Numerical Renormalization Group for Bosonic Systems and Application to the Sub-Ohmic Spin-Boson Model

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We describe the generalization of Wilson's numerical renormalization group method to quantum impurity models with a bosonic bath, providing a general nonperturbative approach to bosonic impurity models which can access exponentially small energies and temperatures. As an application, we consider the spin-boson model, describing a two-level system coupled to a bosonic bath with power-law spectral density, $J(\omega) \propto \omega^s$. We find clear evidence for a line of continuous quantum phase transitions for sub-Ohmic bath exponents $0 < s < 1$; the line terminates in the well-known Kosterlitz-Thouless transition at $s = 1$. Contact is made with results from perturbative renormalization group, and various other applications are outlined.

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The numerical renormalization group method (NRG) developed by Wilson [1] is a powerful tool for the investigation of the Kondo model and its generalizations [1–4]. In these models, a (possibly complex) impurity, such as a localized spin, couples to a fermionic bath. In the case of a spin-$\frac{1}{2}$ impurity coupled antiferromagnetically to a metallic bath, the impurity spin is screened below a characteristic scale T_K, the Kondo temperature [3]. The strength of the NRG lies in its nonperturbative nature and the ability to resolve arbitrarily small energies [1]. A variety of thermodynamic and dynamic quantities can be calculated for a large number of impurity models in the whole parameter space [4,5].

There is, however, a very important class of models for which the NRG method has not yet been developed: models with a coupling of the impurity to a *bosonic* bath [6]. The intensively studied spin-boson model [7,8] belongs to this class; its Hamiltonian is given by

$$H = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \sum_i \omega_i a_i^\dagger a_i + \frac{\sigma_z}{2}\sum_i \lambda_i (a_i + a_i^\dagger). \quad (1)$$

Here the Pauli matrices σ_j describe a spin, i.e., a generic two-level system, which is linearly coupled to a bath of harmonic oscillators, with creation (annihilation) operators $a_i^\dagger$ (a_i). The bare tunneling amplitude between the two spin states $|\uparrow\rangle$ and $|\downarrow\rangle$ is given by Δ, and ϵ is an additional bias. The ω_i are the oscillator frequencies and λ_i the coupling strengths between the oscillators and the local spin. The coupling between spin and bosonic bath is completely specified by the bath spectral function

$$J(\omega) = \pi \sum_i \lambda_i^2 \delta(\omega - \omega_i). \quad (2)$$

Of particular interest are power-law spectra

$$J(\omega) = 2\pi\alpha\omega_c^{1-s}\omega^s, \qquad 0 < \omega < \omega_c, \qquad s > -1, \quad (3)$$

where the dimensionless parameter α characterizes the dissipation strength, and ω_c is a cutoff energy. The value $s = 1$ corresponds to the case of Ohmic dissipation.

The spin-boson model is a generic model describing quantum dissipation; it has been discussed in the context of a great variety of physical problems [7,8] ranging from the effect of friction on the electron transfer in biomolecules [9] to the description of the quantum entanglement between a qubit and its environment [10–12].

Considering the wealth of applications, the question arises whether Wilson's NRG method can be exploited for this class of models; and it is the purpose of this Letter to show that this is indeed the case. What we have in mind here is the direct mapping of models like (1) to a semi-infinite chain form typical for the NRG [1]. As described below, bosonic operators constitute the sites of the chain, and the Hamiltonian is solved by iterative numerical diagonalization [13]. This approach is different from previous NRG calculations in Refs. [10,14], where the mapping of the spin-boson model (1) to the anisotropic *fermionic* Kondo model was employed — such a mapping is restricted to the Ohmic case $J(\omega) \propto \omega$.

Bosonic NRG.—Let us now describe the generalization of the NRG method to a bosonic bath with a continuous spectrum. The strategy is similar to the one used for the Kondo or single-impurity Anderson model [1,2]. There are, however, important differences which we outline here; a more detailed discussion will appear elsewhere. Here we present explicit equations for the spin-boson model (1); the generalization to other impurity models or multiple bosonic baths is straightforward.

