Entanglement between a qubit and the environment in the spin-boson model

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The quantitative description of the quantum entanglement between a qubit and its environment is considered. Specifically, for the ground state of the spin-boson model, the entropy of entanglement of the spin is calculated as a function of α, the strength of the ohmic coupling to the environment, and ε, the level asymmetry. This is done by a numerical renormalization group treatment of the related anisotropic Kondo model. For $\varepsilon=0$, the entanglement increases monotonically with α, until it becomes maximal for $\alpha\rightarrow 1^-$. For fixed $\varepsilon>0$, the entanglement is a maximum as a function of α for a value, $\alpha=\alpha_M<1$.

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Due to the promise of quantum computation there is currently considerable interest in the relationship between entanglement, decoherence, entropy, and measurement. Motivated by quantum information theory several authors have recently investigated entanglement in quantum many-body systems [2,1,3,4]. It is often stated that decoherence or a measurement causes a system to become entangled with its environment. The purpose of this paper is to make these ideas quantitative by a study of the simplest possible model, the spin-boson model [5,6]. This describes a qubit (two-level system) interacting with an infinite collection of harmonic oscillators that model the environment responsible for decoherence and dissipation. Specifically, we show how the entanglement between a superposition state of the qubit and the environment changes as the coupling between the qubit and environment increases. One interesting result is that we find that the qubit becomes maximally entangled with the environment when the coupling α approaches a particular finite value ($\alpha\rightarrow 1^-$). Furthermore, at this value the model undergoes a quantum phase transition, which is consistent with recent observations that often entanglement is largest near quantum critical points [2,1,3,4].

The spin-boson model. The Hamiltonian is [5,6]

$$H_{SB}=\frac{1}{2}\Delta\sigma_x+\frac{1}{2}\varepsilon\sigma_z+\sum_i \omega_i\left(a_i^\dagger a_i+\frac{1}{2}\right)+\frac{1}{2}\sigma_z\sum_i \lambda_i(a_i+a_i^\dagger), \quad (1)$$

where Δ is the bare tunneling amplitude between the two quantum-mechanical states $\uparrow$ and $\downarrow$, ε is the level asymmetry (or bias), ω_i are the frequencies of the oscillators, and λ_i is the strength with which they couple to the two quantum-mechanical states. The effect of the oscillator bath is completely determined by the spectral function $J(\omega)$, defined below [5]. We will only consider the ohmic case, where it is has a linear dependence on frequency

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

for $\omega\ll\omega_c$, and α is the dimensionless dissipation strength. The cutoff frequency $\omega_c\gg\Delta$. This model can describe the decoherence of Josephson junction qubits, such as those recently realized experimentally [7], due to voltage fluctuations in the electronic circuit [8], and α can be expressed in terms of resistances and capacitances in the circuit and so this is an experimentally tunable parameter. Recent results show it is possible to construct devices with $\alpha\ll 1$, the regime required for quantum computation. However, when modeling measurements one has $\alpha\sim 1$.

The dynamical properties of the model have been extensively studied. In particular, suppose the spin (qubit) is initially in a pure state which is a product state of up spin and the environment state, then the coherent Rabi oscillations that would be observed in the absence of coupling to the environment are modified as follows. One finds distinct behavior for $0<\alpha<1/2$ (damped coherent oscillations), $1/2<\alpha<1$ (exponential decay), and $1<\alpha$ (localization, i.e., the spin remains in the up state) [5,6,9,15].

Entropy of entanglement. We now consider a quantitative description of the entanglement of the qubit with the environment. A good entanglement measure for a pure state is the von Neumann entropy or entropy of entanglement [10,11]

$$E(\rho)=-\mathrm{Tr}(\rho\log_2\rho), \quad (2)$$

where ρ is the reduced density matrix of the qubit. This is a two by two matrix given by

$$\rho=\frac{1}{2}\left(1+\sum_{a=x,y,z}\langle\sigma_a\rangle\sigma_a\right), \quad (3)$$

where $\langle\sigma_a\rangle$ denotes the expectation value in the state of interest. In this case Eq. (2) reduces to

$$E(\rho)=-p_+\log_2 p_+-p_-\log_2 p_-, \quad (4)$$

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where $p_\pm$ are the eigenvalues of the density matrix,

$$p_\pm = \frac{1}{2}(1 \pm |\langle \vec{\sigma} \rangle|). \tag{5}$$

For $\varepsilon = 0$ the only nonzero value of $\langle \sigma_a \rangle$ is $\langle \sigma_x \rangle$. At $T = 0$ it is given by

