

# Quantum phase transition of the sub-Ohmic rotor model

Manal Al-Ali and Thomas Vojta

*Department of Physics, Missouri University of Science and Technology, Rolla, Missouri 65409, USA*

(Received 18 October 2011; published 28 November 2011)

We investigate the behavior of an  $N$ -component quantum rotor coupled to a bosonic dissipative bath having a sub-Ohmic spectral density  $J(\omega) \propto \omega^s$  with  $s < 1$ . With increasing dissipation strength, this system undergoes a quantum phase transition from a delocalized phase to a localized phase. We determine the exact critical behavior of this transition in the large- $N$  limit. For  $1 > s > 1/2$ , we find nontrivial critical behavior corresponding to an interacting renormalization group fixed point, while we find mean-field behavior for  $s < 1/2$ . The results agree with those of the corresponding long-range interacting classical model. The quantum-to-classical mapping is therefore valid for the sub-Ohmic rotor model.

DOI: [10.1103/PhysRevB.84.195136](https://doi.org/10.1103/PhysRevB.84.195136)

PACS number(s): 05.10.Cc, 05.30.Jp

## I. INTRODUCTION

Quantum phase transitions are abrupt changes in the ground state properties of a quantum many-particle system that occur when a nonthermal control parameter is varied.<sup>1</sup> In analogy to thermal phase transitions, they can be classified as either first-order or continuous transitions. Continuous quantum phase transitions, also called quantum-critical points, are characterized by large-scale temporal and spatial fluctuations that lead to unconventional behavior in systems ranging from strongly correlated electron materials to ultracold quantum gases (for reviews see, e.g., Refs. 2–7).

Impurity quantum phase transitions<sup>8</sup> are an interesting class of quantum phase transitions at which only the degrees of freedom of a finite-size (zero-dimensional) subsystem become critical at the transition point. The rest of the system (the “bath”) does not undergo a transition. Impurity quantum phase transitions can occur, e.g., in systems composed of a single quantum spin coupled to an infinite fermionic or bosonic bath. Fermionic examples include the anisotropic Kondo model<sup>9</sup> and the pseudogap Kondo model.<sup>10</sup>

The prototypical system involving a bosonic bath is the dissipative two-state system,<sup>11,12</sup> also called the spin-boson model, which describes a two-level system coupled to a single dissipative bath of harmonic oscillators. Its ground-state phase diagram depends on the behavior of the bath spectral density  $J(\omega)$  for small frequencies  $\omega$ . Power-law spectra  $J(\omega) \propto \omega^s$  are of particular interest. In the super-Ohmic case ( $s > 1$ ), the system is in the delocalized (disordered) phase for any dissipation strength. In contrast, for sub-Ohmic dissipation ( $0 < s < 1$ ), there is a continuous quantum phase transition from a delocalized phase at weak dissipation to a localized (ordered) phase at strong dissipation.<sup>13</sup> In the marginal Ohmic case ( $s = 1$ ), a quantum phase transition exists too, but it is of Kosterlitz-Thouless type.<sup>11,12</sup>

The sub-Ohmic spin-boson model has recently attracted considerable attention in the context of the so-called quantum-to-classical mapping. This concept relates the critical behavior of a quantum phase transition in  $d$  space dimensions to that of a classical transition in  $d + 1$  dimensions. The mapping is usually established by comparing the order-parameter field theories of the transitions: Imaginary time in the quantum problem plays the role of the extra dimension in the corresponding classical system. In the case of the spin-boson

model, the classical counterpart is a one-dimensional Ising model with long-range interactions that decay as  $1/r^{1+s}$  for large distances  $r$ . In recent years, the applicability of the quantum-to-classical mapping to the sub-Ohmic spin-boson model has been controversially discussed after numerical renormalization group results<sup>14</sup> suggested that its critical behavior for  $s < 1/2$  deviates from that of the corresponding Ising model. While there is now strong evidence<sup>15–18</sup> that this conclusion is incorrect and that the quantum-to-classical mapping is actually valid, the issue appears to be still not fully settled.<sup>19</sup> Moreover, possible failures of the quantum-to-classical mapping have also been reported for other impurity models with both Ising<sup>20–22</sup> and higher<sup>23,24</sup> symmetries, and the precise conditions under which it is supposed to hold are not resolved.

In the present paper, we therefore investigate the large- $N$  limit of the sub-Ohmic quantum rotor model. Analogous to the spin-boson model, this system undergoes a quantum phase transition with increasing dissipation strength from a delocalized phase to a localized phase.<sup>25,26</sup> We exactly solve the critical properties of this transition. Our analysis yields nontrivial critical behavior corresponding to an interacting renormalization group fixed point for  $1 > s > 1/2$ , while we find mean-field behavior for  $s < 1/2$ . All critical exponents agree with those of the corresponding long-range interacting classical model,<sup>27</sup> implying that the quantum-to-classical mapping is valid.

Our paper is organized as follows. We define the sub-Ohmic rotor model in Sec. II. In Sec. III, we derive its partition function, and we solve the self-consistent large- $N$  constraint at zero and finite temperatures as well as with and without an external field. Section IV is devoted to a discussion of observables and the resulting critical behavior. We conclude in Sec. V.

