Quantum Phase Transitions in the Sub-Ohmic Spin-Boson Model: Failure of the Quantum-Classical Mapping

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The effective theories for many quantum phase transitions can be mapped onto those of classical transitions. Here we show that the naive mapping fails for the sub-Ohmic spin-boson model which describes a two-level system coupled to a bosonic bath with power-law spectral density, $J(\omega) \propto \omega^s$. Using an ϵ expansion we prove that this model has a quantum transition controlled by an *interacting* fixed point at small s, and support this by numerical calculations. In contrast, the corresponding classical long-range Ising model is known to display mean-field transition behavior for $0 < s < 1/2$, controlled by a *noninteracting* fixed point. The failure of the quantum-classical mapping is argued to arise from the long-ranged interaction in imaginary time in the quantum model.

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Low-energy theories for certain classes of quantum phase transitions in clean systems with d spatial dimensions are known to be equivalent to the ones of classical phase transitions in $(d + z)$ dimensions, where z is the dynamical exponent of the quantum transition [1]. This mapping is usually established in a path integral formulation of the effective action for the order parameter, where imaginary time in the quantum problem takes the role of z additional space dimensions in the classical counterpart. The tuning parameter for the phase transition, being the ratio of certain coupling constants in the quantum problem (where T is fixed to zero), becomes temperature for the classical transition. For the quantum Ising model, where the transverse field can drive the system into a disordered phase at $T = 0$, the quantum-classical equivalence in the scaling limit can be explicitly shown using transfer matrix techniques [1]. While this formal proof is applicable only for *short-range* interactions in the time direction, it is believed that it also holds for long-range interactions, which can arise upon integrating out gapless degrees of freedom coupled to the order parameter. (Counterexamples are phase transitions in itinerant magnets, where the elimination of low-energy fermions produces nonanalyticities in the resulting order parameter field theory [2].) A paradigmatic example is the spin-boson model [3,4], where an Ising spin (i.e., a generic two-level system) is coupled to a bath of harmonic oscillators: eliminating the bath variables leads to a retarded self-interaction for the local spin degree of freedom, which decays as $1/\tau^2$ in the well-studied case of Ohmic damping. Interestingly, the same model is obtained as the low-energy limit of the anisotropic Kondo model which describes a spin-1/2 magnetic impurity coupled to a gas of conduction electrons [5,6].

The purpose of this Letter is to point out that the naive quantum-classical mapping can fail for long-ranged interactions in imaginary time even for the simplest case of $(0 + 1)$ dimensions and Ising symmetry. We shall explicitly prove this failure for the sub-Ohmic spin-boson model, by showing that the phase transitions in the quantum problem and in the corresponding classical long-range Ising model fall in different universality classes.

The spin-boson model is described by the Hamiltonian

$$\mathcal{H}_{\mathrm{SB}} = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \sum_i \omega_i a_i^\dagger a_i + \frac{\sigma_z}{2}\sum_i \lambda_i (a_i + a_i^\dagger) \tag{1}$$

in standard notation. The coupling between spin σ and the bosonic bath with oscillators $\{a_i\}$ is completely specified by the bath spectral function

$$J(\omega) = \pi \sum_i \lambda_i^2 \delta(\omega - \omega_i), \tag{2}$$

conveniently parametrized as

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

where the dimensionless parameter α characterizes the dissipation strength, and ω_c is a cutoff energy. The value $s = 1$ represents the case of Ohmic dissipation, where a Kosterlitz-Thouless transition separates a delocalized phase at small α from a localized phase at large α. These two phases asymptotically correspond to the eigenstates of σ_x and σ_z, respectively.