$$\langle \sigma_x \rangle = 2\frac{\partial E_0}{\partial \Delta}, \tag{6}$$

where E_0 is the ground-state energy of the Hamiltonian (1), and use has been made of the Feynman-Hellmann theorem. That the other values are zero can be seen by symmetry as follows. In general the Hamiltonian is invariant under the reflection in spin space, $\sigma_y \to -\sigma_y$. Hence, all eigenstates must have a definite parity under this transformation. Thus, $\langle \sigma_y \rangle = -\langle \sigma_y \rangle$ for all states and so $\langle \sigma_y \rangle = 0$ at any temperature. For $\varepsilon = 0$ the Hamiltonian is also invariant under the joint transformation $\sigma_z \to -\sigma_z$ and $a_i \to -a_i$ and so $\langle \sigma_z \rangle = 0$ at any temperature, provided there is no symmetry breaking.

The challenge is now to evaluate the ground-state expectation values $\langle \sigma_x \rangle$ and $\langle \sigma_z \rangle$. For $\alpha > 1/2$ and particularly for $\alpha \sim 1$ this is a highly nontrivial problem because in this regime nonperturbative effects become important [5,6]. However, we show how these expectation values can be evaluated using the numerical renormalization group (NRG) applied to the equivalent anisotropic Kondo model.

Anisotropic Kondo Model. The above model is equivalent to the anisotropic Kondo model (AKM), defined by [12]

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{J_\perp}{2}(c^\dagger_{0\uparrow} c_{0\downarrow} S^- + c^\dagger_{0\downarrow} c_{0\uparrow} S^+) + \frac{J_\parallel}{2}(c^\dagger_{0\uparrow} c_{0\uparrow} - c^\dagger_{0\downarrow} c_{0\downarrow}) S^z + g\mu_B h S_z. \tag{7}$$

The first term represents a free electron conduction band. We use a flat density of states $\rho_0 = 1/2D_0$ per spin, with $2D_0$ the bandwidth. The second and third terms represent the transverse and longitudinal parts of the exchange interaction between a $S = 1/2$ impurity and the local conduction-electron spin density, and the last term represents a Zeeman term for a magnetic-field coupling only to the impurity spin. The correspondence between H and H_{SB}, established via bosonization [13,14], implies $\varepsilon = g\mu_B h$, $\Delta/\omega_c = \rho_0 J_\perp$, and $\alpha = (1 + 2\delta/\pi)^2$, where $\tan \delta = -\pi \rho_0 J_\parallel / 4$. δ is the phase shift for scattering of electrons from a potential $J_\parallel/4$ [5,15,13]. We choose $\omega_c = 2D_0$ so that $\Delta = J_\perp$. This equivalence has been used extensively to make predictions about the dynamics [15] and thermodynamics [14] of the ohmic spin-boson model. The relevant low-energy scale for the thermodynamics is the Kondo scale $T_K(J_\perp, J_\parallel)$ which is identified with the renormalized tunneling amplitude Δ_r of the spin-boson model,

$$\frac{\Delta_r}{\omega_c} = \left(\frac{\Delta}{\omega_c}\right)^{1/(1-\alpha)}. \tag{8}$$

We restrict ourselves in this paper to the longitudinal sector of the AKM, i.e., to $J_\perp < |J_\parallel|$, where the simple parameter correspondence between the models given above remains valid to lowest order in $\Delta/\omega_c = \rho_0 J_\perp$. For larger values of Δ/ω_c, α will acquire a renormalization due to finite $\Delta = J_\perp$, as indicated by the scaling analysis of the AKM in Refs. [12,14]. This renormalization, however, is important mainly for the transverse sector of the AKM, $J_\perp > |J_\parallel|$, which we do not consider in this paper.

We turn now to the evaluation of $\langle \sigma_x \rangle$. The equivalence between models ensures that the AKM has (to within an additive constant) the same ground-state energy E_0 as that of the spin-boson model. At $T = 0$, we therefore find, in analogy to Eq. (6) applied to the AKM with $\Delta = J_\perp$, that

$$\langle \sigma_x \rangle = \langle c^\dagger_{0,\uparrow} c_{0,\downarrow} S^- + \text{H.c.} \rangle, \tag{9}$$

i.e., $\langle \sigma_x \rangle$ can be obtained from a *local* static correlation function. Another way of seeing that this relation is valid, is to note that the unitary transformation in bosonization which transforms H into H_{SB} also transforms $(c^\dagger_{0,\uparrow} c_{0,\downarrow} S^- + \text{H.c.})$ into σ_x of the spin-boson model (details of this mapping can be found in Ref. [13] and in greater detail in Appendix A of Ref. [14]). The same unitary transformation on the AKM transforms $\langle S_z \rangle$ into $\sigma_z/2$ of the spin-boson model. The latter can therefore be calculated directly within the AKM as a thermodynamic average $\langle 2S_z \rangle$.