## II. SUB-OHMIC ROTOR MODEL

A quantum rotor can be understood as a point moving on an  $N$ -dimensional hypersphere of radius  $N^{1/2}$ . It can be represented by an  $N$ -component vector  $\mathbf{S}$  satisfying  $\mathbf{S}^2 = N$ . The rotor has a momentum  $\mathbf{P}$ ; the position and momentum components fulfill the usual canonical commutation relations  $[S_\alpha, P_\beta] = i\delta_{\alpha\beta}$ . In the large- $N$  limit  $N \rightarrow \infty$ , the hard constraint  $\mathbf{S}^2 = N$  can be replaced by one for the thermodynamic

average  $\langle S^2 \rangle = N$ , because fluctuations of the magnitude of  $\mathbf{S}$  are suppressed by the central limit theorem. The large- $N$  quantum rotor is thus equivalent to the quantum spherical model of Ref. 28, which is given by the Hamiltonian

$$H_S = \frac{1}{2}P^2 + \frac{1}{2}\omega_0^2 S^2 - hS + \mu(S^2 - 1). \quad (1)$$

Here,  $S$  and  $P$  represent the position and momentum of one rotor component,  $\mu$  is a Lagrange multiplier enforcing the constraint  $\langle S^2 \rangle = 1$ , and  $h$  is an external symmetry-breaking field.<sup>29</sup>

We now couple (every component of) the rotor to a bath of harmonic oscillators.<sup>30</sup> In the conventional linear-coupling form, the Hamiltonian describing the bath and its coupling to  $S$  reads

$$H_B = \sum_j \left[ \frac{p_j^2}{2m_j} + \frac{m_j}{2} \omega_j^2 q_j^2 + \lambda_j q_j S + \frac{\lambda_j^2}{2m_j \omega_j^2} S^2 \right], \quad (2)$$

with  $q_j$ ,  $p_j$ , and  $m_j$  being the position, momentum, and mass of the  $j$ th oscillator. The  $\omega_j$  are the oscillator frequencies and  $\lambda_j$  the coupling strengths between the oscillators and  $S$ . The last term in the bracket is the usual counter term which insures that the dissipation is invariant under translations in  $S$ .<sup>11</sup> The coupling between the rotor and the bath is completely characterized by the spectral density

$$J(\omega) = \frac{\pi}{2} \sum_j \frac{\lambda_j^2}{m_j \omega_j} \delta(\omega - \omega_j), \quad (3)$$

which we assume to be of power-law form

$$J(\omega) = 2\pi \bar{\alpha} \omega_c^{1-s} \omega^s, \quad (0 < \omega < \omega_c). \quad (4)$$

Here,  $\bar{\alpha}$  is the dimensionless dissipation strength and  $\omega_c$  is a cutoff frequency. We will be interested mostly in the case of sub-Ohmic dissipation,  $0 < s < 1$ .

### III. PARTITION FUNCTION AND CONSTRAINT EQUATION

#### A. Path integral formulation

We now derive a representation of the partition function in terms of an imaginary-time functional integral. Because the sub-Ohmic rotor model  $H = H_S + H_B$  is equivalent to a system of coupled harmonic oscillators (with an additional self-consistency condition), this can be done following Feynman's path integral approach<sup>31</sup> with position and momentum eigenstates as basis states. After integrating out the momentum variables, we arrive at the partition function

$$Z = \int D[S(\tau)] D[q_j(\tau)] e^{-\mathcal{A}_S - \mathcal{A}_B}. \quad (5)$$

The Euclidian action is given by

$$\mathcal{A}_S = \int_0^\beta d\tau \left[ \frac{1}{2} (\dot{S}^2 + \omega_0^2 S^2) - hS + \mu(S^2 - 1) \right] \quad (6)$$

$$\mathcal{A}_B = \int_0^\beta d\tau \sum_j \left[ \frac{m_j}{2} (\dot{q}_j^2 + \omega_j^2 q_j^2) + S \lambda_j q_j + \frac{\lambda_j^2 S^2}{2m_j \omega_j^2} \right], \quad (7)$$

where the dot marks the derivative with respect to imaginary time  $\tau$ , and  $\beta = 1/T$  is the inverse temperature.

The bath action is quadratic in the  $q_j$ ; we can thus exactly integrate out the bath modes. After a Fourier transformation from imaginary time  $\tau$  to Matsubara frequency  $\omega_n$ , this yields  $\int D[\tilde{q}_i(\omega_n)] \exp(-\mathcal{A}_B) = Z_B^0 \exp(-\mathcal{A}_B')$ , where  $Z_B^0$  is the partition function of the unperturbed bath and

$$\mathcal{A}_B' = T \sum_{\omega_n} \sum_j \frac{\lambda_j^2}{2m_j} \frac{\omega_n^2}{\omega_j^2(\omega_n^2 + \omega_j^2)} \tilde{S}(\omega_n) \tilde{S}(-\omega_n). \quad (8)$$