In the following, we are interested in sub-Ohmic damping, $0 < s < 1$ [7,8]. The standard approach is to integrate out the bath, leading to an effective interaction

$$S_{\mathrm{int}} = \int d\tau d\tau' \sigma_z(\tau) g(\tau - \tau') \sigma_z(\tau') \tag{4}$$

with $g(\tau) \propto 1/\tau^{1+s}$ at long times. Numerical renormalization group (NRG) calculations in Refs. [9,10], performed directly for the sub-Ohmic spin-boson model, have established that a second-order quantum transition occurs for all $0 < s < 1$. Here we use an analytical renormalization group (RG) expansion, controlled by the small parameter s, to establish that the spin-boson transition at small s is governed by an interacting fixed point with strong hyperscaling properties. This analytical result is supported by NRG calculations. In contrast, the transition in the classical Ising model is known to display mean-field behavior for $0 < s < 1/2$ [11,12].

Scaling and critical exponents.—A scaling ansatz for the impurity part of the free energy takes the form

$$F_{\rm imp} = T f(|\alpha - \alpha_c| T^{-1/\nu}, \epsilon T^{-y_\epsilon}), \tag{5}$$

where $|\alpha - \alpha_c|$ measures the distance to criticality. The bias ϵ takes the role of a local field (with scaling exponent y_ϵ), and ν is the correlation length exponent which describes the vanishing of the energy scale T^*, above which quantum critical behavior is observed [1]: $T^* \propto |\alpha - \alpha_c|^\nu$. The ansatz (5) assumes the fixed point to be interacting; for a Gaussian fixed point the scaling function also depends upon dangerously irrelevant variables.

With the local magnetization $M_{\rm loc} = \langle \sigma_z \rangle = -\partial F_{\rm imp}/\partial\epsilon$ and the susceptibility $\chi_{\rm loc} = -\partial^2 F_{\rm imp}/(\partial\epsilon)^2$, we can define critical exponents (see also Ref. [13]):

$$\begin{aligned}
&M_{\rm loc}(\alpha > \alpha_c, T = 0, \epsilon = 0) \propto (\alpha - \alpha_c)^\beta,\\
&\chi_{\rm loc}(\alpha < \alpha_c, T = 0) \propto (\alpha_c - \alpha)^{-\gamma},\\
&M_{\rm loc}(\alpha = \alpha_c, T = 0) \propto |\epsilon|^{1/\delta},\\
&\chi_{\rm loc}(\alpha = \alpha_c, T) \propto T^{-x},\\
&\chi''_{\rm loc}(\alpha = \alpha_c, T = 0, \omega) \propto |\omega|^{-y}{\rm sgn}(\omega).
\end{aligned} \tag{6}$$

The last equation describes the dynamical scaling of $\chi_{\rm loc}$.

In the absence of a dangerously irrelevant variable there are only two independent exponents, e.g., ν and y_ϵ. The scaling form (5) yields hyperscaling relations:

$$\beta = \gamma\frac{1-x}{2x}, \qquad 2\beta + \gamma = \nu, \qquad \gamma = \nu x, \qquad \delta = \frac{1+x}{1-x}. \tag{7}$$

Hyperscaling also implies $x = y$, which is equivalent to so-called ω/T scaling in the dynamical behavior.

Long-range Ising model.—The classical counterpart of the spin-boson model (1) is the one-dimensional Ising model [3,4]

$$\mathcal{H}_{\rm cl} = -\sum_{\langle ij\rangle} J_{ij} S_i^z S_j^z + \mathcal{H}_{\rm SR} \tag{8}$$

with interaction $J_{ij} = J/|i-j|^{1+s}$. $\mathcal{H}_{\rm SR}$ contains an additional generic short-range interaction which arises from the transverse field, but is believed to be irrelevant for the critical behavior [11,12]. As proven by Dyson [14] this model displays a phase transition for $0 < s \le 1$. Both analytical arguments, based on the equivalence to a O(1) ϕ^4 theory [11], and extensive numerical simulations [12] show that the upper-critical dimension for the d-dimensional long-range Ising model is $d_c^+ = 2s$; i.e., in $d = 1$ the transition obeys nontrivial critical behavior for $1/2 < s < 1$. In contrast, mean-field behavior obtains for $0 < s < 1/2$, with exponents [11,12] $\beta = 1/2$, $\gamma = 1$, $\delta = 3$, $\nu = 1/s$, $y = s$ violating hyperscaling.

