

## Quantum phase transitions in the spin-boson model: Monte Carlo method versus variational approach à la Feynman

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The effectiveness of the variational approach à la Feynman is proved in the spin-boson model, i.e., the simplest realization of the Caldeira-Leggett model able to reveal the quantum phase transition from delocalized to localized states and the quantum dissipation and decoherence effects induced by a heat bath. After exactly eliminating the bath degrees of freedom, we propose a trial, nonlocal in time, interaction between the spin and itself simulating the coupling of the two-level system with the bosonic bath. It stems from a Hamiltonian where the spin is linearly coupled to a finite number of harmonic oscillators whose frequencies and coupling strengths are variationally determined. We show that a very limited number of these fictitious modes is enough to get a remarkable agreement, up to very low temperatures, with the data obtained by using an approximation-free Monte Carlo approach, predicting (1) in the Ohmic regime, a Berezinski-Thouless-Kosterlitz quantum phase transition exhibiting the typical universal jump at the critical value; and (2) in the sub-Ohmic regime ( $s \leq 0.5$ ), mean-field quantum phase transitions, with logarithmic corrections for  $s = 0.5$ .

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*Introduction.* The spin-boson model is a paradigmatic minimal model used for describing the quantum phase transition (QPT) from delocalized to localized states induced by the environment [1–3]. It also plays a significant role in understanding the relaxation processes, in particular the dissipation and decoherence effects, in quantum systems [4,5]. The model consists of a two-level system, i.e., a single quantum qubit or spin, interacting with an infinite number of quantum oscillators whose frequencies and coupling strengths obey specific distributions. Due to its versatility, it can catch the physics of a large range of different physical systems going from defects in solids and quantum thermodynamics [6] to physical chemistry and biological systems [7–9]. It has been also used to study trapped ions [10], quantum emitters coupled to surface plasmons [11], quantum heat engines [12], or superconducting qubits strongly interacting with a set of individual microwave resonators that reside in a restricted frequency range [13]. In spite of its simplicity, an exact solution is not available and a variety of approximated approaches have been adopted to investigate the ground state physical properties of the quasi-particle formed by the two-level system surrounded by the virtual excitation cloud induced by the spin-bath coupling, i.e., the spin polaron [14–18]. Actually in the spin-boson model a quantum critical transition between localized and delocalized states is expected by increasing the coupling strength between

the two-level system and the bosonic bath [2]. In particular, in the Ohmic regime and for finite values of the bath cutoff, in the literature there are predictions on this QPT, inferred from the mapping between the spin-boson model and the Kondo model that is based on the well-known equivalences between Fermi and Bose operators in one dimension that, in turn, are strictly valid only in the limit of a divergent cutoff [1,19]. In this Rapid Communication we solve this long-standing problem, definitely determining the nature of the QPT and the exact values of the critical couplings by using two different approaches at finite temperature. The first one is unbiased, exact from the numerical point of view, and based on the worldline Monte Carlo (MC) technique. The other one is variational and based on the idea of Feynman to describe the charge polaron in the Fröhlich model [20]. We predict (1) in the Ohmic regime, a Berezinski-Thouless-Kosterlitz (BTK) QPT exhibiting the typical universal jump at the critical value; and (2) in the sub-Ohmic regime ( $s \leq 0.5$ ), mean-field quantum phase transitions, with logarithmic corrections for  $s = 0.5$ .