Method. The above local correlation function can be calculated from Wilson's NRG method [16] which has been shown to give very reliable results for quantum impurity models such as the AKM [17]. The approach used here allows in addition the calculation of local dynamical quantities, such as the dynamical susceptibility $\langle\langle c^\dagger_{0,\uparrow} c_{0,\downarrow} S^-; c^\dagger_{0,\downarrow} c_{0,\uparrow} S^+ \rangle\rangle$ [18]. In outline (see Ref. [16] for the details), the procedure consists of introducing a logarithmic mesh of k points $k_n = \Lambda^{-n}, \Lambda > 1$ for the conduction band and performing a unitary transformation of the $c_{k\sigma}$ such that $f_{0\sigma} = \Sigma_k c_{k\sigma}$ is the first operator in a new basis $f_{n\sigma}, n = 0,1,\ldots,$ which tridiagonalizes $H_c = \Sigma_{k\mu} \epsilon_{k\mu} c^\dagger_{k\mu} c_{k\mu}$ in k space. The Hamiltonian (7) with the discretized form of the kinetic energy is now diagonalized by the following iterative process: (a) One defines a sequence of finite-size Hamiltonians $H_N = \Sigma_\mu \Sigma_{n=0}^{N-1} \xi_n \Lambda^{-n/2} (f^\dagger_{n+1\mu} f_{n\mu} + \text{H.c.}) + (J_\perp/2)(f^\dagger_{0\uparrow} f_{0\downarrow} S^- + f^\dagger_{0\downarrow} f_{0\uparrow} S^+) + (J_\parallel/2)(f^\dagger_{0\uparrow} f_{0\uparrow} - f^\dagger_{0\downarrow} f_{0\downarrow}) S^z$ for $N \gg 0$ and $\xi_n \to 1$ for $n \gg 1$ [16]; (b) The sequence of Hamiltonians H_N for $N = 0,1,\ldots$ is iteratively diagonalized within a product basis of, typically, up to 1200 states for each iteration, up to a maximum value $N = N_m$. This gives the excitations and many-body eigenstates at a corresponding set of energy scales ω_N defined by the lowest scale $\omega_N = \Lambda^{-(N-1)/2}$ in H_N. The matrix elements $\langle m | O_{x,z} | n \rangle_N$ for the operators $O_x = c^\dagger_{0,\uparrow} c_{0,\downarrow} S^-$ and $O_z = S_z$, required to calculate $\langle \sigma_x \rangle$ and $\langle \sigma_z \rangle$, are also calculated iteratively. The choice of N_m depends on the Kondo scale $T_K = \Delta_r$ and hence on α, but for given α (i.e., for given $J_\perp, J_\parallel$) should be large enough such that $\omega_{N_m} \ll \Delta_r$. A discretization parameter $\Lambda = 1.5$ was used throughout and we checked that the above expectation values remained unchanged on further increasing N_m. This

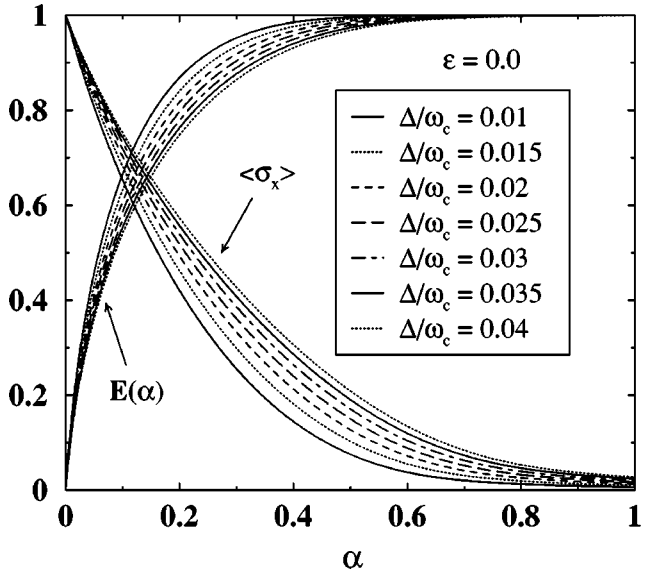

FIG. 1. The dependence of (i) the ground-state expectation value $\langle\sigma_x\rangle$ as a function of the dimensionless coupling α to the environment for $\varepsilon=0$ and (ii) the entanglement entropy E of a qubit ohmically coupled to an environment as a function of α for $\varepsilon=0$. The different curves correspond to different values of the ratio of the bare tunneling amplitude Δ to the cutoff frequency of the boson bath ω_c. Note that as $\alpha\rightarrow 1^-$ the qubit becomes maximally entangled with the environment.

suggested that our approximation of using a finite N_m to calculate the thermodynamic expectation values of the infinite system is a very good one.

