Real-Time-RG Analysis of the Dynamics of the Spin-Boson Model

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(March 21, 2022)

Using a real-time renormalization group method we determine the complete dynamics of the spin-boson model with ohmic dissipation for coupling strengths α ≲ 0.1 − 0.2. We calculate the relaxation and dephasing time, the static susceptibility and correlation functions. Our results are consistent with quantum Monte Carlo simulations and the Shiba relation. We present for the first time reliable results for finite cutoff and finite bias in a regime where perturbation theory in α or in tunneling breaks down. Furthermore, an unambiguous comparison to results from the Kondo model is achieved.

Introduction. The spin-boson model is one of the most fundamental quantum dissipative systems [1,2]. It plays an important role in describing defect tunneling in solids [3,4], quantum tunneling between flux states in a SQUID [5], electron tunneling between quantum dots [6], or electron transfer in chemical and biological reactions [7]. The latter is known as the noninteracting blip [8]. The latter exactly using numerical renormalization group (NRG) [9], Bethe ansatz [10], or conformal field theory (CFT) [11]. However, NRG and Bethe ansatz provide only spectral properties or dynamics at very short time scales [7], and CFT has solved so far only the unbiased case ε = 0 for the diagonal elements of p(t). Furthermore, and most importantly, the mapping on the Kondo model can not be proven rigorously, and the relation of the parameters is not precisely known [2,18]. It is known that the mapping is incorrect for finite cutoff D, but it is at least established that the scaling behaviour agrees with that of the spin-boson model [2,3,4,10].

In this paper, we will present for the first time a solution of the complete dynamics of the spin-boson model for α ≲ 0.1 − 0.2. We study the diagonal and nondiagonal part of the reduced density matrix p(t) starting from an arbitrary nonequilibrium state p₀. From the asymptotic behaviour we determine the relaxation and dephasing time. Furthermore, we calculate the spin susceptibility and correlation functions. Especially, and in contrast to many other methods, we solve directly the spin-boson model and present results at finite cutoff D and finite bias ε. Therefore, our results provide for the first time the possibility for a quantitative and unambiguous comparison to results obtained from the mapping of the spin-boson model on the Kondo model. We find that for ε = 0 the relaxation parameters agree with those of CFT and in the scaling limit the susceptibility agrees rather well with Bethe-ansatz results, but for the latter deviations occur at finite bias. To demonstrate the reliability of our results, we show the consistency with chromostochastic quantum dynamics (CSQD) [11], and check the Shiba-relation as well as the scaling behaviour.

To obtain our results, we will use a recently developed real-time renormalization group (RTRG) method [13,20]. This method has been successfully applied to equilibrium problems [19,21], and to the study of nonequilibrium stationary states [23]. Here we will apply it for the first time to the dynamics of the reduced density matrix, and generalize it to the evaluation of correlation functions as
well. Since this technique is rather straightforward and easily generalized to other models, this may open a new possibility for the study of various kinds of dissipative quantum systems, like e.g. many-level systems, magnetic nanoparticles interacting with phonons, coupled quantum dots or other kinds of dissipative environments.

Kinetic equation and RTRG approach. The RTRG approach is based on a kinetic equation for the density matrix, see Ref. [20] for details. We only mention the main steps:

1. The time evolution of the reduced density matrix is written in Liouville space as
   
   \[ p(t) = \text{Tr}_B \exp(-iLt) p_0 \rho_Z^B, \]
   
   where \( \text{Tr}_B \) denotes the trace over the bath degrees of freedom, and \( L = [H, \cdot] = L_0 + L_B + L_V \) is the Liouville operator. The initial density matrix is assumed to decouple into an arbitrary nonequilibrium distribution \( p_0 \) for the two-level system and an equilibrium distribution \( \rho_Z^B \) for the oscillator bath.

2. The propagator \( \exp(-iLt) \) is expanded in the interaction part \( L_V \), and the trace \( \text{Tr}_B \) over the bath degrees of freedom is performed by application of Wick’s theorem. In this way we obtain a series of terms where vertices \( G_p \) of the local system (originating from the \( \sigma_z/2 \) factor in \( V \)) are connected by pair contractions \( \gamma_{pp'}(t) \) of the bath. Here, \( p = \pm \) indicates wether the interaction takes place on the forward or the backward propagator. With \( j = \sum_q g_q (a_q^+ + a_q) \) and \( \gamma(t) = \text{Tr}_B \rho_Z^B j(t) \), we obtain
   
   \[ \gamma_{pp'}(t) = R(t) + iS(t), \]
   
   where we restricted ourselves to the physically relevant situation \( D \gg T \).