The sum over  $j$  can be turned into an integral over the spectral density  $J(\omega)$ . Carrying out this integral gives

$$\mathcal{A}_B' = \frac{1}{2} T \sum_{\omega_n} \alpha \omega_c^{1-s} |\omega_n|^s \tilde{S}(\omega_n) \tilde{S}(-\omega_n), \quad (9)$$

with the dimensionless coupling constant  $\alpha = 2\pi \bar{\alpha} \operatorname{cosec}(\pi s/2)$ . Combining  $\mathcal{A}_S$  and  $\mathcal{A}_B'$  yields the effective action of the sub-Ohmic rotor model as

$$\begin{aligned} \mathcal{A}_{\text{eff}} = & -\beta\mu + \frac{T}{2} \sum_{\omega_n} (\epsilon + \alpha \omega_c^{1-s} |\omega_n|^s) \tilde{S}(\omega_n) \tilde{S}(-\omega_n) \\ & - T \sum_{\omega_n} \tilde{h}(\omega_n) \tilde{S}(-\omega_n), \end{aligned} \quad (10)$$

where  $\epsilon = \omega_0^2 + 2\mu$  is the renormalized distance from quantum criticality. The  $\omega_n^2$  term in  $\mathcal{A}_S$  is subleading in the limit  $\omega_n \rightarrow 0$ . It is thus irrelevant for the critical behavior at the quantum critical point and has been dropped. The theory then needs a cutoff for the Matsubara frequencies which we chose to be  $\omega_c$ . Because the effective action is Gaussian, the partition function  $Z = Z_B^0 \int D[\tilde{S}(\omega_n)] \exp(-\mathcal{A}_{\text{eff}})$  is easily evaluated. We find

$$\begin{aligned} Z = & Z_B^0 \exp(\beta\mu) \prod_{\omega_n} \left[ \frac{2\pi}{T(\epsilon + \alpha \omega_c^{1-s} |\omega_n|^s)} \right]^{1/2} \\ & \times \exp \left[ \frac{T}{2} \sum_{\omega_n} \frac{\tilde{h}(\omega_n) \tilde{h}(-\omega_n)}{\epsilon + \alpha \omega_c^{1-s} |\omega_n|^s} \right]. \end{aligned} \quad (11)$$

#### B. Solving the spherical constraint

The spherical (large  $N$ ) constraint  $\langle S^2 \rangle = 1$  can be easily derived from the free energy  $F = -T \ln Z$  by means of the relation  $0 = \partial F / \partial \mu$ . In the case of a time-independent external field  $h$  with Fourier components  $\tilde{h}(\omega_n) = \delta_{n,0} h / T$ , this yields

$$T \sum_{\omega_n} \frac{1}{\epsilon + \alpha \omega_c^{1-s} |\omega_n|^s} + \frac{h^2}{\epsilon^2} = 1. \quad (12)$$

We now solve this equation, which gives the renormalized distance from criticality  $\epsilon$  as a function of the external parameters  $\alpha$ ,  $T$ , and  $h$ , in various limiting cases.

##### 1. $T = 0$ and $h = 0$

At zero temperature, the sum over the Matsubara frequencies turns into an integral, and the constraint equation reads

$$\frac{1}{\pi} \int_0^{\omega_c} d\omega \frac{1}{\epsilon + \alpha \omega_c^{1-s} \omega^s} = 1. \quad (13)$$

For sub-Ohmic dissipation  $s < 1$ , a solution  $\epsilon \geq 0$  to this equation only exists for dissipation strengths  $\alpha$  below a critical value  $\alpha_c$  because the integral converges at the lower bound even for  $\epsilon = 0$ . The value of  $\alpha_c$  defines the location of the quantum critical point. Performing the integral for  $\epsilon = 0$ , we find  $\alpha_c = 1/[\pi(1-s)]$ . As we are interested in the critical behavior, we now solve the constraint equation for dissipation strengths close to the critical one  $\alpha \lesssim \alpha_c$ . We need to distinguish two cases:  $1 > s > 1/2$  and  $s < 1/2$ .

In the first case, the calculation can be performed by subtracting the constraint equations at  $\alpha$  and at  $\alpha_c$  from each other. After moving the cutoff  $\omega_c$  to  $\infty$ , the resulting integral can be easily evaluated giving

$$\epsilon = \alpha \omega_c A^{s/(s-1)} (\alpha_c - \alpha)^{s/(1-s)} \quad (s > 1/2), \quad (14)$$

where  $A = -(1/s) \operatorname{cosec}(\pi/s)$ . In the case  $s < 1/2$ , Eq. (13) can be evaluated by a straight Taylor expansion in  $\alpha_c - \alpha$ , resulting in

$$\epsilon = \alpha_c \omega_c B^{-1} (\alpha_c - \alpha) \quad (s < 1/2), \quad (15)$$

with  $B = 1/[\pi(1-2s)]$ . For  $s < 1/2$ , the functional dependence of  $\epsilon$  on  $\alpha_c - \alpha$  thus becomes linear, independent of  $s$ . As we will see later, this causes the transition to be of mean-field type.

For dissipation strengths above the critical value  $\alpha_c$ , the spherical constraint can only be solved by *not* transforming the sum over the Matsubara frequencies in Eq. (12) into the frequency integral in Eq. (13). Instead, the  $\omega_n = 0$  Fourier component has to be treated separately.<sup>32</sup> Alternatively, one can explicitly introduce a nonzero average for one of the  $N$  order parameter components (see, e.g., Ref. 1). Both approaches are equivalent; we will follow the first route in the next subsection.