As the exponent s exclusively determines the power laws of spectra and correlations in a long-range model once spatial dimensionality ($d = 1$) is fixed, s takes the role of a "dimension"; i.e., we refer to $s = 1/2$ as the upper-critical "dimension" of the classical Ising chain.

Near $s = 1$ the phase transition can be analyzed using a kink-gas representation of the partition function, where the kinks represent Ising domain walls [15]. This expansion, controlled by the smallness of the kink fugacity, is done around the ordered phase of the Ising model, corresponding to the localized fixed point of the spin-boson quantum problem. For small $(1 - s)$ the results obtained via the perturbative kink-gas RG are consistent with the NRG data for the spin-boson transition [9], indicating that the quantum-classical mapping works in the asymptotic vicinity of the localized fixed point.

Spin-boson model: perturbative RG.—We now describe a novel RG expansion which is performed around the *delocalized* fixed point of the spin-boson model. NRG indicates that the critical fixed point merges with the delocalized one as $s \to 0^+$; thus we expect that the expansion will allow access to the quantum phase transition for small s. As shown below, the expansion is done about the *lower-critical* dimension $s = 0$; it yields an interacting fixed point, and mean-field critical behavior for small s does *not* obtain. For convenience we assume equal couplings, $\lambda_i \equiv \lambda$, then the energy dependence of $J(\omega)$ is contained in the density of states of the oscillator modes ω_i, and we have $\alpha \propto \lambda^2$.

How can a suitable RG expansion be set up? Power counting about the free-spin fixed point, $\lambda = \Delta = 0$, gives the scaling dimensions $\dim[\lambda] = (1 - s)/2$ and $\dim[\Delta] = 1$. Thus, both parameters are strongly relevant for small s. A better starting point is the delocalized fixed point, corresponding to *finite* Δ. Eigenstates of the impurity are $|\!\rightarrow_x\rangle$ and $|\!\leftarrow_x\rangle$, with an energy splitting of Δ. The low-energy Hilbert space contains the state $|\!\rightarrow_x\rangle$ only, and interaction

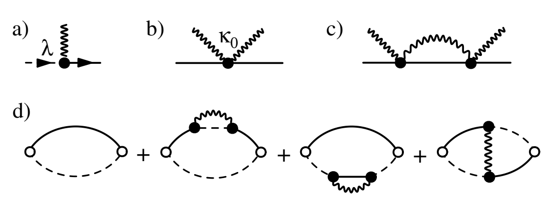

FIG. 1. Feynman diagrams occurring in the perturbation theory for the spin-boson model. Full and dashed lines denote the propagators of the $|\!\rightarrow_x\rangle$ and $|\!\leftarrow_x\rangle$ impurity states—the two states are separated by a gap of size Δ. The wiggly line is the local bath boson $G_{\rm loc}$. (a) Interaction vertex λ. (b) Interaction vertex κ_0 in the low-energy sector. (c) One-loop renormalization of κ. (d) Diagrams for the local susceptibility $\chi_{\rm loc}$.

processes with the bath arise in second-order perturbation theory, proportional to $\kappa_0 = \lambda^2/\Delta$. Power counting with respect to the $\lambda = 0$ limit now gives $\dim[\kappa_0] = -s$; i.e., κ_0 is marginal at $s = 0$, indicating that an ϵ-type expansion for small s is possible.

To lowest order, the RG can be performed within the low-energy sector, i.e., for the κ_0 vertex [Fig. 1(b)] and the propagator for the $|\rightarrow_x\rangle$ state. Consequently, our approach is valid as long as $\lambda \ll \Delta, \omega_c$. We introduce a renormalized coupling κ according to $\kappa_0 = \Lambda^{-s}\kappa$ where Λ is the running cutoff, $\Lambda = \omega_c$ initially. The one-loop beta function can be derived using the familiar momentum shell method, i.e., by successively eliminating high-energy bath bosons. To one-loop order only the coupling-constant renormalization in Fig. 1(c) enters, and we obtain

$$\beta(\kappa) = -s\kappa + \kappa^2. \tag{9}$$

Besides the stable delocalized fixed point $\kappa = 0$ this flow equation displays an infrared unstable fixed point at

$$\kappa^* = s + \mathcal{O}(s^2), \tag{10}$$

which controls the transition between the delocalized and localized phases. No (dangerously) irrelevant variables are present in this theory, so we conclude that the critical fixed point (10) is interacting [16].

