Transition between quantum coherence and incoherence

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We show that a transformed Caldeira-Leggett Hamiltonian has two distinct families of fixed points rather than a single unique fixed point as often conjectured based on its connection to the anisotropic Kondo model. The two families are distinguished by a sharp qualitative difference in their quantum coherence properties and we argue that this distinction is best understood as the result of a transition in the model between degeneracy and nondegeneracy in the spectral function of the ''spin-flip'' operator. [S1063-651X(97)05006-X]

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The prototypical model for studying the loss of quantum coherence is the Caldeira-Leggett or two-level system (TLS) model. This model describes a two-state degree of freedom coupled to a bath of harmonic oscillators and the Hamiltonian is given by

$$H_{\rm TLS}=\Delta\sigma_x+\frac{1}{2}\sigma_z\sum_i C_i x_i+\sum_i\left(\frac{1}{2}m_i\omega_i^2x_i^2+\frac{1}{2m_i}p_i^2\right). \tag{1}$$

Here C_i is the coupling to the ith oscillator and m_i, ω_i, x_i, and p_i are the mass, frequency, position, and momentum of the ith oscillator, respectively. We restrict our discussion of the model to zero temperature and the so-called Ohmic regime [1] where the spectral density of the bath is given by

$$J(\omega)=\frac{\pi}{2}\sum_i\frac{C_i^2}{m_i\omega_i}\delta(\omega-\omega_i)=2\pi\alpha\omega\exp(-\omega/\omega_c). \tag{2}$$

In connection with questions of quantum coherence, the spin is taken to represent a macroscopic variable and the oscillators an environmental bath of unobservable, microscopic degrees of freedom. If the coupling to this bath is strong enough, then the quantum interference effects that the isolated spin would exhibit can be wiped out by the effects of the environment. A quantity frequently studied in this context is $P(t)=\langle\sigma^z(t)\rangle$. Here $t>0$ and the state of the system is obtained by evolving forward in time from a $t=0$ state with $\sigma^z=1$ and the oscillator bath in its equilibrium state for σ^z clamped to $\sigma^z=1$. For vanishing coupling to the environment, $P(t)=\cos 2\Delta t$, with the oscillations resulting from the interference between the various possible histories of $\sigma^z(t')$, $0<t'<t$. As the coupling to the bath is turned on these interference effects are expected to be gradually wiped out, representing the generic loss of observability of interference effects between the different possible histories of $\sigma^z(t')$. This corresponds to the quantum to classical crossover for this model and it is known that for $\alpha=\frac{1}{2}$ [2], there are no oscillations of any kind and the interference effects are completely unobservable: $P(t)=\exp(-\Gamma t)$ with $\Gamma=\Delta^2/\omega_c$.

This behavior is naturally understood in a model obtained by making a canonical transformation [1] on the Hamiltonian [Eq. (1), hereafter referred to as TLS]: $H'_{\rm TLS}=\hat{U}H_{\rm TLS}\hat{U}^{-1}$, where

$$\hat{U}=\exp\left(-\frac{1}{2}\sigma_z\sum_i\frac{C_i}{m_i\omega_i^2}\hat{p}_i\right). \tag{3}$$

The new Hamiltonian takes the form

$$H'_{\rm TLS}=\frac{1}{2}\Delta(\sigma^+e^{-i\Omega}+{\rm H.c.})+H_{\rm oscillators}, \tag{4}$$

where $\Omega=\Sigma_i(C_i/m_i\omega_i^2)p_i$. Hereafter, we refer to Eq. (4) as the transformed Caldeira-Leggett (XCL) model.

