must be greater than any time scale of interest.^{41,42} Throughout this

work, we will use $N_b = 20\,000$ and $\omega_{\max} = 4\omega_c$, resulting in a recurrence time $T_p = 10\,000\pi$ that places our simulations at a safe distance from the Poincaré recurrence. Correspondingly, from the integration of the spectral density over ω ,

$$\sum_{l=1}^{N_b} \lambda_l^2 = \int_0^\infty d\omega J(\omega) \approx \sum_{l=1}^{N_b} J(\omega_l) \Delta\omega, \quad (23)$$

we obtain that $\lambda_l^2 = J(\omega_l) \Delta\omega$. It is found that under the factorized bath initial condition, the simulation results are insensitive to the number of phonon modes. Under the polarized initial condition, the number of the phonon modes has a considerable influence on the dynamics, which is especially true in the strong coupling regime. However, our numerical tests show that good convergence is reached when $N_b = 20\,000$ for the time periods considered.

As shown in Fig. 1, under the polarized initial condition, the population difference as a function of time, $P_z(t)$, manifests coherent oscillations even for very large couplings $\alpha = 0.3 \approx 13\alpha_c$, where $\alpha_c \approx 0.022$ ^{11,43} is the critical coupling for the quantum phase transition. It is clearly seen that oscillatory behavior emerges even for very strong coupling far beyond α_c . Furthermore, the characteristic oscillation frequency of $P_z(t)$ increases with increasing α . Our results agree with those of Kast *et al.* obtained using the real-time path integral Monte Carlo simulation.¹⁵ It is widely accepted that under the polarized initial condition, a quantum dissipative system such as the spin-boson model is expected to display classical over-damped behavior (or incoherent phase) at strong spin-bath couplings. Our results reveal that this is not the case for $0 < s < 0.5$. However, such apparent contradictions only appear for the polarized bath initial condition. For the factorized initial bath condition, the persistent coherence does not occur. The upper panel of Fig. 2 shows the population difference as a function of time under the factorized bath initial condition. It is found that the critical coupling strength for the coherent-incoherent transition is $\alpha_{\text{CI}}^{(f)} \approx 0.1 \approx 4.5\alpha_c$. In the lower panel of Fig. 2, we also plot the relative deviation²² of

FIG. 1. Under the polarized bath initial conditions, the time dependent population difference $P_z(t)$ for $s = 0.25$ ($\alpha_c \approx 0.022$) and $\Delta/\omega_c = 0.1$ is presented. Seven values of α are taken. The inset is a magnified figure for large couplings.

FIG. 2. Time dependent population difference $P_z(t)$ (upper panel) and relative deviation $\sigma(t)$ (lower panel) for $s = 0.25$ ($\alpha_c \approx 0.022$) and $\Delta/\omega_c = 0.1$ under the factorized bath initial conditions. Seven values of α are used for comparison.

the trial state $|D_s(t)\rangle$ defined as

$$\sigma(t) = \frac{\sqrt{\langle \delta(t) | \delta(t) \rangle}}{\bar{E}_{\text{bath}}}, \quad (24)$$

where $\bar{E}_{\text{bath}}$ denotes the average energy of bath within the time interval considered, and $|\delta(t)\rangle$ is the deviation vector quantifying how faithfully $|D_s(t)\rangle$ follows the Schrödinger equation:

$$|\delta(t)\rangle = (i\partial_t - \hat{H})|D_s(t)\rangle. \quad (25)$$

In other words, the smaller the relative deviation $\sigma(t)$, the more faithfully the trial state $|D_s(t)\rangle$ obeys the Schrödinger equation. To compare with the ML-MCTDH method, a calculation is carried out for four values of s . The upper panel of Fig. 3 shows the time-dependent population difference $P_z(t)$ for $\alpha = 0.2$, $\omega_c/\Delta = 5$, in good agreement with corresponding results in Ref. 17. As shown in the lower panel of Fig. 3, the relative deviation $\sigma(t)$ gradually increases with time before reaching a saturation value that has a strong dependence on the exponent s , indicating that the smaller the exponent s is, the more accurate our ansatz becomes.