## 2. $T > 0$ and $h = 0$

At small but nonzero temperatures, an approximate solution of the spherical constraint (12) can be obtained by keeping the  $\omega_n = 0$  term in the frequency sum discrete while representing all other modes in terms of an  $\omega$  integral. This gives

$$\frac{T}{\epsilon} + \frac{1}{\pi} \int_0^{\omega_c} d\omega \frac{1}{\epsilon + \alpha \omega_c^{1-s} \omega^s} = 1. \quad (16)$$

We now solve this equation on the disordered side of the transition ( $\alpha < \alpha_c$ ), at the critical dissipation strength  $\alpha_c$ , and on the ordered side of the transition ( $\alpha > \alpha_c$ ). We again need to distinguish the cases  $1 > s > 1/2$  and  $s < 1/2$ .

In the first case, we subtract the quantum critical ( $T = 0, h = 0, \alpha = \alpha_c$ ) constraint from Eq. (16). After evaluating the emerging integral, the following results are obtained in the limit  $T \rightarrow 0$  and  $|\alpha - \alpha_c|$  small but fixed,

$$\epsilon = \frac{\alpha}{\alpha - \alpha_c} T \quad (\alpha > \alpha_c, s > 1/2), \quad (17a)$$

$$\epsilon = A^{-s} \alpha_c \omega_c^{1-s} T^s \quad (\alpha = \alpha_c, s > 1/2), \quad (17b)$$

$$\epsilon = \epsilon_0 + \frac{\alpha}{\alpha_c - \alpha} \frac{s}{1-s} T \quad (\alpha < \alpha_c, s > 1/2). \quad (17c)$$

Here,  $\epsilon_0$  is the zero-temperature value given in Eq. (14), and  $A = -(1/s) \operatorname{cosec}(\pi/s)$  as above. For  $s < 1/2$ , we expand (16) in  $\alpha - \alpha_c$  and find

$$\epsilon = \frac{\alpha}{\alpha - \alpha_c} T \quad (\alpha > \alpha_c, s < 1/2), \quad (18a)$$

$$\epsilon = B^{-1/2} \alpha_c \omega_c^{1/2} T^{1/2} \quad (\alpha = \alpha_c, s < 1/2), \quad (18b)$$

$$\epsilon = \epsilon_0 + \frac{\alpha}{\alpha_c - \alpha} T \quad (\alpha < \alpha_c, s < 1/2), \quad (18c)$$

with  $\epsilon_0$  given in Eq. (15) and  $B = 1/[\pi(1-2s)]$  as above.

## 3. $T = 0$ and $h \neq 0$

At zero temperature, but in the presence of an external field, the spherical constraint reads

$$\frac{1}{\pi} \int_0^{\omega_c} d\omega \frac{1}{\epsilon + \alpha \omega_c^{1-s} \omega^s} + \frac{h^2}{\epsilon^2} = 1. \quad (19)$$

Proceeding in analogy to the last subsection, we determine the distance  $\epsilon$  from criticality in the limit  $h \rightarrow 0$  and  $|\alpha - \alpha_c|$  small but fixed. In the case  $1 > s > 1/2$ , we obtain

$$\epsilon = \left( \frac{\alpha}{\alpha - \alpha_c} \right)^{1/2} h \quad (\alpha > \alpha_c, s > 1/2), \quad (20a)$$

$$\epsilon = (A^{-s} \alpha_c \omega_c^{1-s} h^{2s})^{1/(s+1)} \quad (\alpha = \alpha_c, s > 1/2), \quad (20b)$$

$$\epsilon = \epsilon_0 + \frac{\alpha}{\alpha_c - \alpha} \frac{s}{1-s} \frac{h^2}{\epsilon_0} \quad (\alpha < \alpha_c, s > 1/2), \quad (20c)$$

where  $\epsilon_0$  is the zero-field value given in Eq. (14) and  $A = -(1/s) \operatorname{cosec}(\pi/s)$  as above. For  $s < 1/2$ , the corresponding results read

$$\epsilon = \left( \frac{\alpha}{\alpha - \alpha_c} \right)^{1/2} h \quad (\alpha > \alpha_c, s < 1/2), \quad (21a)$$

$$\epsilon = (B^{-1} \alpha_c^2 \omega_c h^2)^{1/3} \quad (\alpha = \alpha_c, s < 1/2), \quad (21b)$$

$$\epsilon = \epsilon_0 + \frac{\alpha}{\alpha_c - \alpha} \frac{h^2}{\epsilon_0} \quad (\alpha < \alpha_c, s < 1/2), \quad (21c)$$

with  $\epsilon_0$  given in Eq. (15) and  $B = 1/[\pi(1-2s)]$  as above.

## IV. OBSERVABLES AT THE QUANTUM PHASE TRANSITION

### A. Magnetization

After having solved the spherical constraint, we now turn to the behavior of observables at the quantum critical point. The magnetization  $M = \langle S \rangle$  follows from Eq. (11) via  $M = -\partial F / \partial h = T \partial (\ln Z) / \partial h$ . This simply gives

$$M = h / \epsilon. \quad (22)$$

To find the zero-temperature spontaneous magnetization in the ordered phase, we need to evaluate Eq. (22) for  $T = 0, \alpha > \alpha_c$ , and  $h \rightarrow 0$ . Using Eqs. (20a) and (21a), we find

$$M = \sqrt{(\alpha - \alpha_c) / \alpha} \quad (23)$$

for the entire range  $1 > s > 0$ . The order parameter exponent  $\beta$  thus takes the value  $1/2$  in the entire  $s$  range. For  $T > 0$ ,  $\epsilon$  does not vanish even in the limit  $h \rightarrow 0$ . The spontaneous

magnetization is therefore identical to zero for any nonzero temperature, independent of the dissipation strength  $\alpha$ .