3. From the diagrammatic language one can derive a formally exact kinetic equation for \( p(t) \)
   
   \[ \dot{p}(t) + iL_0 p(t) = \int_0^t dt' \Sigma(t-t') p(t'), \]
   
   where \( \Sigma(t-t') \) is a superoperator acting on \( p(t') \) and is defined by the sum over all irreducible diagrams. In Laplace space we get the formal solution
   
   \[ p(z) = \Pi(z) p_0 \]
   
   with \( \Pi(z) = i/(z - L_0 - i \Sigma(z)) \).

4. The kernel \( \Sigma(z) \) is calculated by a renormalization group procedure. Short time scales of \( \gamma(t) \) are integrated out first by introducing a short-time cutoff \( t_c \) into the correlation function \( \gamma(t) \rightarrow \gamma(t, t_c) \). In each renormalization group step, the time scales between \( t_c \) and \( t_c + dt_c \) are integrated out, starting from \( t_c = 0 \) and ending at \( t_c = \infty \). As a consequence, one generates RG equations for \( \Sigma(z), L_0, G_p \), and the two boundary vertex operators \( A^p \) and \( B^p \) (defined as the rightmost and leftmost vertex of the kernel \( \Sigma(z) \)). Within the scheme of a perturbative RG analysis, generation of multiple vertex-operators is neglected here, as in Ref. [22].

For the present model, we choose the cutoff dependence either as \( \gamma(t, t_c) = \gamma(t) \Theta(t-t_c) \) (choice I) or

\[ \gamma(t, t_c) = \frac{d}{dt} \left( \tilde{R}(t) \Theta(t-t_c) \right) + iS(t) \Theta(t-t_c), \]

with \( R(t) = (d/dt) \tilde{R}(t) \) (choice II). It turns out that choice I is better for \( t_c > \Delta \), whereas choice II is needed for small \( t_c \) in order to avoid unphysical linear dependencies on the cutoff \( D \). At \( t_c = 0 \) we use a smooth crossover from choice I to choice II. Solving the RG equations numerically gives the kernel \( \Sigma(z) \) in Laplace space, and the reduced density matrix can be deduced. The static susceptibility follows from \( \chi_0 = - (d/d\epsilon) \text{Tr}_0 \Sigma_{zz} \), where \( \text{Tr}_0 \) is the trace over the local system, and \( p_{st} \) denotes the stationary solution \( p_{st} = \lim_{t \rightarrow \infty} p(t) \).

5. To calculate correlation functions of the form
   
   \( \chi(t) = \frac{1}{2} \text{Tr} \{ \sigma_z(t), \sigma_z \sigma_{eq} \} \)
   
   we have to generalize the RG procedure. With \( C = G^+ + G^- \) we get in Laplace space

\[ \chi(z) = \text{Tr}_0 \{ \sigma_z \Pi(z) (C + \Sigma_C(z)) p_{st} \}, \]

where \( \Sigma_C(z) \) is analogously defined to \( \Sigma(z) \) but contains the “vertex” \( C \) at any time point. Within the framework of Ref. [20], the RG equation for \( \Sigma_C(z) \) can be easily derived and reads

\[ \frac{d}{dt_c} \Sigma_C(z) = \sum_{pp'} \int_0^\infty dt \int_0^t dt' \frac{d}{dt_c} \gamma_{pp'}(t, t_c), \]

where \( B^p = B^p|_{z=0} \).