In this model, the point $\alpha=\frac{1}{2}$ is special in that the Hamiltonian can be converted into that of the so-called resonant level model [3], which in turn is equivalent to the anisotropic Kondo problem at the Toulouse point [4]. In general, the XCL model can be connected in the limit of vanishing Δ to the anisotropic Kondo model Hamiltonian (AKM)

$$H_{\rm Kondo}=\sum_{k,\sigma}\epsilon_k c^\dagger_{k,\sigma}c_{k,\sigma}+\frac{J_{xy}}{2}\sum_{k,q}(c^\dagger_{k,\uparrow}c_{q,\downarrow}S^-+{\rm H.c.})+\frac{J_z}{2}\sum_{k,q}(c^\dagger_{k,\uparrow}c_{q,\uparrow}-c^\dagger_{k,\downarrow}c_{q,\downarrow})S^z \tag{5}$$

via the mapping

$$\Delta=\omega_c\rho J_{xy}, \tag{6}$$

$$\alpha=\left[1-\frac{2}{\pi}\arctan\left(\frac{\pi\rho J_z}{4}\right)\right]^2, \tag{7}$$

where ρ is the density of states that follows from ϵ_k. The AKM has a unique fixed point for all antiferromagnetic J_z $(0<\alpha<1)$ [5] and it has therefore been argued that the TLS and XCL Hamiltonians also have unique fixed points. However, the study of the XCL Hamiltonian by Guinea *et al.* [6] concluded that there was a line of fixed points for $0<\alpha<\frac{1}{2}$ and that only for $\alpha\geqslant\frac{1}{2}$ was the system described by the unique Kondo fixed point. It would have great intuitive appeal if the ''incoherent'' and ''coherent'' phases of the TLS model corresponded to different fixed points; however, a different study by Guinea [7] and another recent study [8,9] of the long-time behavior of $\langle \sigma^z(t)\sigma^z(0)\rangle$ concluded that asymptotic behavior is $\sim t^{-2}$ for any α with $0<\alpha<1$. This result is consistent with a unique fixed point. Thus, while there is some uncertainty, the accepted wisdom is that all three Hamiltonians exhibit only a single fixed point and that, consequently, no true, long-time distinction exists between the coherent and incoherent phases. The purpose of this paper is to demonstrate that, while the anisotropic Kondo model may possess a unique fixed point for antiferromagnetic J_z and we find no evidence for multiple fixed points in the regime $0<\alpha<1$ for the TLS Hamiltonian, the XCL Hamiltonian *does possess* an entire family of fixed points distinguished by different values of α [10]. Further, there is a true, qualitative, long-time distinction between the behavior for $0<\alpha<\frac{1}{2}$ and $\frac{1}{2}<\alpha<1$. This distinction is directly related to questions of quantum (in)coherence and, we believe, to the effective transition between degeneracy and nondegeneracy of the action of the spin-flip operator.

As mentioned, questions of quantum coherence have traditionally focused on the quantity $P(t)$ defined above and the question of whether or not it exhibits oscillations at ''intermediate times'' (times of order the Kondo scale). In the XCL model, there exists a more direct probe of quantum coherence: the off-diagonal components of the density matrix describing the two-state degree of freedom when the oscillator bath is traced over [11,12]. The sum of the two off-diagonal components of the density matrix is given by $\langle \sigma^x\rangle$, so we choose as our probes of quantum coherence the correlation functions of σ^x.

First, consider the behavior of the time symmetrized correlation: $F(t)=\frac{1}{2}\langle\{\sigma^x(t),\sigma^x(0)\}\rangle$ in the solvable limits $\alpha=0$ and $\alpha=1/2$. At $\alpha=0$, the problem is trivial and $F(t)=1$ because $\langle\sigma^x\rangle=1$; the system has maximal quantum coherence in the sense that the off-diagonal components of the density matrix are as large as the diagonal. At $\alpha=1/2$, the Toulouse refermionization may be used and $F(t)=\exp(-\Gamma t)$, which is identical to $P(t)$. At this point there is no sign of any quantum coherence: not only is $\langle\sigma^x\rangle=0$, but the correlations of σ^x entering into $F(t)$ decay faster than any power of t.

Now consider other values of α; here we follow the numerical approach of [8] and study the imaginary time correlation function $\langle\sigma^x(\tau)\sigma^x(0)\rangle$ using the Coulomb gas (CG) language [13]. Recall that the CG model related to the AKM is a one-dimensional model with alternating plus and minus charges that interact with a logarithmic Coulomb interaction whose strength is proportional to α [13]. We choose to use an inverse squared Ising (ISI) model as a specific realization of the CG with a short-distance regularization provided by the lattice. The ISI model is defined on N sites with the Hamiltonian

$$H_I=-\frac{J_{NN}}{2}\sum_{0\geqslant i<N} S_iS_{i+1}-\frac{J_{LR}}{2}\sum_{i<j}\frac{(\pi/N)^2S_iS_j}{\sin^2[\pi(j-i)/N]}, \tag{8}$$

where $J_{LR}=\alpha$, $N=\beta_{\mathrm{XCL}}$, and $\Delta\sim 2\exp[-J_{NN}-J_{LR}(1+\gamma)]$, with γ Euler's constant.