We emphasize that the variational approaches present in the literature are limited to zero temperature, and none of them is able to correctly describe the BTK QPT in the Ohmic regime for finite values of the bath cutoff. In this Rapid Communication we introduce a variational approach at finite temperature providing an excellent description of different quantities of physical interest at the thermodynamic equilibrium. It borrows from the idea of Feynman, based on the path integrals, to describe the charge polaron. In the Fröhlich

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model, the high accuracy of the predicted free energy, polaron mass, and optical properties by the Feynman approach has been confirmed by numerically exact methods [21–23]. Here we use a variational approach à la Feynman in the spin-boson model. After exactly eliminating the bath degrees of freedom, in analogy with the charge-polaron problem, we introduce a simple trial retarded interaction between the spin and itself simulating the true retarded spin-bath interaction. It stems from a not exactly solvable model Hamiltonian where the spin is coupled to a finite number of harmonic oscillators whose frequencies and coupling strengths are variationally determined. The comparison with the approximation-free MC approach shows that a very limited number of these fictitious modes is enough to correctly describe, up to very low temperatures, any physical property. In particular, we show that the more one increases the number of fictitious harmonic oscillators, simulating the coupling with the bath, the more one is able to correctly describe the relevant physical properties at lower and lower temperatures, correctly predicting the QPT in both the Ohmic and sub-Ohmic regimes for any value of the bath cutoff.

*The model.* The spin-boson Hamiltonian is written as

$$H = H_Q + H_B + H_I, \quad (1)$$

where (1)  $H_Q = -\frac{\Delta}{2}\sigma_x$  represents the free qubit contribution: here  $\Delta$  is the tunneling matrix element; (2)  $H_B = \sum_i \omega_i a_i^\dagger a_i$  describes the bath, modeled by means of a collection of bosonic oscillators of frequencies  $\omega_i$ ; and (3)  $H_I = \sigma_z \sum_i \lambda_i (a_i^\dagger + a_i)$  is the spin-bath interaction:  $\lambda_i$  represents the coupling strength with the  $i$ th oscillator. In Eq. (1),  $\sigma_x$  and  $\sigma_z$  are Pauli matrices with eigenvalues 1 and  $-1$ , and  $a_i$  and  $a_i^\dagger$  denote bosonic creation and annihilation operators. The spin-bath couplings  $\lambda_i$  are determined by the spectral function  $J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i) = \frac{\alpha}{2} \omega_c^{1-s} \omega^s \Theta(\omega_c - \omega)$ , where  $\omega_c$  is a cutoff frequency. Here the adimensional parameter  $\alpha$  measures the strength of the coupling, while the parameter  $s$  distinguishes among the three different kinds of dissipation: Ohmic ( $s = 1$ ), sub-Ohmic ( $s < 1$ ), and super-Ohmic ( $s > 1$ ). We use units such that  $\hbar = k_B = 1$ .

*The methods.* We investigate the physical features of this Hamiltonian, at thermal equilibrium, by using two different approaches. The first of them is based on the path integral technique. Here the elimination of the bath degrees of freedom leads to an effective Euclidean action [2,24]:

$$S = \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \sigma_z(\tau) K(\tau - \tau') \sigma_z(\tau'), \quad (2)$$

where the kernel is expressed in terms of the spectral density  $J(\omega)$  and the bath propagator:  $K(\tau) = \int_0^\infty d\omega J(\omega) \frac{\cosh[\omega(\frac{\beta}{2} - \tau)]}{\sinh(\frac{\beta\omega}{2})}$ . In particular, for  $\frac{1}{\omega_c} \ll \tau \ll \beta/2$ , it has the behavior  $K(\tau) \simeq \frac{\alpha(\omega_c)^{1-s} \Gamma(1+s)}{2\tau^{1+s}}$ , that for  $s = 1$  becomes simply  $K(\tau) = \frac{\alpha}{2\tau^2}$ . The functional integral has to be done, with Poissonian measure, over all the possible piecewise constant functions, i.e., the worldlines  $\sigma_z(\tau)$ , with values 1 and  $-1$ , periodic of period  $\beta = 1/T$ , where  $T$  is the system temperature. We emphasize that  $\beta$  represents the size of the classical interacting spin system. An efficient sampling of the path integral can be performed adopting a cluster algorithm [24–26], based on the Swendsen and Wang

approach [27]. The critical properties of the spin-boson model in the sub-Ohmic regime have been successfully investigated through this MC technique [24]. Here we extend this kind of calculation to the Ohmic regime. We emphasize that this approach is exact from a numerical point of view and it is equivalent to the sum of all the Feynman diagrams. It will be used also as a test for the variational approach described below.