The critical magnetization-field curve of the quantum phase transition can be determined by analyzing Eq. (22) for  $T = 0$ ,  $\alpha = \alpha_c$ , and nonzero  $h$ . In the case of  $1 > s > 1/2$ , inserting Eq. (20b) into Eq. (22) yields

$$M = (A^s \alpha_c^{-1} \omega_c^{-(1-s)} h^{1-s})^{1/(1+s)} \quad (s > 1/2), \quad (24)$$

which implies a critical exponent  $\delta = (1 + s)/(1 - s)$ . For  $s < 1/2$ , we instead get the relation

$$M = (B \alpha_c^{-2} \omega_c^{-1} h)^{1/3} \quad (s < 1/2). \quad (25)$$

The critical exponent  $\delta$  thus takes the mean-field value of 3.

### B. Susceptibility

The Matsubara susceptibility can be calculated by taking the second derivative of  $\ln Z$  in Eq. (11) with respect to the Fourier components of the field, yielding

$$\chi(i\omega_n) = \frac{1}{\epsilon + \alpha \omega_c^{1-s} |\omega_n|^s}. \quad (26)$$

We first discuss the static susceptibility  $\chi_{\text{st}} = \chi(0) = 1/\epsilon$  in the case of  $1 > s > 1/2$ . To find the zero-temperature, zero-field susceptibility in the disordered (delocalized) phase  $\alpha < \alpha_c$ , we use Eq. (14) for  $\epsilon$ , which results in

$$\chi_{\text{st}} = \alpha^{-1} \omega_c^{-1} A^{s/(1-s)} (\alpha_c - \alpha)^{-s/(1-s)} \quad (s > 1/2). \quad (27)$$

The susceptibility exponent thus takes the value  $\gamma = s/(1 - s)$ .

For dissipation strengths  $\alpha \geq \alpha_c$ , the susceptibility diverges in the limit  $T \rightarrow 0$ . The temperature dependencies follow from substituting Eqs. (17a) and (17b) into  $\chi_{\text{st}} = 1/\epsilon$ . This yields

$$\chi_{\text{st}} = \frac{\alpha - \alpha_c}{\alpha} T^{-1} \quad (\alpha > \alpha_c, s > 1/2), \quad (28a)$$

$$\chi_{\text{st}} = \omega_c^{s-1} \alpha_c^{-1} A^s T^{-s} \quad (\alpha = \alpha_c, s > 1/2). \quad (28b)$$

In the ordered (localized) phase, we thus find Curie behavior with an effective moment of  $M^2 = (\alpha - \alpha_c)/\alpha$  in agreement with Eq. (23).

The static susceptibility in the case  $s < 1/2$  is obtained analogously. Using Eq. (15), the zero-temperature, zero-field susceptibility reads

$$\chi_{\text{st}} = \alpha^{-1} \omega_c^{-1} B (\alpha_c - \alpha)^{-1} \quad (s < 1/2), \quad (29)$$

implying that the susceptibility exponent takes the mean-field value  $\gamma = 1$ . From Eq. (18b), we obtain the temperature dependence of  $\chi_{\text{st}}$  at the critical damping strength,

$$\chi_{\text{st}} = \omega_c^{-1} \alpha_c^{-1/2} B^{1/2} T^{-1/2} \quad (\alpha = \alpha_c, s < 1/2). \quad (30)$$

In the ordered phase, the behavior for  $s < 1/2$  is identical to that for  $s > 1/2$  given in Eq. (28a).

We now turn to the dynamic susceptibility. To compute the retarded susceptibility  $\chi(\omega)$ , we need to analytically continue the Matsubara susceptibility by performing a Wick rotation to real frequencies,  $i\omega_n \rightarrow \omega + i0$ . A direct transformation of Eq. (26) is hampered by the nonanalytic frequency dependence  $|\omega_n|^s$ . We therefore go back to a representation of the dynamic term in the susceptibility in terms of discrete bath modes [see

the action (8)]. As this representation is analytic in  $\omega_n$ , the Wick rotation can be performed easily. We then carry out the integration over the spectral density *after* the Wick rotation. The resulting dynamical susceptibility reads

$$\chi(\omega) = \frac{1}{\epsilon + \alpha \omega_c^{1-s} |\omega|^s [\cos(\pi s/2) - i \sin(\pi s/2) \text{sgn}(\omega)]}. \quad (31)$$

At quantum criticality ( $\alpha = \alpha_c$ ,  $T = 0$ ,  $h = 0$ ), the real and imaginary parts of the dynamic susceptibility simplify to

$$\text{Re}\chi(\omega) = \frac{\cos(\pi s/2)}{\alpha_c \omega_c^{1-s} |\omega|^s}, \quad \text{Im}\chi(\omega) = \frac{\sin(\pi s/2) \text{sgn}(\omega)}{\alpha_c \omega_c^{1-s} |\omega|^s} \quad (32)$$

in the entire range  $1 > s > 0$ . Comparing this with the temperature dependencies (28b) and (30), we note that the results for  $s < 1/2$  violate  $\omega/T$  scaling, while those for  $1 > s > 1/2$  are compatible with it.