Symmetric case. For $\varepsilon=0$ and $\alpha<1$ only $\langle\sigma_x\rangle$ is nonvanishing. We show this in Fig. 1 at $T=0$ versus dimensionless dissipation strength α in the range $0<\alpha<1$, and for several values of the dimensionless tunneling amplitude Δ/ω_c. The limiting noninteracting value $\langle\sigma_x\rangle\rightarrow 1$ is recovered as $\alpha\rightarrow 0$. In the limit $\Delta/\omega_c\rightarrow 0$ it vanishes at the quantum critical point of the spin-boson model $\alpha=1$ where $\Delta_r\rightarrow 0$. For any finite fixed Δ/ω_c, however, our use of the AKM implies that the critical behavior occurs at $\alpha_c>1$ with $\alpha_c\rightarrow 1$ as $J_\perp\rightarrow 0$ (specifically, this critical behavior occurs at the ferromagnetic-antiferromagnetic boundary $J_\perp=-J_\parallel$). Figure 1 also shows the $T=0$ entropy of entanglement of the qubit. The entropy vanishes as $\alpha\rightarrow 0$ and approaches its maximum value as $\alpha\rightarrow 1^-$ (see also Ref. [20] for weak dissipation results for E). For $\alpha>1$, we are in the ferromagnetic sector of the AKM where $\langle\sigma_z\rangle=1,\langle\sigma_x\rangle=0$, and the reduced density matrix eigenvalues $p_\pm=0,1$ giving $E=0$, i.e., $E(\alpha)$ drops discontinuously at the quantum critical point $\alpha=1$ [19]. It is interesting that for a spin qubit coupled to two bosonic baths it is possible to remain in the delocalized phase (i.e., $\langle\sigma_z\rangle=0$) for all dissipation strengths [21]. Finally, we note that the entropy of entanglement is quite different from the thermodynamic entropy of the boundary (or impurity spin entropy). The latter is usually defined as $S(\alpha)-S(\alpha=0)$ where $S(\alpha)$ is the total thermodynamic entropy of the system [14]. The impurity spin entropy is zero for $\alpha<1$ because the ground state of the AKM is a spin singlet for $J_\parallel>0$.

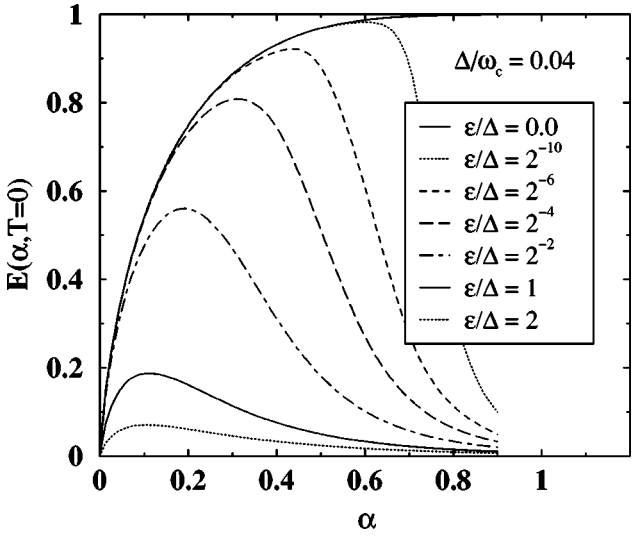

FIG. 2. The dependence of the entanglement entropy of the ground state on the coupling to the environment α and the level asymmetry ε for $\Delta/\omega_c=0.04$. Note that for $\varepsilon>0$, the entanglement is a maximum at $\alpha=\alpha_M<1$.