The second method is based on the variational principle and it is strictly related to the approach introduced by Feynman within the Fröhlich model [20]. For the sake of clarity we resume the main steps. In general, in a many-body problem, one uses the Feynman-Dyson perturbation theory [28,29] starting from the Hamiltonian without interactions, so the more the strength of the coupling increases, the more the number of Feynman diagrams to be considered increases. To overcome this difficulty, in the charge polaron problem, Feynman introduced, as a starting point for the perturbation theory, a smart variational action that the expansion to the first order is already enough to obtain an excellent description of the physics for arbitrary coupling strength. Here we follow this idea. We adopt the ordered operator calculus [30], i.e., the operator equivalent of the Feynman path integral [31]. The first step is the calculation of the partition function [28,29]  $Z = \text{Tr}[e^{-\beta H}] = Z_0 U(\beta)$ , where  $U(\beta) = \langle T_\tau e^{-\int_0^\beta d\tau H_I^{(0)}(\tau')} \rangle_0$ . Here  $Z_0$  is the free partition function (related to  $H_0 = H_Q + H_B$ ),  $T_\tau$  is the time ordering operator,  $H_I^{(0)}$  represents the Hamiltonian  $H_I$  in the interaction representation, and  $\langle \dots \rangle_0$  denotes the ensemble average with respect to  $H_0$ . By choosing, for the trace, the basis of  $H_0$  (it is factorized), it is possible to exactly eliminate the bath degrees of freedom by using the Bloch-DeDominicis theorem [28,29]. The partition function becomes

$$Z = Z_Q Z_B \langle T_\tau e^\phi \rangle_Q, \quad (3)$$

where

$$\phi = \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \sigma_z^{(0)}(\tau) K(\tau - \tau') \sigma_z^{(0)}(\tau'). \quad (4)$$

Note that, in Eq. (3), the ensemble average is with respect to  $H_Q$  and that, differently from the path-integral representation, i.e., Eq. (2), in Eq. (4) spin operators and not their eigenvalues appear. So far no approximation has been used. In order to go ahead with the calculation, one can expand the exponential and use the standard perturbation theory in the many-body problem. In order to avoid evaluating a huge number of diagrams when the coupling with the bath increases, we follow Feynman's idea and introduce a trial Hamiltonian ( $H_{\text{tr}}$ ), where we replace the bath, characterized by a continuum distribution of harmonic oscillators, with a discrete collection of  $N$  bosonic fictitious modes:

$$H_{\text{tr}} = H_Q + \sum_{i=1}^N \tilde{\omega}_i b_i^\dagger b_i + \sigma_z \sum_{i=1}^N \tilde{\lambda}_i (b_i^\dagger + b_i), \quad (5)$$

where the parameters  $\tilde{\omega}_i$  and  $\tilde{\lambda}_i$  have to be variationally determined as specified in the following. Also in this case, due to the linearity of the coupling term, we can exactly eliminate