We start from the following form of the model (1):

$$H = H_{\mathrm{loc}} + \int_0^1 d\varepsilon g(\varepsilon) a_\varepsilon^\dagger a_\varepsilon + \frac{\sigma_z}{2}\int_0^1 d\varepsilon h(\varepsilon)(a_\varepsilon + a_\varepsilon^\dagger), \quad (4)$$

with $H_{\mathrm{loc}} = -\Delta\sigma_x/2 + \epsilon\sigma_z/2$. In this model, $g(\varepsilon)$ characterizes the dispersion of a bosonic bath in a one-dimensional representation, with upper cutoff 1 for ε. The coupling between the spin and the bosonic bath is given by $h(\varepsilon)$. These two energy-dependent functions are related to the spectral function $J(\omega)$ via

$$\frac{1}{\pi}J(x) = \frac{d\varepsilon(x)}{dx}h^2[\varepsilon(x)], \qquad x \in [0, \omega_c], \qquad (5)$$

where $\varepsilon(x)$ is the inverse function of $g(x)$, $g[\varepsilon(x)] = x$. As discussed in Ref. [15] for the Anderson model, Eq. (5) does not uniquely determine $g(x)$ and $h(x)$, and a specific choice for $h(x)$ is used to simplify the calculations.

The NRG procedure starts by dividing the energy interval $[0, 1]$ into intervals $[\Lambda^{-(n+1)}, \Lambda^{-n}]$ ($n = 0, 1, 2, \dots$). An orthonormal set of functions $\psi_{np}(\varepsilon) \propto e^{i\omega_n p\varepsilon}$ is introduced for each interval so that the operators a_ε can be represented in this basis. Choosing $h(\varepsilon)$ as constant in each interval [15] and dropping the ($p \neq 0$) components as in [1,2], the Hamiltonian of the spin-boson model then takes the following form:

$$H = H_{\rm loc} + \sum_{n=0}^{\infty} \xi_n a_n^\dagger a_n + \frac{\sigma_z}{2\sqrt{\pi}} \sum_{n=0}^{\infty} \gamma_n (a_n + a_n^\dagger),$$

$$\xi_n = \gamma_n^{-2} \int_{\Lambda^{-(n+1)}\omega_c}^{\Lambda^{-n}\omega_c} dx J(x) x, \qquad \gamma_n^2 = \int_{\Lambda^{-(n+1)}\omega_c}^{\Lambda^{-n}\omega_c} dx J(x). \qquad (6)$$

The transformation to a semi-infinite chain form yields

$$H_{\rm sem} = H_{\rm loc} + \sqrt{\frac{\eta_0}{\pi}} \frac{\sigma_z}{2} (b_0 + b_0^\dagger) + \sum_{n=0}^{+\infty} [\epsilon_n b_n^\dagger b_n + t_n (b_n^\dagger b_{n+1} + b_{n+1}^\dagger b_n)], \qquad (7)$$

with $\eta_0 = \int dx J(x)$. The spin now couples to the first site of the bosonic chain only, and the remaining part of the chain is characterized by on-site energies ϵ_n and hopping parameters t_n. The parameters η_0, ϵ_n, and t_n can be calculated numerically from a given spectral function $J(\omega)$ [15]. Note that here the spectrum is restricted to positive frequencies; this results in hopping matrix elements falling off as $t_n \propto \Lambda^{-n}$ (which allows one to work with $\Lambda = 2$ while keeping a relatively small number of states), in contrast to the fermionic case where the discretization is performed for both negative and positive energies, in this case $t_n \propto \Lambda^{-n/2}$. The on-site energies also fall off as $\epsilon_n \propto \Lambda^{-n}$ so that a fixed but s-dependent ratio t_n/ϵ_n emerges for large n, where s is the bath exponent in (3).

The Hamiltonian (7) is solved by iterative numerical diagonalization [1,2]. At each step, one bosonic site of the chain is added. The infinite bosonic Hilbert space has to be cut off, by restricting the basis of each new bosonic site to a finite number of states N_b. After diagonalizing the enhanced cluster, the N_s lowest lying many-particle states are kept, and the procedure is repeated [16]. The calculation of static and dynamic observables can be done in analogy to the fermionic NRG. In general, and as known from the fermionic case, the accuracy of the cutoff procedure has to be tested for each application, and we will show results below.

Application to the spin-boson model.—To investigate the feasibility of the bosonic NRG, we performed extensive calculations for the spin-boson model with bath exponents $0 < s \leq 1$, bias $\epsilon = 0$, and $\omega_c = 1$. In the Ohmic case $s = 1$, it is known that a Kosterlitz-Thouless quantum transition separates a localized phase at $\alpha \geq \alpha_c$ from a delocalized phase at $\alpha < \alpha_c$ [7,8]. In the localized regime, the tunnel splitting between the two levels renormalizes to zero, whereas it is finite in the delocalized phase. For $\Delta \ll \omega_c$ the transition occurs at $\alpha_c = 1$.