### C. Correlation time

To find the inverse correlation time (characteristic energy)  $\Delta = \xi_t^{-1}$ , we parametrize the inverse susceptibility as  $\epsilon + \alpha \omega_c^{1-s} |\omega_n|^s = \epsilon(1 + |\omega_n/\Delta|^s)$ . This implies the relation

$$\Delta = (\epsilon \alpha^{-1} \omega_c^{s-1})^{1/s}. \quad (33)$$

The dependence of the inverse correlation time on the tuning parameter  $\alpha$  at zero temperature and field in the case of  $1 > s > 1/2$  is obtained by inserting Eq. (14) into Eq. (33). In the disordered phase,  $\alpha < \alpha_c$ , this gives

$$\Delta = \omega_c A^{-1/(1-s)} (\alpha_c - \alpha)^{1/(1-s)} \quad (s > 1/2). \quad (34)$$

The correlation-time critical exponent therefore reads  $\nu z = 1/(1 - s)$ . Note that this exponent is sometimes called just  $\nu$  rather than  $\nu z$  in the literature on impurity transitions. We follow the general convention for quantum phase transitions where  $\nu$  describes the divergence of the correlation *length* while  $\nu z$  that of the correlation *time*. By substituting Eq. (17b) into Eq. (33), we can also determine the dependence of  $\Delta$  on temperature at  $\alpha = \alpha_c$  and  $h = 0$ . We find  $\Delta = A^{-1} T$ . The characteristic energy thus scales with  $T$ , as expected from naive scaling.

In the case of  $s < 1/2$ , the zero-temperature, zero-field correlation time in the disordered phase behaves as [using Eq. (15)]

$$\Delta = \omega_c B^{-1/s} (\alpha_c - \alpha)^{1/s} \quad (s < 1/2), \quad (35)$$

resulting in the mean-field value  $\nu z = 1/s$  for the correlation time critical exponent. The dependence of  $\Delta$  on temperature at  $\alpha = \alpha_c$  and  $h = 0$  follows from Eq. (18b); it reads  $\Delta = B^{-1/(2s)} \omega_c^{(2s-1)/(2s)} T^{1/(2s)}$ . The characteristic energy thus scales differently than the temperature, in disagreement with naive scaling.

### D. Scaling form of the equation of state

A scaling form of the equation of state for  $1 > s > 1/2$  can be determined by subtracting the quantum critical ( $T = 0$ ,

$h = 0, \alpha = \alpha_c$ ) spherical constraint from the general constraint (12). After performing the resulting integral, we find

$$\frac{\alpha_c - \alpha}{\alpha} + \frac{h^2}{\epsilon^2} + \frac{T}{\epsilon} = A\epsilon^{-1+1/s}\alpha^{-1/s}\omega_c^{1-1/s}. \quad (36)$$

We substitute  $\epsilon = h/M$  [from Eq. (22)], and after some lengthy but straightforward algebra, this equation can be written in the scaling form

$$X(M/r^{1/2}, h/r^{(1+s)/(2-2s)}, T/r^{1/(1-s)}) = 0, \quad (37)$$

with  $X$  being the scaling function and  $r = (\alpha - \alpha_c)/\alpha$  being the reduced distance from criticality. This scaling form can be used to reproduce the critical exponents  $\beta = 1/2$ ,  $\gamma = s/(1-s)$ , and  $\delta = (1+s)/(1-s)$  found above. For  $s < 1/2$ , the same approach gives a scaling equation containing the mean-field exponents  $\beta = 1/2$ ,  $\gamma = 1$ , and  $\delta = 3$ . Moreover, an explicit dependence on the cutoff for the Matsubara frequencies remains.

### E. Entropy and specific heat

Within our path integral approach, thermal properties are somewhat harder to calculate than magnetic properties because the measure of the path integral explicitly depends on temperature. As the spherical model is equivalent to a set of coupled harmonic oscillators, we can use the ‘‘remarkable formulas’’ derived by Ford *et al.*,<sup>33</sup> which express the free energy (and internal energy) of a quantum oscillator in a heat bath in terms of its susceptibility and the free energy (and internal energy) of a free oscillator. For our spherical model, they read

$$F_S = -\mu + \frac{1}{\pi} \int_0^\infty d\omega F_f(\omega, T) \operatorname{Im} \left[ \frac{d}{d\omega} \ln \chi(\omega) \right], \quad (38)$$

$$U_S = -\mu + \frac{1}{\pi} \int_0^\infty d\omega U_f(\omega, T) \operatorname{Im} \left[ \frac{d}{d\omega} \ln \chi(\omega) \right]. \quad (39)$$

Here,  $F_f(\omega, T) = T \ln[2 \sinh(\omega/2T)]$  and  $U_f(\omega, T) = (\omega/2) \coth(\omega/2T)$ . The extra  $-\mu$  terms stem from the spherical constraint. Note that the free energy in Eq. (38) is the difference between the free energy of the coupled rotor-bath system and that of the unperturbed bath,  $F_S = F - F_B^0 = -T \ln(Z/Z_B^0)$ . The same holds true for the internal energy  $U_S = U - U_B^0$ .