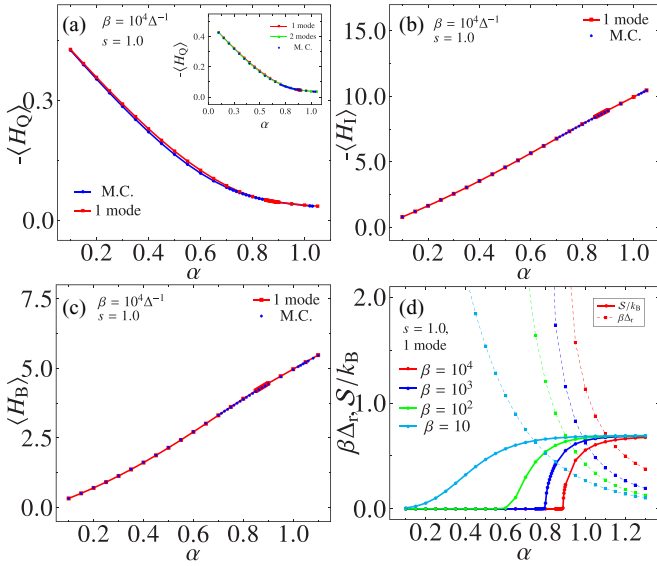


FIG. 1. (a), (b), and (c)  $-\langle H_Q \rangle$ ,  $-\langle H_I \rangle$ , and  $\langle H_B \rangle$  (measured with respect to the value in the absence of interaction), in units of  $\Delta$ , vs  $\alpha$  for  $\omega_c = 10\Delta$ : comparison between the MC method and the variational approach with one fictitious mode (in the inset  $-\langle H_Q \rangle$  for  $N = 2$ ); (d)  $\Delta_r/T$  (dashed line) and the entropy (solid line) vs  $\alpha$ .

the bosonic degrees of freedom, getting

$$Z_{\text{tr}} = Z_Q Z_{B_{\text{tr}}} \langle T_{\tau} e^{\phi_{\text{tr}}} \rangle_Q, \quad (6)$$

where

$$\phi_{\text{tr}} = \frac{1}{2} \int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sigma_z^{(0)}(\tau) K_{\text{tr}}(\tau - \tau') \sigma_z^{(0)}(\tau'), \quad (7)$$

and  $K_{\text{tr}}(\tau)$  contains the propagator of these trial modes and the coupling strengths:  $K_{\text{tr}}(\tau) = \sum_{i=1}^N \tilde{\lambda}_i^2 \frac{\cosh[\tilde{\omega}_i(\frac{\beta}{2} - \tau)]}{\sinh(\frac{\beta \tilde{\omega}_i}{2})}$ . Now it is straightforward to prove that the second derivative of the function  $f(x) = -T \ln \langle T_{\tau} e^{\phi_{\text{tr}} + x(\phi - \phi_{\text{tr}})} \rangle_S$  is negative for any value of  $x$  in the range  $[0, 1]$  [32]. This property gives rise to the following inequality:  $f(x=1) - f(x=0) \leq f'(x=0, 0)$ , i.e., an upper bound for the free energy  $F = -T \ln Z$ :

$$F - F_B \leq F_{\text{tr}} - F_{B_{\text{tr}}} - T \frac{\langle T_{\tau} e^{\phi_{\text{tr}}} (\phi - \phi_{\text{tr}}) \rangle_Q}{\langle T_{\tau} e^{\phi_{\text{tr}}} \rangle_Q}. \quad (8)$$

This is exactly the same inequality found by Feynman within the Fröhlich model (Feynman-Jensen inequality) [20,33]: it is a generalization of the well-known Bogoliubov inequality [33]. We emphasize that, in this variational formulation, only the free energy of the model Hamiltonian and the first correction enter. The knowledge of the eigenvalues and eigenvectors of  $H_{\text{tr}}$ , through numerical diagonalization [34,35], allows us to calculate the right side of Eq. (8) [36] and then the parameters  $\tilde{\omega}_i$  and  $\tilde{\lambda}_i$ . Finally, by considering the partial derivative of the free energy with respect to  $\Delta$ ,  $\omega_i$ , and  $\lambda_i$ , and replacing, at the end of the calculation,  $\phi$  with  $\phi_{\text{tr}}$ , it is possible to obtain the average values of the three terms of the Hamiltonian, i.e.,  $\langle H_Q \rangle$ ,  $\langle H_B \rangle$ , and  $\langle H_I \rangle$ .