Thus, the bath initial conditions play an important role in the dynamics of the sub-Ohmic spin-boson model. In Ref. 15, the authors studied out-of-equilibrium bath preparations with respect to the initial state of the spin. The polarized bath initial

FIG. 3. Time-dependent population difference $P_z(t)$ (upper panel) and relative deviation $\sigma(t)$ (lower panel) for $\alpha = 0.5$, $\omega_c/\Delta = 5$, and four values of the exponent s : $s = 0.25, 0.5, 0.75$, and 1. The factorized bath initial condition is taken.

condition corresponds to the case where the bath distribution is fully equilibrated with the initial state of the spin, while the factorized bath initial condition corresponds to the one most displaced from the equilibrium. We note that our results for $\alpha = 0.1$ in Fig. 1 and in the upper panel of Fig. 2 are consistent

FIG. 4. Population difference $P_z(t)$ as a function of time for $s = 0.25$ ($\alpha_c \approx 0.022$) and $\Delta/\omega_c = 0.1$ with polarized and factorized bath initial conditions.

FIG. 5. Von Neumann entropy calculated with the polarized bath initial condition for $s = 0.25$ ($\alpha_c \approx 0.022$) and $\Delta/\omega_c = 0.1$.

with those in Ref. 15, where it was found that compared with the polarized initial condition, the factorized one yields decreased oscillation frequency of the dynamics and increased initial loss in population (cf. the pink lines in Fig. 1 and the upper panel of Fig. 2).

An explicit comparison between the polarized and factorized initial conditions is given in Fig. 4, where substantial differences are revealed between the two bath initial conditions for $\alpha = 0.9\alpha_c$ and $\alpha = 1.3\alpha_c$. Under the factorized bath initial condition, the oscillations occur around $P_z = 0$ in both the localized and delocalized phases, and the population difference $P_z(t)$ is in a delocalized phase even for $\alpha > \alpha_c$, a parameter regime where the state is expected to be localized. In contrast, the oscillations occur around finite values of P_z even in the delocalized phase for the polarized initial condition. Also, the steady state value of $P_z(t)$ is an increasing function of α . Similar results are also found by Nalbach and Thorwart using the quasiadiabatic propagator path integral.¹¹

We also monitor the entanglement between the spin and the bath via the von Neumann entropy. At $t = 0$, the systems are in a separable state, so that $S(0) = 0$. Equation (21) mani-

FIG. 6. Von Neumann entropy calculated under with the factorized bath initial condition for $s = 0.25$ ($\alpha_c \approx 0.022$) and $\Delta/\omega_c = 0.1$.

festes that the entropy S increases monotonously with ω_+ from 0 and reaches its maximum at $\omega_+ = 1/2$, before decreasing monotonously to 0. Figures 5 and 6 show that there are substantial differences in the time evolution of the entropy under the polarized and factorized bath initial conditions. Under the polarized initial condition, overall the entropy decreases with an increase in α as shown in Fig. 5. For strong coupling strengths, the entropy eventually vanishes as expected.⁶ Under the factorized initial condition, the entropy establishes its steady state value quickly for various coupling strengths. Interestingly, the steady state value is not a monotonous function of α , and reaches its maximum at approximately $\alpha \approx 0.07$.

IV. CONCLUSIONS AND DISCUSSIONS

Although quite a number of numerical approaches have been applied to study the ground state and dynamical properties of the sub-Ohmic spin-boson model, few analytical treatments have been available. Recently, Chin *et al.*⁴³ used an extension of the Silbey-Harris variational wave function to study the ground state of the sub-Ohmic spin-boson model with $0 < s < 0.5$, and found that such a trial state generates correct mean-field exponents for the continuous localization-delocalization transition. The asymmetrically displaced-oscillator (ADO) trial state used in Ref. 43 is of the form,

$$|\psi\rangle_{\text{ADO}} = A|+\rangle \exp\left[\sum_l (f_l b_l^\dagger - h.c.)\right]|0\rangle_{\text{ph}} + B|-\rangle \exp\left[\sum_l (g_l b_l^\dagger - h.c.)\right]|0\rangle_{\text{ph}}, \quad (26)$$

where the variational parameters $A, B, f_l/s$, and g_l/s are all real numbers to be determined by the ground-state energy minimization. It is interesting to note that our ansatz, Eq. (6), gets reduced to Eq. (26) if we restrict all variational parameters to be real, and consequently, the Dirac-Frenkel variation employed in this work gets reduced to the conventional variational principle for the ground state used in Ref. 43. Therefore, we have successfully extended the static trial state of Eq. (26) to its dynamical counterpart, which is similar in form to the Davydov D_1 ansatz. The foregoing connection also helps in mapping out the validity regime of our ansatz. As pointed out by Nazir *et al.*, although the ADO state works well for the sub-Ohmic baths with $s < 0.5$, it becomes unstable and deviates from the well-established results for the Ohmic case and strong coupling (the cause of which is still under investigation).⁴⁴ Thus, it is expected that our ansatz reliably reveals the dynamics of the sub-Ohmic spin-boson model for $s \ll 1$, but may lose accuracy for large s .