We proceed with the calculation of critical exponents. Expanding the RG beta function around the fixed point (10) gives the correlation length exponent

$$1/\nu = s + \mathcal{O}(s^2), \tag{11}$$

i.e., ν diverges as $s \rightarrow 0^+$, as is characteristic for a lower-critical dimension. Parenthetically, we note that the RG structure for $s \rightarrow 1^-$ is also similar to that near a lower-critical dimension: The line of second-order transitions for $0 < s < 1$ terminates in a Kosterlitz-Thouless transition at $s = 1$ and is thus bounded by *two lower-critical "dimensions"*—a similar situation was recently found in the pseudogap Kondo problem, which, however, is in a different universality class [17]. As is usual for RG expansions around a lower-critical dimension the present RG can capture only one of the two phases (the delocalized one), whereas runaway flow occurs on the localized side.

The exponents associated with the local field ϵ can be obtained in straightforward renormalized perturbation theory. To calculate observables, the diagrams are written down using the original model with couplings λ and Δ and both $|\rightarrow_x\rangle$, $|\leftarrow_x\rangle$ states. The perturbation theory turns out to be organized in powers of λ^2/Δ, as expected. Some of the relevant diagrams are displayed in Fig. 1(d), and details will appear elsewhere. Restricting ourselves to the lowest-order results for the disordered and quantum critical regimes we find

$$\begin{aligned} &\gamma = 1 + \mathcal{O}(s), \qquad x = y = s + \mathcal{O}(s^2), \\ &1/\delta = 1 - 2s + \mathcal{O}(s^2). \end{aligned} \tag{12}$$

Interestingly, we are able to derive an *exact* result for the exponents x, y, employing an argument along the lines of Refs. [18,19], based on the diagrammatic structure of $\chi_{\rm loc}$. We obtain

$$x = y = s. \tag{13}$$

(Notably, $y = s$ was found to be the exact decay exponent of the critical spin correlations in the long-range Ising model for all s [11,20].) Hyperscaling yields $\delta = (1 + s)/(1 - s)$, consistent with the lowest-order result (12).

As an aside, we note that at $s = 0$ the bath coupling is marginally relevant. Therefore the impurity is always localized as $T \rightarrow 0$, with a localization temperature given by $T^* = \omega_c \exp(-\Delta\omega_c/\lambda^2)$.

Spin-boson model: Numerical results.—We have performed extensive NRG calculations [10] to evaluate the critical exponents of the spin-boson transition; see Refs. [9,10] for numerical details [21]. Results are shown in Figs. 2 and 3: these exponents obey hyperscaling including $x = y$ (ω/T scaling). They are in excellent agreement with the small-s RG expansion, but at variance with the exponents of the long-range Ising model: the mean-field predictions are $\beta = 1/2$, $\delta = 3$ which are clearly violated by our results in Fig. 2.

Within error bars the mean-field exponents are realized *at* $s = 1/2$. Further, the one-loop results for ν (11) and γ (12) appear to be exact for all $0 < s < 1/2$, and logarithmic corrections to the power laws are observed at $s = 1/2$. This suggests that the spin-boson transition *does* change its character at $s = 1/2$, but the critical fixed points for both $0 < s < 1/2$ and $1/2 < s < 1$ are interacting and obey hyperscaling (the latter one being equivalent to that of the classical Ising model).