*The results.* We first focus our attention on the most interesting case from the physical point of view, i.e., Ohmic regime  $s = 1$ . In Figs. 1(a), 1(b), and 1(c), we plot  $-\langle H_Q \rangle$ ,

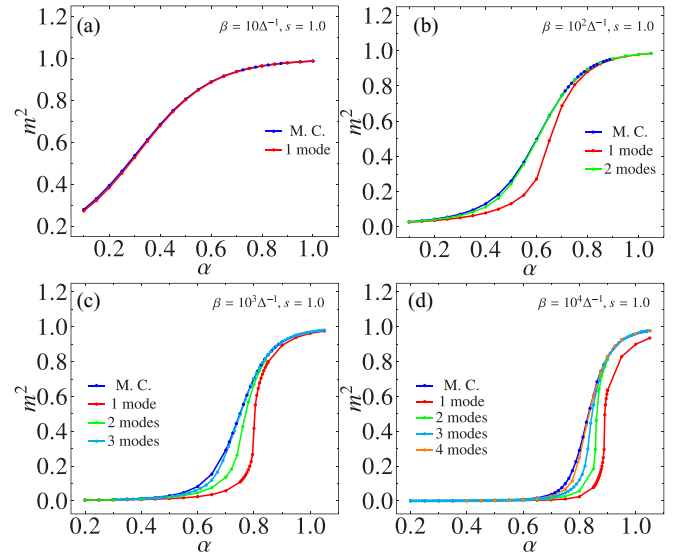


FIG. 2.  $m^2$  vs  $\alpha$  for four temperatures: comparison between the MC method and the variational approach with different fictitious modes for  $\omega_c = 10\Delta$ .

$-\langle H_I \rangle$ , and  $\langle H_B \rangle$ , respectively, as a function of  $\alpha$ , at  $T = 10^{-4}\Delta$ , by using only one fictitious mode [ $N = 1$  in Eq. (5)]. As expected, by increasing the coupling spin-bath strength  $\alpha$ ,  $-\langle H_Q \rangle$  reduces, indicating a progressive decrease of the tunneling between the two spin levels, whereas  $\langle H_B \rangle$  and the absolute value of  $\langle H_I \rangle$  increase. It is also clear that the Feynman picture provides very good estimates of the average values at thermal equilibrium independently of the value of the coupling  $\alpha$ . We emphasize that, for a fixed  $N$ , the agreement between the two approaches improves more and more by increasing the temperature. By fixing  $T$ , the very small differences between the two approaches practically vanish by increasing the number of fictitious modes [see inset of Fig. 1(a)]. In Fig. 1(d) we plot the gap between the first two eigenvalues of the model Hamiltonian,  $\Delta_r$ , scaled with  $T$ , and the thermodynamic entropy as a function of  $\alpha$ , for different temperatures and  $N = 1$ . The plot points out that, at any temperature, there is a value of  $\alpha$  where  $\Delta_r$  becomes smaller than  $T$  and, at the same time, the entropy increases from zero to  $\ln 2$ . This behavior suggests the presence of an incipient QPT. Actually, the existence of a QPT in the spin-boson model has been largely debated in literature [1,37,38]. Usually the critical properties are inferred from the mapping between the spin-boson and Kondo model that is based on the well-known equivalences between Fermi and Bose operators in one dimension that, in turn, are strictly valid only in the limit of  $\omega_c \rightarrow \infty$  [1,19]. It is also worth noting that the renormalization-group equations of the two models are identical [39,40]. On the basis of these reasonings, it is generally believed that, at  $s = 1$ , the QPT belongs to the class of BTK transitions with a critical value of  $\alpha$ ,  $\alpha_c$ , around 1. In order to clarify the existence of a QPT and characterize it, we study the temperature dependence of the squared magnetization  $m^2 = \frac{1}{\beta} \int_0^{\beta} d\tau \langle \sigma_z(\tau) \sigma_z(0) \rangle$ . In Fig. 2 we plot  $m^2$  as a function of  $\alpha$  for different temperatures. The behavior of  $m^2$ , from about 0 to about 1 by increasing the coupling strength, in a steeper and