The frequency derivative of  $\ln \chi(\omega)$  can be calculated from Eq. (31), giving

$$\begin{aligned} & \operatorname{Im} \left[ \frac{d}{d\omega} \ln \chi(\omega) \right] \\ &= \frac{\epsilon s \alpha \omega_c^{1-s} \omega^{s-1} \sin(\pi s/2)}{[\epsilon + \alpha \omega_c^{1-s} \omega^s \cos(\pi s/2)]^2 + [\alpha \omega_c^{1-s} \omega^s \sin(\pi s/2)]^2}. \end{aligned} \quad (40)$$

To calculate the impurity entropy  $S_S = (U_S - F_S)/T$ , we insert Eq. (40) into Eqs. (38) and (39) and perform the resulting integral. In the disordered phase  $\alpha < \alpha_c$ , the entropy behaves as

$$S_S = D \alpha \omega_c^{1-s} T^s / \epsilon_0 \quad (41)$$

in the limit  $T \rightarrow 0$  for all  $s$  in the sub-Ohmic range  $1 > s > 0$ . Here,  $\epsilon_0$  is the zero-temperature renormalized distance from

criticality given in Eq. (14), and  $D$  is an  $s$ -dependent constant. Upon approaching criticality  $\alpha \rightarrow \alpha_c$ , the prefactor of the  $T^s$  power-law diverges, suggesting a weaker temperature dependence at criticality. The specific heat can be calculated from  $C_S = T(\partial S_S/\partial T)$ , it thus behaves as  $D s \alpha \omega_c^{1-s} T^s / \epsilon_0$ .

We now turn to the critical dissipation strength  $\alpha = \alpha_c$ . For  $1 > s > 1/2$ , we find a temperature-independent but nonuniversal ( $s$ -dependent) entropy in the limit of low temperatures. For  $s < 1/2$ , the impurity entropy diverges logarithmically as  $\ln(\omega_0/T)$  with  $T \rightarrow 0$ . In the ordered phase  $\alpha > \alpha_c$ , we find a logarithmically diverging entropy for all  $s$  between 0 and 1.

At first glance, these logarithmic divergencies appear to violate the third law of thermodynamics. We emphasize, however, that the impurity entropy represents the difference between the entropy of the coupled rotor-bath system and that of the unperturbed bath. Because the bath is infinite, the entropy thus involves an *infinite* number of degrees of freedom and does not have to remain finite. Whether the logarithmic divergence occurs only in the large- $N$  limit or also for finite- $N$  rotors remains a question for the future.

We note in passing that the entropy of classical spherical models<sup>27,34</sup> also diverges in the limit  $T \rightarrow 0$  (even when measured per degree of freedom). In these models, the divergence occurs because the classical description becomes invalid at sufficiently low temperatures. It can be cured by going from the classical spherical model to the quantum spherical model.<sup>28</sup> This implies that the diverging entropy in the ordered phase of the sub-Ohmic rotor model is caused by a different mechanism than that in the classical spherical model.

### V. CONCLUSIONS

In summary, we have investigated the quantum critical behavior of a large- $N$  quantum rotor coupled to a sub-Ohmic bosonic bath characterized by a power-law spectral density  $J(\omega) \sim \omega^s$  with  $0 < s < 1$ . As this model can be solved exactly, it provides a reliable reference point for the discussion of more complex and realistic impurity quantum phase transitions. We find that all critical exponents take their mean-field values if the bath exponent  $s$  is below  $1/2$ . In contrast, for  $1 > s > 1/2$ , the exponents display nontrivial,  $s$ -dependent values. A summary of the exponent values in both cases is shown in Table I. The exponent  $\eta$  sticks to its mean-field value  $2 - s$  in the entire region  $1 > s > 0$ , in agreement with renormalization group arguments on the absence of field renormalization for long-range interactions.<sup>35</sup> The fact that the order parameter exponent  $\beta$  is  $1/2$  in the entire range  $1 > s > 0$  is a result of the large- $N$  limit; it generically takes this value in spherical models.

TABLE I. Critical exponents of the sub-Ohmic quantum rotor model.

	$1 > s > 1/2$	$s < 1/2$
$\beta$	$1/2$	$1/2$
$\gamma$	$s/(1-s)$	$1$
$\delta$	$(1+s)/(1-s)$	$3$
$\nu z$	$1/(1-s)$	$1/s$
$\eta$	$2-s$	$2-s$

Moreover, the behaviors of the dynamic susceptibility and inverse correlation time are compatible with  $\omega/T$  scaling for  $1 > s > 1/2$ , while they violate  $\omega/T$  scaling for  $s < 1/2$ . We conclude that the quantum phase transition of the sub-Ohmic quantum rotor model is controlled by an interacting renormalization group fixed point in the case  $1 > s > 1/2$ . In contrast, the transition is controlled by a noninteracting (Gaussian) fixed point for  $s < 1/2$ .

We now turn to the question of the quantum-to-classical mapping. The classical counterpart of the sub-Ohmic quantum rotor model is a one-dimensional classical Heisenberg chain with long-range interactions that decay as  $1/r^{1+s}$  with distance  $r$ . The spherical (large- $N$ ) version of this model was solved by Joyce,<sup>27</sup> its critical exponents are identical to that of the sub-Ohmic quantum rotor found here. The quantum-to-classical mapping is thus valid.

The properties of our quantum *rotor* model must be contrasted with the behavior of the Bose-Kondo model which describes a continuous symmetry quantum *spin* coupled to a bosonic bath. For this system, the quantum-to-classical mapping appears to be inapplicable.<sup>23</sup> A related observation has been made in a Bose-Fermi-Kondo model.<sup>24</sup> The main difference between a rotor and a quantum spin is the presence of the Berry phase term in the action of the latter. Our results thus support the conjecture that this Berry phase term, which is complex and has no classical analog, causes the inapplicability of the quantum-to-classical mapping.