Asymmetric case. For $\varepsilon>0$, $\langle\sigma_z\rangle$ acquires a finite value analogous to the magnetization $\langle S_z\rangle$ in a local magnetic field $g\mu_B h=\varepsilon$ in the AKM. The entanglement entropy E now depends on $|\langle\vec{\sigma}\rangle|=(|\langle\sigma_x\rangle|^2+|\langle\sigma_z\rangle|)^{1/2}$ via Eq. (3) and is shown in Fig. 2. The behavior of E as a function of α and ε is understood from the behavior of $\langle\sigma_x\rangle$ and $\langle\sigma_z\rangle$ shown in Fig. 3. In particular, we now find that for arbitrary small ε, the entanglement entropy first increases with increasing α before reaching a maximum value at $\alpha=\alpha_M<1$ and then decreasing as $\alpha\rightarrow 1$. This behavior arises from the competition between the α dependence of $\langle\sigma_x\rangle$ and $\langle\sigma_z\rangle$ in Fig. 3. Whereas $\langle\sigma_x\rangle$ continues to decrease monotonically with increasing α (as for $\varepsilon=0$), it is seen that $\langle\sigma_z\rangle$ increases mono-

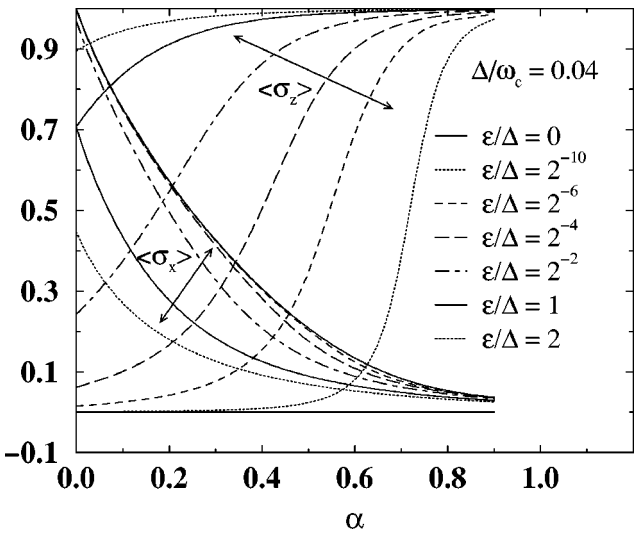

FIG. 3. The dependence of the ground-state expectation values $\langle\sigma_x\rangle$, $\langle\sigma_z\rangle$ on α and ε for $\Delta/\omega_c=0.04$. For $\alpha=0$ the noninteracting values $\langle\sigma_x\rangle=\Delta/\sqrt{\varepsilon^2+\Delta^2}$ and $\langle\sigma_z\rangle=\varepsilon/\sqrt{\varepsilon^2+\Delta^2}$ are recovered for all values of ε/Δ.

tonically with increasing α, with $\langle\sigma_z\rangle\to 1$ as $\alpha\to 1$. The condition for full polarization, $\langle\sigma_z\rangle\approx 1$, is $\varepsilon\gg\Delta_r$. For any $\varepsilon>0$, this condition is always satisfied since $\Delta_r\to 0$ as $\alpha\to 1$. It follows that $|\langle\vec{\sigma}\rangle|$ has a minimum as a function of α and that the entanglement entropy, for $\varepsilon>0$, has a maximum at $\alpha=\alpha_M<1$ before decreasing again as $\alpha\to 1$.

Finally, we suggest several directions for future work.

(i) This work focused solely on static properties of the spin-boson model. It would be interesting to consider dynamics, for example, the longitudinal and the transverse dynamical susceptibilities, and hence extract the decoherence and relaxation rates for an ohmically coupled qubit. In addition, it is interesting to ask how the entanglement varies with time if the initial state has no entanglement of the qubit and the environment.

(ii) The AKM is integrable by the Bethe ansatz [22]. The AKM can also be related to a free boson field theory with a boundary sine-Gordon term [9,23] which is also integrable by the Bethe ansatz. Exact expressions can be obtained for the free energy. It involves solving a set of thermodynamic Bethe ansatz (TBA) equations. At $T=0$ the impurity ground-state energy is going to be related to T_K. The real problem is getting results for arbitrary anisotropies (dissipation strengths) [24].

(iii) Recently it was shown [4] that if in a quantum critical system one calculates the entropy of entanglement of a subsystem of size L with the rest of the system this equals the geometric entropy previously calculated for the corresponding conformal field theory (motivated by questions concerning black-hole thermodynamics!) [25]. It would be interesting to perform similar calculations for the relevant boundary field theory.

(iv) The NRG can also be used to reliably calculate properties of the spin-boson model at nonzero temperature [19]. However, calculating the entanglement at nonzero temperature is an open problem because it involves a mixed state and it is not practical to evaluate the measure of entanglement that has been proposed for such states [10].

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