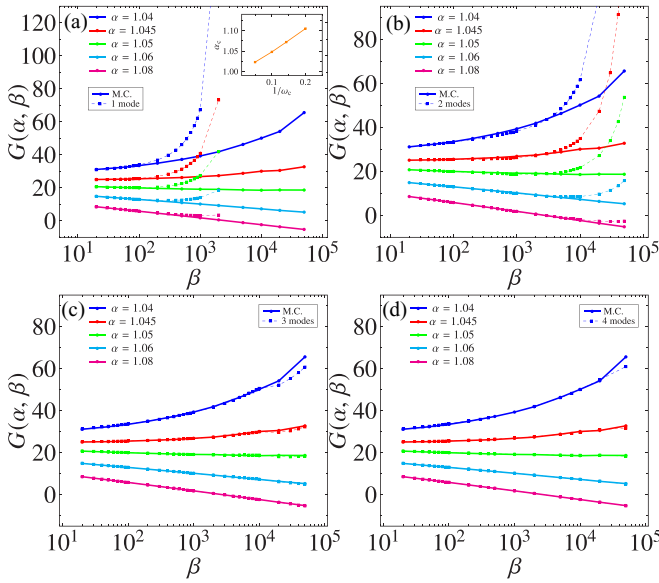


FIG. 3. The function  $G(\alpha, \beta)$  vs  $\beta$  for five values of  $\alpha$  around  $\alpha_c$ : comparison between the MC method and the variational approach with different fictitious modes for  $\omega_c = 10\Delta$ . In the inset  $\alpha_c$  vs  $1/\omega_c$ .

steeper way by lowering  $T$ , signals again an incipient QPT. Indeed, in the BTK transition, the quantity  $m^2$  should exhibit a discontinuity, just at  $\alpha_c$ , for  $T = 0$  [41,42]. The plots point out that the variational approach provides excellent agreement with the numerically exact data of the MC method, although one has to introduce more and more modes by decreasing the temperature.

In order to get a precise estimation of  $\alpha_c$ , we adapt the approach suggested by Minnhagen *et al.* in the framework of the  $X$ - $Y$  model, where the logarithmic behavior of the chirality as a function of the system size at the critical point is exploited [43,44]. In the present context, the roles of the chirality and the lattice size are played by squared magnetization and inverse temperature  $\beta$ , respectively. Defining the scaled order parameter  $\Psi(\alpha, \beta) = \alpha m^2$ , the BTK theory predicts

$$\frac{\Psi(\alpha_c, \beta)}{\Psi_c} = 1 + \frac{1}{2(\ln \beta - \ln \beta_0)}, \quad (9)$$

where  $\beta_0$  is the only fitting parameter and  $\Psi_c = \Psi(\alpha_c, \beta \rightarrow \infty)$  is the universal jump that is expected to be equal to 1. In this scenario, the function  $G(\alpha, \beta) = \frac{1}{\Psi(\alpha, \beta) - 1} - 2 \ln \beta$  should not show any dependence on  $\beta$  at  $\alpha = \alpha_c$ . In order to test the validity of this scenario, in Fig. 3 we plot the function  $G(\alpha, \beta)$  as a function of  $\ln \beta$  for different values of  $\alpha$  around 1. The plots clearly show that there is a value of  $\alpha$  such that  $G$  is independent of  $\beta$ . It determines  $\alpha_c$ , that, for  $\omega_c = 10\Delta$ , turns out to be about 1.05. In the inset of Fig. 3(a) we plot the value of  $\alpha_c$  for different values of  $\omega_c$ . The data point out that  $\alpha_c$  is always greater than 1 and tends to 1 only when  $\omega_c \rightarrow \infty$ . We emphasize that  $\Psi_c = 1$  and  $\alpha_c > 1$  imply  $m^2 < 1$  for  $\alpha > \alpha_c$  and  $T = 0$ . The presence of residual tunneling, due to a not full magnetization, explains why  $\langle H_Q \rangle$ , in Fig. 1(a), assumes, for  $\alpha > \alpha_c$ , a finite value different from zero. It is also worth noting that four fictitious bosonic modes, variationally determined á la Feynman, provide excellent agreement with the