#### ACKNOWLEDGMENTS

We acknowledge helpful discussions with M. Vojta and S. Kirchner. This work has been supported in part by the NSF under Grant No. DMR-0906566.

- 
- <sup>1</sup>S. Sachdev, *Quantum phase transitions* (Cambridge University Press, Cambridge, 1999).
- <sup>2</sup>S. L. Sondhi, S. M. Girvin, J. P. Carini, and D. Shahar, *Rev. Mod. Phys.* **69**, 315 (1997).
- <sup>3</sup>T. Vojta, *Ann. Phys. (Berlin)* **9**, 403 (2000).
- <sup>4</sup>M. Vojta, *Rep. Prog. Phys.* **66**, 2069 (2003).
- <sup>5</sup>P. Coleman and A. J. Schofield, *Nature (London)* **433**, 226 (2005).
- <sup>6</sup>P. Gegenwart, Q. Si, and F. Steglich, *Nat. Phys.* **4**, 186 (2008).
- <sup>7</sup>S. Sachdev, *Nat. Phys.* **4**, 173 (2008).
- <sup>8</sup>M. Vojta, *Philos. Mag.* **86**, 1807 (2006).
- <sup>9</sup>P. W. Anderson, G. Yuval, and D. R. Hamann, *Phys. Rev. B* **1**, 4464 (1970).
- <sup>10</sup>D. Withoff and E. Fradkin, *Phys. Rev. Lett.* **64**, 1835 (1990).
- <sup>11</sup>A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, *Rev. Mod. Phys.* **59**, 1 (1987).
- <sup>12</sup>U. Weiss, *Quantum dissipative systems* (World Scientific, Singapore, 1993).
- <sup>13</sup>R. Bulla, N.-H. Tong, and M. Vojta, *Phys. Rev. Lett.* **91**, 170601 (2003).
- <sup>14</sup>M. Vojta, N.-H. Tong, and R. Bulla, *Phys. Rev. Lett.* **94**, 070604 (2005).
- <sup>15</sup>A. Winter, H. Rieger, M. Vojta, and R. Bulla, *Phys. Rev. Lett.* **102**, 030601 (2009).
- <sup>16</sup>A. Alvermann and H. Fehske, *Phys. Rev. Lett.* **102**, 150601 (2009).
- <sup>17</sup>M. Vojta, R. Bulla, F. Gütge, and F. Anders, *Phys. Rev. B* **81**, 075122 (2010).
- <sup>18</sup>N.-H. Tong and Y.-H. Hou, e-print arXiv:1012.5615.
- <sup>19</sup>S. Kirchner, *J. Low Temp. Phys.* **161**, 282 (2010).
- <sup>20</sup>M. T. Glossop and K. Ingersent, *Phys. Rev. Lett.* **95**, 067202 (2005).
- <sup>21</sup>S. Kirchner, Q. Si, and K. Ingersent, *Phys. Rev. Lett.* **102**, 166405 (2009).
- <sup>22</sup>M. Cheng, M. T. Glossop, and K. Ingersent, *Phys. Rev. B* **80**, 165113 (2009).
- <sup>23</sup>S. Sachdev, C. Buragohain, and M. Vojta, *Science* **286**, 2479 (1999).
- <sup>24</sup>L. Zhu, S. Kirchner, Q. Si, and A. Georges, *Phys. Rev. Lett.* **93**, 267201 (2004).
- <sup>25</sup>L. F. Cugliandolo, D. R. Grempel, G. Lozano, H. Lozza, and C. A. da Silva Santos, *Phys. Rev. B* **66**, 014444 (2002).
- <sup>26</sup>S. Drewes, D. P. Arovas, and S. Renn, *Phys. Rev. B* **68**, 165345 (2003).
- <sup>27</sup>G. S. Joyce, *Phys. Rev.* **146**, 349 (1966).
- <sup>28</sup>T. Vojta, *Phys. Rev. B* **53**, 710 (1996); T. Vojta and M. Schreiber, *ibid.* **53**, 8211 (1996).
- <sup>29</sup>For the original rotor, this corresponds to a field coupling to all components,  $\mathbf{h} = h(1, 1, \dots, 1)$ . This convention is convenient because the components remain equivalent even in the presence of a field.
- <sup>30</sup>Equivalently, the  $N$ -component rotor is coupled to  $N$ -component oscillators.
- <sup>31</sup>R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
- <sup>32</sup>This is analogous to the usual analysis of Bose-Einstein condensation where the  $\mathbf{q} = 0$  mode has to be treated separately below the condensation temperature.
- <sup>33</sup>G. W. Ford, J. T. Lewis, and R. F. O'Connell, *Phys. Rev. Lett.* **55**, 2273 (1985); *Ann. Phys. (NY)* **185**, 270 (1988).
- <sup>34</sup>T. H. Berlin and M. Kac, *Phys. Rev.* **86**, 821 (1952).
- <sup>35</sup>M. E. Fisher, S.-K. Ma, and B. G. Nickel, *Phys. Rev. Lett.* **29**, 917 (1972); M. Suzuki, *Prog. Theor. Phys.* **49**, 424 (1973); **49**, 1106 (1973).