The sub-Ohmic case [11,17] is less clear. For $\Delta/\omega_c \to 0$ the system is localized for any nonzero coupling; however, the behavior at finite Δ was not discussed in Refs. [7,8]. For large Δ a delocalized phase was argued to exist [17,18], and Ref. [17] proposed a first-order transition scenario. In the following, we will resolve this issue and show that a continuous transition with associated critical behavior occurs for all $0 < s < 1$.

Notably, the spin-boson model can be mapped onto a one-dimensional Ising model with long-range couplings falling off as r^{-s-1}; the localized phase of the spin-boson model then corresponds to the ordered phase of the Ising magnet [7]. As shown by Dyson [19], this Ising model features a transition for $0 < s \leq 1$, but the results for $s < 1$ have not been systematically carried over to the spin-boson model thus far.

Our NRG calculations provide clear evidence for a phase transition in the spin-boson model for all $0 < s \leq 1$, which is continuous for $0 < s < 1$ and of Kosterlitz-Thouless type for $s = 1$. The numerical results are summarized in Fig. 1(a), which shows the phase boundaries determined from the NRG flow for fixed NRG parameters $\Lambda = 2$, $N_b = 8$, and $N_s = 100$ [16]. (No transition occurs for $s > 1$: the system is always delocalized.) As displayed in Fig. 1(b), the critical coupling α_c closely follows a power law as a function of the bare tunnel splitting, $\alpha_c \propto \Delta^x$ for small Δ, with an s-dependent exponent x. Our data are consistent with $x = 1 - s$; see below.

In the Ohmic case, $s = 1$, the critical α_c approaches a *finite* value as $\Delta \to 0$. For the quoted NRG parameters we find $\alpha_c \approx 1.18$, being slightly larger than the established value $\alpha_c(s = 1, \Delta \to 0) = 1$. This deviation is solely due to the NRG discretization; calculations with different Λ show that in the limit $\Lambda \to 1$ we recover $\alpha_c = 1$. The general behavior is illustrated in Fig. 2, which shows α_c for fixed Δ and $s = 0.9$. Keeping Λ fixed, we observe a rapid convergence of α_c with increasing N_b and N_s. As expected from the iterative diagonalization scheme, the values of N_b and N_s necessary for convergence increase with decreasing Λ [16]. The converged data for $\alpha_c(\Lambda)$

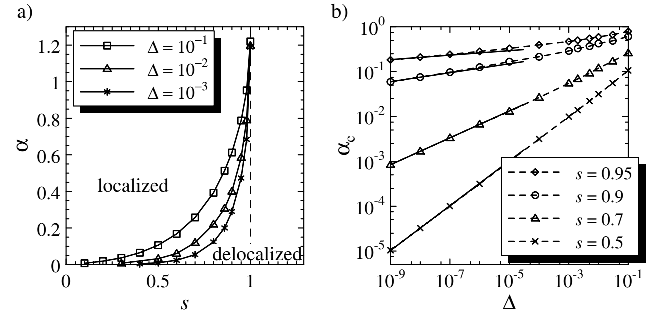

FIG. 1. (a) Phase diagram for the transition between delocalized ($\alpha < \alpha_c$) and localized phases ($\alpha > \alpha_c$) of the spin-boson model (1) for bias $\epsilon = 0$ and various values of Δ, deduced from the NRG flow. (b) Δ dependence of the critical coupling α_c for various values of the bath exponent s. The dashed lines are guides to the eye; the solid lines are fits to Eq. (10) using the $\Delta < 10^{-7}$ points only. For s close to 1 the asymptotic regime is reached only for very small Δ. NRG parameters here and in Figs. 3–5 are $\Lambda = 2$, $N_b = 8$, and $N_s = 100$.

show a linear Λ dependence in the range $1.8 < \Lambda < 3$, with a deviation of about 15% at $\Lambda = 2$ from the extrapolated $\Lambda \to 1$ value. The same holds for the Ohmic case (data not shown) and the extrapolation results in $\alpha_c(s = 1, \Delta = 10^{-4}, \Lambda \to 1) = 0.99 \pm 0.02$; our data are consistent with the renormalization group (RG) result $\alpha_c = 1 + \mathcal{O}(\Delta/\omega_c)$ [7].