For the sub-Ohmic spin-boson model with $0 < s < 1/2$, detailed dynamics in the strong coupling regime is still surrounded by contention. The hierarchy of the Davydov *Ansätze* of varying sophistication has been known to be competent in handling polaron dynamics in the strong coupling regime.^{22,23} Using a version of the most accurate of the hierarchy, the Davydov D_1 ansatz, we have carried out a time-dependent variational calculation with regard to the dynamic

properties of the sub-Ohmic spin-boson model. It is a simple, yet extremely efficient approach to investigate the dynamics of a quantum dissipative system, such as the population disparity $P_z(t)$ of the sub-Ohmic spin-boson model. Our results are consistent with those obtained using advanced numerical methods that are computationally much more expensive, such as the path integral Monte Carlo simulations^{11,15} and the ML-MCTDH technique.¹⁷ It is found that the bath initial conditions have considerable influence over the dynamics of this many-body dissipative system. Even in the very strong coupling regime, quantum coherence features still manage to survive under the polarized bath initial condition, while such features are absent under the factorized bath initial condition. The onset of the incoherent phase occurs at $\alpha = 0.1$ for $s = 0.25$ under the factorized bath initial condition. Our findings are consistent with those in Ref. 15, which first reported the persistence of coherent quantum dynamics at strong dissipation under the polarized bath initial condition. Furthermore, the Davydov D_1 ansatz has been employed successfully to study excitation energy transfer across light-harvesting complexes in photosynthesis.²⁴ Our approach may turn out to be a competitive tool to investigate sustained quantum coherence recently discovered to reside in pigment networks even at elevated temperatures.^{45–47}

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¹J. A. Leggett, *Rev. Mod. Phys.* **59**, 1 (1987).

²U. Weiss, *Quantum Dissipative Systems*, 3rd ed. (World Scientific, Singapore, 2007).

³P. Bocchieri and A. Loinger, *Phys. Rev.* **107**, 337 (1957); L. Barreira, "Poincaré recurrence: old and new," in *Proceedings of the Fourth International Congress on Mathematical Physics* (World Scientific, 2006), pp. 415–422.

⁴A. O. Caldeira and A. J. Leggett, *Physica A* **121**, 587 (1983).

⁵R. A. Marcus and N. Sutin, *Biochim. Biophys. Acta* **811**, 265 (1985); A. Garg *et al.*, *J. Chem. Phys.* **83**, 4491 (1985).

⁶T. A. Costi and R. H. McKenzie, *Phys. Rev. A* **68**, 034301 (2003); K. L. Hur, P. D. Beaupre, and W. Hofstetter, *Phys. Rev. Lett.* **99**, 126801 (2007).

⁷D. V. Khveshchenko, *Phys. Rev. B* **69**, 153311 (2004); M. Thorwart and P. Hanggi, *Phys. Rev. A* **65**, 012309 (2001).

⁸K. G. Wilson, *Rev. Mod. Phys.* **47**, 773 (1975).

⁹R. Bulla, N.-H. Tong, and M. Vojta, *Phys. Rev. Lett.* **91**, 170601 (2003); M. Vojta, N.-H. Tong, and R. Bulla, *ibid.* **94**, 070604 (2005); F. B. Anders, R. Bulla, and M. Vojta, *ibid.* **98**, 210402 (2007).

¹⁰N. Makri and D. E. Makarov, *J. Chem. Phys.* **102**, 4600 (1995); **102**, 4611 (1995); N. Makri, *J. Math. Phys.* **36**, 2430 (1995); M. Thorwart, P. Reimann, P. Jung, and R. F. Fox, *Chem. Phys.* **235**, 61 (1998); M. Thorwart, P. Reimann, and P. Hanggi, *Phys. Rev. E* **62**, 5808 (2000).

¹¹P. Nalbach and M. Thorwart, *Phys. Rev. B* **81**, 054308 (2010).

¹²A. Winter, H. Rieger, M. Vojta, and R. Bulla, *Phys. Rev. Lett.* **102**, 030601 (2009).

¹³A. Alvermann and H. Fehske, *Phys. Rev. Lett.* **102**, 150601 (2009).

¹⁴R. Egger and C. H. Mak, *Phys. Rev. B* **50**, 15210 (1994); L. Muhlbacher and J. Ankerhold, *J. Chem. Phys.* **122**, 184715 (2005); L. Muhlbacher, J. Ankerhold, and A. Komnik, *Phys. Rev. Lett.* **95**, 220404 (2005).