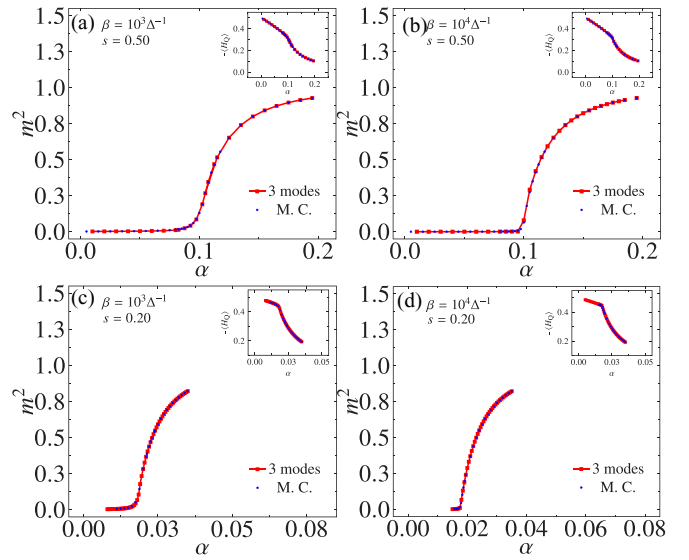


FIG. 4.  $m^2$  vs  $\alpha$  for two different values of  $s$ :  $s = 0.5$  in (a) and (b), and  $s = 0.2$  in (c) and (d). In the insets  $-\langle H_Q \rangle$ , in units of  $\Delta$ , vs  $\alpha$ . Comparison between the MC method and the variational approach à la Feynman for  $\omega_c = 10\Delta$ .

numerically exact MC data, even around the critical value of the spin-bath coupling, up to  $T \simeq 10^{-4} - 10^{-5} \Delta$ . This confirms the power of this variational approach: in this regard, it is worth mentioning that, so far, there is no other variational formulation, based on the wave functions and without using the time-ordered operators, able to restore the above found variational results.

In Fig. 4, we plot  $m^2$  and  $-\langle H_Q \rangle$  vs  $\alpha$  at two different values of  $\beta$ , for  $s = 0.5$  and  $s = 0.2$ , i.e., sub-Ohmic regime [26]. The variational approach á la Feynman with three fictitious modes provides remarkable agreement with the MC data, again confirming the effectiveness of this approach in any regime and for any value of the spin-bath coupling. Furthermore we emphasize that our data are in perfect agreement with the results obtained by Winter *et al.* [24] both at  $s = 0.2$  and  $s = 0.5$ . In particular, the finite  $\beta$  scaling analysis for  $s = 0.5$  points out the presence of logarithmic corrections to the mean-field theory.

**Conclusion.** We investigated the spin-boson model by using two different approaches: one unbiased, exact from the numerical point of view and based on the worldline MC technique, and the other one variational and based on the method proposed by Feynman to treat the charge polaron problem. We proved that this variational approach is extremely powerful and efficient providing an excellent description of the physical features of the spin polaron in any regime. In particular, we confirmed that, within the Ohmic regime, a BTK quantum phase transition sets in, proving that  $\alpha_c > 1$  and  $\alpha_c \rightarrow 1$  when  $\omega_c \rightarrow \infty$ . These results can open the way to the study of out-of-equilibrium properties [45,46], such as ultrafast processes and dynamics in the presence of strong driving fields, where standard perturbation theories fail. Work in this direction is in progress.

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