The NRG flow of the many-particle levels of the Hamiltonian, displayed in Fig. 3, can be used to analyze the low-temperature behavior. For all values of $0 < s < 1$, we can identify two stable fixed points, corresponding to the localized and delocalized phases of the impurity spin, and a third NRG fixed point, which is infrared unstable and corresponds to a critical fixed point. In contrast, for $s = 1$ we find (in addition to the delocalized fixed point) a *line* of fixed points for $\alpha \geq \alpha_c$, and *no* critical fixed point, as expected for a Kosterlitz-Thouless transition.

The energy scale T^*, describing the crossover from the critical to a stable fixed point, is shown in Fig. 4. For $0 < s < 1$, T^* is found to vary in a power-law fashion with the distance from criticality, $T^* \propto |\alpha - \alpha_c|^{\nu z}$, where we have introduced the correlation length and dynamical exponents ν and z; note that $1/(\nu z)$ is nothing but the scaling dimension of the leading relevant operator at the critical fixed point. Figure 4(a) nicely shows that νz is independent of Δ for fixed s, further supporting the existence of a continuous quantum phase transition with universal behavior. In the Ohmic case $s = 1$, T^* varies exponentially with the distance from the critical coupling, $\ln T^* \propto 1/(\alpha_c - \alpha)$, as expected [Fig. 4(b)].

In Fig. 5(a) we show the s dependence of the exponent νz. We find a divergence for both $s \to 0$ and $s \to 1$, consistent with a Kosterlitz-Thouless transition at $s = 1$, and the system being always localized at $s = 0$. The $s \to 1$ divergence is in good agreement with the perturbative result (9); see below.

The NRG algorithm can be used to compute a variety of static and dynamic observables. As an example, we show $C(\omega)$, being the Fourier transform of the symmetrized autocorrelation function $C(t) = \frac{1}{2}\langle[\sigma_z(t), \sigma_z]_+\rangle$, in Fig. 5(b) for $s = 0.6$ and parameters in the delocalized phase close to the transition. We observe a crossover from $C(\omega) \propto \omega^s$ at small frequencies, characteristic of the

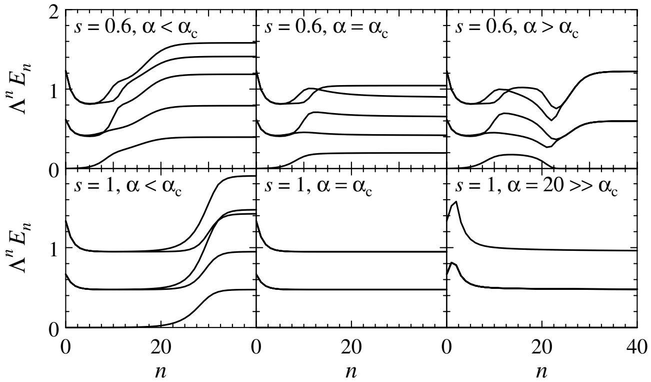

FIG. 3. Sample NRG flow diagrams for the sub-Ohmic (upper panel, $s = 0.6$) and the Ohmic case (lower panel, $s = 1$), close to the phase transition (except for the lower right-hand panel).

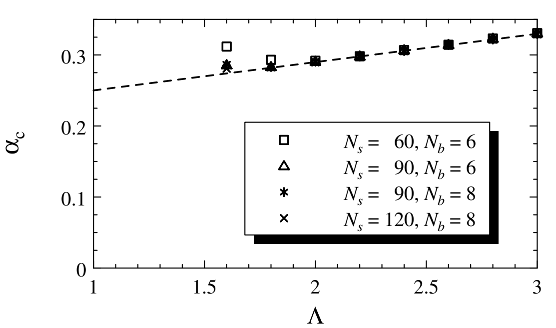

FIG. 2. Λ dependence of the critical coupling α_c at $s = 0.9$, $\Delta = 10^{-3}$, for various NRG parameters N_s and N_b [16]. The dashed line is a linear fit to the $N_s = 120$, $N_b = 8$ data in the range $2 \leq \Lambda \leq 3$.