Discussion.—We have proven that the naive quantum-classical mapping fails for the sub-Ohmic spin-boson model: Using a novel RG expansion around the delocalized fixed point, we have shown that the quantum transition at $0 < s < 1/2$ is controlled by an interacting fixed point, whereas the corresponding classical long-range Ising model shows mean-field behavior. Thus, the spin-boson problem for $s < 1/2$ is equivalent neither to the classical

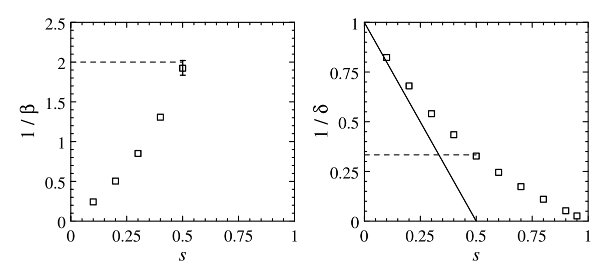

FIG. 2. Left: NRG data for the order parameter exponent $1/\beta$. Right: Magnetization exponent $1/\delta$ from NRG, together with the analytical RG result (12) (solid line). The dashed lines are the mean-field results $\beta = 1/2$, $\delta = 3$.

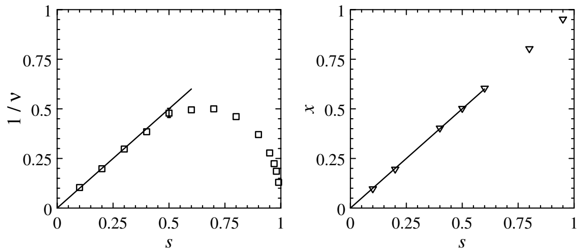

FIG. 3. Left: Numerical data for the correlation length exponent $1/\nu$ obtained from NRG, together with the RG result (11). Right: Susceptibility exponent x from NRG, together with the RG result (13). Here, the mean-field results coincide with the lowest-order perturbative ones.

Ising model nor to the corresponding (quantum or classical) O(1) ϕ^4 theory [12]. In physical terms the inequivalence can be traced back to the different disordered (delocalized) fixed points in the two situations (expansions around these fixed points are suitable to access the critical behavior for small s): In the quantum model the transverse field fully polarizes the spin in the x direction (which can be viewed as a "condensate" of spin flips), whereas the high-temperature limit of the classical Ising model is simply incoherently disordered.

The inequivalence may come unexpectedly—so where does the quantum-classical mapping fail? Formal proofs of the mapping using transfer matrices rely on the short-ranged character of the interaction [1]. For general interactions a Trotter decomposition of the quantum partition function is employed where the imaginary axis of length $\beta = 1/T$ is divided into N slices of size $\Delta\tau = \beta/N$, leading to an Ising chain (8) with N sites. This procedure is exact when the limits $\Delta\tau \to 0$ and $\beta \to \infty$ are taken in this order. However, the limit $\Delta\tau \to 0$ leads to a *diverging* near-neighbor coupling in the term $\mathcal{H}_{\rm SR}$ of the classical Ising model (8) [6]. This may, in fact, change the critical behavior of $\mathcal{H}_{\rm cl}$ (8), as a classical model with finite couplings arises upon taking $\beta \to \infty$ first. In other words, the quantum and classical problems are only equivalent if and only if the low-energy limit of $\mathcal{H}_{\rm cl}$ is independent of the order of the two limits $\Delta\tau \to 0$ and $\beta \to \infty$ [6]. As we have proven the inequivalence of $\mathcal{H}_{\rm SB}$ and $\mathcal{H}_{\rm cl}$ (with finite couplings) we conclude that the two limits cannot be interchanged for $s < 1/2$.

A recent paper [22] investigated a SU(N)-symmetric Bose-Fermi Kondo model in a certain large-N limit and found a critical fixed point with ω/T scaling for all s. The authors argued that the apparent failure of the quantum-classical mapping is due to the quantum nature of the impurity spin. As discussed above, this alone is not sufficient: for short-range interactions in imaginary time the mapping can be proven to be asymptotically exact [1]; *long-range* interactions are essential.

Our results suggest that some conclusions drawn in the past for effectively long-range Ising systems on the basis of the quantum-classical mapping have to be reexamined. Further, we envision that our novel ϵ expansion will have applications for various quantum impurity problems, e.g., two-level systems coupled to multiple baths, Bose-Fermi Kondo models [19,22], and also for quantum dissipative lattice models [23].

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