Results. Figs. 1 and 2 show the time evolution of \( p(t) \) for the unbiased and biased case. Initially, the two-level system is prepared in the spin-up state \( (u) \). For \( \epsilon = 0 \), we achieve a very good agreement with CSQD. Only the real parts of the nondiagonal elements, which correspond to \( \langle \sigma_z \rangle \), exhibit a deviation of approximately 5%. However, the CSQD cannot give an accurate error for \( \langle \sigma_z \rangle \) [23]. The diagonal elements oscillate in time with the frequency \( \Delta_r \sim \Delta (\Delta/D)^{\alpha/(1-\alpha)} \). This agrees with the renormalized tunnel matrix element, which is the characteristic energy scale of the spin boson model [24]. In Fig. 1 we obtain \( \Delta_r = 0.626 \Delta \) (CFT gives \( \Delta_r = 0.625 \Delta \)). In contrast, the real part of the nondiagonal elements is purely decaying for \( \epsilon = 0 \) (only for \( \epsilon \neq 0 \) it also exhibits oscillations). In the scaling limit, i.e. for \( D, \Delta \rightarrow \infty \) such that \( \Delta_r = \text{const} \), the diagonal elements are universal, i.e. they only depend on \( \Delta_r, t \). The nondiagonal elements however have an extra factor of \( \Delta_r/\Delta \) (see inset in Fig. 1) which is consistent with [24]. The long-time behaviour is given by an exponential decay. For \( \epsilon = 0 \) the decay constants of the diagonal (nondiagonal) elements correspond to the relaxation (dephasing) time \( \tau^{rel} (\tau^{dep}) \), see insets in Fig. 1. For \( \tau^{rel} \) we find good agreement with
susceptibility \( \chi \) increases with frequency but fails for \( \omega = \omega_0 \) for a maximum. We note that our results for the correlation functions which demonstrate that the commonly used relation \( \chi' \sim 1/T \) has already an error of 25\% concerning the Shiba-relation and only gives data for the unbiased case. Like the static susceptibility, the correlation function depends strongly on the cutoff \( D \) and the dephasing time are the first ones presented in the literature.

For coupling parameters \( \alpha < 1 \) we obtained for the biased case. A quantitative comparison with recent Bethe ansatz results for the Kondo model shows a very good agreement for the unbiased case (see inset in Fig. 3). However, in the scaling limit the susceptibility is universal. We normalize our results using the zero-temperature value \( \chi_0(T = 0) \). For \( \epsilon = 0 \), the susceptibility is a monotonous function, whereas a local maximum is obtained for the biased case. A quantitative comparison with recent Bethe ansatz results for the Kondo model shows a very good agreement for the unbiased case (see inset in Fig. 3). However, in the scaling limit the susceptibility

The static susceptibility for the unbiased and biased case is shown in Figs. 3 and 4. Clearly, the susceptibility depends strongly on the cutoff \( D \) (see right inset in Fig. 4). For coupling parameters \( \alpha < 0.1 \), we achieved a very good agreement (error smaller than 5\%). Like the static susceptibility, the correlation function depends strongly on the cutoff \( D \), but in the scaling limit, the normalized quantity \( S(\omega)/S(0) \) depends only on \( \omega/\omega_{\text{max}} \) (see inset in Fig. 4), where \( \omega_{\text{max}} \sim \Delta_r \) denotes the frequency where \( S(\omega) \) is maximum. We note that our results for the correlation function are the first ones presented for the spin-boson model for \( \alpha = 0.1 \). NRG results [14] are very accurate for low frequency but fail for \( \omega \sim \Delta_r \). Flow equation methods have already an error of \( \Delta_r \) concern the Shiba-relation [13], and CSQD does not provide a check of the Shiba-relation and only gives data for the unbiased case \( \epsilon = 0 \). [13]

In summary, we investigated the spin-boson model for ohmic dissipation using real-time renormalization group. For coupling parameters \( \alpha \sim 0.1 - 0.2 \) we achieved a full solution of the static and dynamical properties. We calculated the real-time evolution of all matrix elements of the reduced density matrix together with the static susceptibility and correlation functions. In contrast to previous works we are not restricted to zero bias or the scaling limit. The restriction in \( \alpha \) is due to the fact that we neglected double vertex diagrams. Our results show that the RTRG method is a very flexible tool to treat various kinds of dissipative quantum systems.

**Acknowledgments.** We acknowledge useful discussions with K. Schönhammer and U. Weiss. We also thank J. T. Stockburger and T. A. Costi for their numerical data. This work was supported by the "Deutsche Forschungsgemeinschaft" as part of "SFB 345" (M.K.) and "SFB 195" (H.S.).