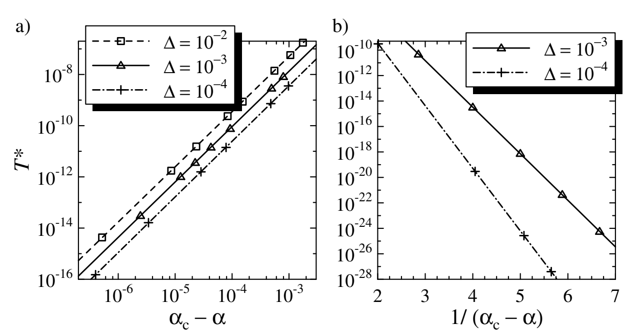

FIG. 4. Crossover scale T^* in the vicinity of the phase transition for $\alpha < \alpha_c$, defined here through the first excited NRG level $\Lambda^n E_{n1}(T^*) = 0.3$. (a) Sub-Ohmic case $s = 0.8$, with power-law fits, (b) Ohmic case $s = 1$, with exponential fits.

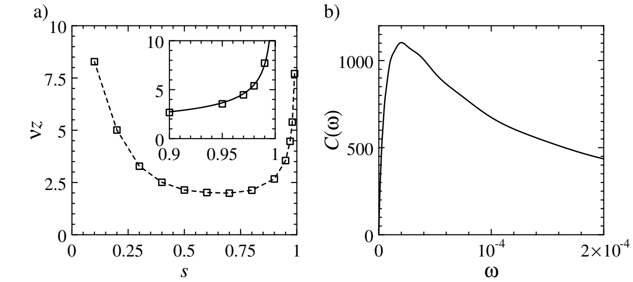

FIG. 5. (a) NRG results for the critical exponent νz, characterizing the vanishing of the crossover energy T^* near the critical point, as a function of the bath exponent s. Inset: data near $s = 1$ together with the function $1/\sqrt{2(1-s)} + 0.5$, Eq. (9). (b) Spin autocorrelation function $C(\omega)$ for $s = 0.6$, $\Delta = 10^{-2}$, and $\alpha = 0.19 \lesssim \alpha_c$ close to the transition.

delocalized phase [17,20], to a quantum critical behavior with a power-law divergence at higher frequencies—this gives rise to a characteristic peak at $\omega \sim T^*$.

Comparison to perturbative results.—The partition function of the spin-boson model can be approximately represented as that of a one-dimensional Ising model with couplings falling off as r^{-s-1}; in this picture, defects in the Ising system correspond to spin flips of the original spin along the imaginary time axis. A RG analysis of this Ising model has been performed by Kosterlitz [21]. Carrying over these results to the spin-boson model, we arrive at the RG equations (see also Ref. [11]),

$$\beta(\alpha) = -\alpha(\bar{\Delta}^2 + s - 1), \qquad \beta(\bar{\Delta}) = \bar{\Delta}(1-\alpha), \quad (8)$$

valid for small $\bar{\Delta}$, where $\bar{\Delta} = \Delta/\omega_c$ is the dimensionless tunneling strength. The RG flow is sketched in Fig. 1 of Ref. [21]. For $s = 1$, these equations are equivalent to the ones known from the anisotropic Kondo model, and describe a Kosterlitz-Thouless transition, with a fixed point line $\bar{\Delta} = 0$, $\alpha \geq 1$. For $s < 1$ there is an unstable fixed point at $\alpha = 1$, $\bar{\Delta}^2 = 1 - s$; clearly it is perturbatively accessible for small values of $(1 - s)$ only. The critical fixed point is characterized by

$$\nu z = 1/\sqrt{2(1-s)} + \mathcal{O}(1). \quad (9)$$

For small α, $\bar{\Delta}$, Eq. (8) yields for the phase boundary

$$\alpha_c \propto \Delta^{1-s} \quad \text{for } \Delta \ll \omega_c, \quad (10)$$

valid for all $0 < s < 1$. The results (9) and (10) are in good agreement with our numerical data in Figs. 5(a) and 1(b), respectively.

Conclusions.—We have presented a generalization of Wilson's NRG to quantum impurity problems with bosonic baths. Applying this novel technique to the sub-Ohmic spin-boson model, we have found a line of continuous boundary quantum phase transitions for all $0 < s < 1$, with exponents varying as a function of s. This line terminates in a Kosterlitz-Thouless transition point at $s = 1$. Near $s = 1$, our numerical results are in agreement with perturbative calculations. The existence of a transition for $s < 1$ implies that weakly damped coherent dynamics *is* possible for qubits coupled to a sub-Ohmic bath, provided that the initial splitting Δ is large.

In close analogy to the fermionic NRG, our method can be easily applied to the calculation of dynamical quantities. Furthermore, generalizations to impurities with multiple bosonic baths or both fermionic and bosonic baths are possible. This will allow the study of large classes of impurity models, e.g., so-called Bose-Kondo and Bose-Fermi-Kondo models.

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