¹⁵D. Kast and J. Ankerhold, *Phys. Rev. Lett.* **110**, 010402 (2013).

¹⁶H. Wang and M. Thoss, *New J. Phys.* **10**, 115005 (2008).

¹⁷H. Wang and M. Thoss, *Chem. Phys.* **370**, 78 (2010).

¹⁸A. Lucke *et al.*, *J. Chem. Phys.* **107**, 8397 (1997).

¹⁹T. Holstein, *Ann. Phys.* **8**, 325 (1959); **8**, 343 (1959).

²⁰A. Scott, *Phys. Rep.* **217**, 1 (1992); A. S. Davydov, *Zh. Eksp. Teor. Fiz.* **78**, 789 (1980) [*Sov. Phys. JETP* **51**, 397 (1980)].

²¹Y. Zhao, D. W. Brown, and K. Lindenberg, *J. Chem. Phys.* **106**, 2728 (1997); **106**, 5622 (1997); **107**, 3159 (1997); **107**, 3179 (1997).

²²J. Sun, B. Luo, and Y. Zhao, *Phys. Rev. B* **82**, 014305 (2010); B. Luo, J. Ye, C. B. Guan, and Y. Zhao, *Phys. Chem. Chem. Phys.* **12**, 15073 (2010).

²³B. Luo, J. Ye, and Y. Zhao, *Phys. Status Solidi C* **8**, 70 (2011).

²⁴J. Ye *et al.*, *J. Chem. Phys.* **136**, 245104 (2012).

²⁵P. A. M. Dirac, *Proc. Cambridge Philos. Soc.* **26**, 376 (1930); J. Frenkel, *Wave Mechanics* (Oxford University Press, 1934).

²⁶Y. Zhao, S. Yokojima, and G. Chen, *J. Chem. Phys.* **113**, 4016 (2000).

²⁷I. Burghardt, H.-D. Meyer, and L. S. Cederbaum, *J. Chem. Phys.* **111**, 2927 (1999).

²⁸I. Burghardt, M. Nest, and G. A. Worth, *J. Chem. Phys.* **119**, 5364 (2003).

²⁹R. Martinazzo, M. Nest, P. Saalfrank, and G. F. Tantardini, *J. Chem. Phys.* **125**, 194102 (2006).

³⁰S. Sawada and H. Metiu, *J. Chem. Phys.* **84**, 227 (1986).

³¹D. V. Shalashilin and I. Burghardt, *J. Chem. Phys.* **129**, 084104 (2008).

³²M. H. Beck, A. Jackle, G. A. Worth, and H.-D. Meyer, *Phys. Rep.* **324**, 1 (2000).

³³G. A. Worth and I. Burghardt, *Chem. Phys. Lett.* **368**, 502 (2003).

³⁴K. Huang and A. Rhys, *Proc. R. Soc. London, Ser. A* **204**, 406 (1950).

³⁵N. Wu, K. W. Sun, Z. Chang, and Y. Zhao, *J. Chem. Phys.* **136**, 124513 (2012).

³⁶Y. Y. Zhang, Q. H. Chen, and K. L. Wang, *Phys. Rev. B* **81**, 121105(R) (2010).

³⁷C. H. Bennett *et al.*, *Phys. Rev. A* **54**, 3824 (1996); M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2004).

³⁸Y. Zhao, P. Zanardi, and G. H. Chen, *Phys. Rev. B* **70**, 195113 (2004); J. Sun, Y. Zhao, and W. Z. Liang, *ibid.* **79**, 155112 (2009).

³⁹L. Amico *et al.*, *Rev. Mod. Phys.* **80**, 517 (2008).

⁴⁰G. Stock, *J. Chem. Phys.* **103**, 1561 (1995).

⁴¹S. L. Lopez *et al.*, *J. Chem. Phys.* **134**, 014102 (2011).

⁴²K. H. Hughes *et al.*, *J. Chem. Phys.* **131**, 024109 (2009).

⁴³A. W. Chin *et al.*, *Phys. Rev. Lett.* **107**, 160601 (2011).

⁴⁴A. Nazir, D. P. S. McCutcheon, and A. W. Chin, *Phys. Rev. B* **85**, 224301 (2012).

⁴⁵G. S. Engel *et al.*, *Nature (London)* **446**, 782 (2007).

⁴⁶T. R. Calhoun *et al.*, *J. Phys. Chem. B* **113**, 16291 (2009).

⁴⁷E. Collini *et al.*, *Nature (London)* **463**, 644 (2010).