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FIG. 1. Real part of $p(t)$ for $\alpha = 0.1$, $\epsilon = 0$, $D = 100\Delta$ and $T = 0$. Solid lines: RTRG. Dashed lines: CSQD; Inset: Rescaled real part of $p(t)$. Solid lines: $D = 100\Delta$. Dashed lines: $D = 1000\Delta$.

FIG. 2. Real part of $p(t)$ for $\alpha = 0.1$, $\epsilon = 0.1\Delta$, $D = 100\Delta$ and $T = 0$; Left inset: $\tau^{rel}$ as a function of $\alpha$ for $D = 100\Delta$ and $T = 0$. Solid line: $\epsilon = 0$. Dashed line: $\epsilon = 0.5\Delta$. Long dashed line: CFT, $\epsilon = 0$; Right inset: $\tau^{dep}$ as a function of $\alpha$ for $D = 100\Delta$ and $T = 0$. Solid line: $\epsilon = 0$. Dashed line: $\epsilon = 0.5\Delta$.

FIG. 3. Static susceptibility as a function of temperature for $\epsilon = 0$, $D \gg \Delta$, and $\alpha = 0.01,0.05,0.1,0.125,0.2$ (from top to bottom); Left inset: $\alpha = 0.125$. Solid line: RTRG. Dashed line: Bethe ansatz; Right inset: Cutoff dependence for $\alpha = 0.1$. Solid line: $D = 100\Delta$. Dashed line: $D = 1000\Delta$.

FIG. 4. Static susceptibility as a function of temperature for $\alpha = 0.1$, $D \gg \Delta$, and $\epsilon/\Delta = 0,0.1,0.2,0.5,1$ (from top to bottom).

FIG. 5. $S$ as a function of $\omega$ for $\alpha = 0.1$, $T = 0$. Solid line: $\epsilon = 0$, $D = 100\Delta$. Dotted line: $\epsilon = 0.1\Delta$, $D = 100\Delta$. Dashed line: $\epsilon = 0$, $D = 1000\Delta$. Dot-dashed line: $\epsilon = 0.1\Delta$, $D = 1000\Delta$; Inset: Rescaled $S$. Upper curve: $\epsilon = 0$. Lower curve: $\epsilon = 0.1\Delta$ (for $D = 1000\Delta$ we rescaled $\epsilon = (1000/100)^{\alpha/(1-\alpha)} \times 0.1\Delta = 10^{1/9} \times 0.1\Delta$).

| $\alpha$ | $\epsilon/\Delta$ | $D/\Delta$ | $\chi_0\Delta$ | $\lim_{\omega \to 0} \Delta^2 S(\omega)$ | error |
|----------|------------------|------------|----------------|---------------------------------|-------|
| 0.01     | 0.0              | 100        | 1.0511         | 0.0680                          | 2.04% |
| 0.05     | 0.0              | 100        | 1.2899         | 0.5083                          | 2.80% |
| 0.1      | 0.0              | 100        | 1.6868         | 1.8343                          | 2.57% |
| 0.2      | 0.0              | 100        | 3.2400         | 12.3085                         | 6.93% |
| 0.01     | 0.0              | 1000       | 1.0772         | 0.0711                          | 2.50% |
| 0.05     | 0.0              | 1000       | 1.4534         | 0.6445                          | 2.92% |
| 0.1      | 0.0              | 1000       | 2.1804         | 3.0880                          | 3.33% |
| 0.2      | 0.0              | 1000       | 5.7219         | 35.4919                         | 14.75%|
| 0.01     | 0.01             | 100        | 1.6859         | 1.8390                          | 2.49% |
| 0.01     | 0.05             | 100        | 1.6671         | 1.7523                          | 0.34% |
| 0.1      | 0.1              | 100        | 1.6036         | 1.6209                          | 0.32% |
| 0.1      | 0.01             | 1000       | 2.1778         | 3.0911                          | 3.66% |
| 0.01     | 0.05             | 1000       | 2.1369         | 2.7233                          | 5.21% |
| 0.1      | 0.1              | 1000       | 2.0187         | 2.4377                          | 4.91% |

TABLE I. Shiba-relation for different $\alpha$, $\epsilon$ and $D$. 

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