The correlation function $\mathcal{G}(\tau)=\langle\sigma^+(\tau)\sigma^-(0)\rangle$ is given by the ratio of a certain ''twisted'' CG partition function to the usual partition function. The twisted partition function is defined by restricting the sum over states to those where the charges on either side $x=0$ are positive and those on either side of $x=\tau$ are negative and requiring that, elsewhere, the charges alternate as usual. This ratio can be computed in the ISI language as the inverse of the usual ISI partition function times the sum over all states that have $\sigma^z(0)=1$ and $\sigma^z(\tau)=1$ of a Boltzmann-like term $\exp(-E_{\mathrm{modified}})$. E_{modified} is defined by $E_{\mathrm{modified}}=2E'+2E''-E-3E^0$. E, E', E'', and E^0 are the energies computed using the ISI Hamiltonian and, respectively, the actual configuration considered, the configuration obtained from the actual by removing all domain walls from spins 1 to τ, the configuration obtained from the actual by removing all domain walls from spins $\tau+1$ to N, and the fully polarized configuration. In the CG language, this reverses the signs of all the charges between $x=0$ and $x=\tau$, the appropriate operation for the change in allowed configurations induced by $\sigma^+(\tau)\sigma^-(0)$.

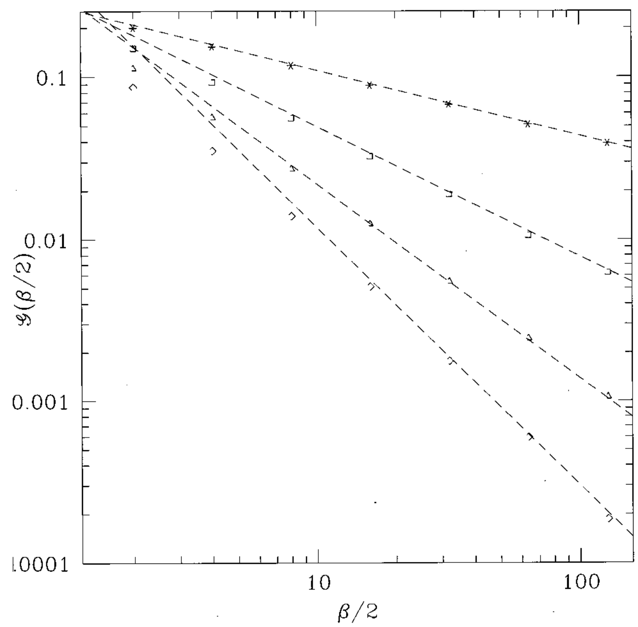

FIG. 1. A log-log plot of $\mathcal{G}(\tau=\beta/2=N/2)$ versus $\beta/2=N/2$. * correspond to $\alpha=0.2$, T_K (as defined in Ref. [7]) ~ 0.70; $\square$ to $\alpha=0.4$, $T_K\sim 0.66$; $\triangle$ to $\alpha=0.6$, $T_K\sim 0.62$; and $\diamond$ to $\alpha=0.8$, $T_K\sim 0.62$. Dashed lines are guides to the eye with slopes of 0.4, 0.8, 1.2, and 1.6, the expected behaviors if $\mathcal{G}(\tau=\beta/2=N/2)\propto\tau^{-2\alpha}$.

We have used Monte Carlo methods to study $\mathcal{G}(\tau)$ and typical results are depicted in Figs. 1 and 2. For distances large compared to the Kondo scale, the results are clearly well described by a power decay of $\mathcal{G}(\tau)$ as $\tau^{-2\alpha}$. The long-time behavior of $\mathcal{G}$ is therefore different for different α, which establishes that the XCL model possesses a line of fixed points, not a single strong-coupling fixed point [14]. The result can be simply understood in the CG language where the insertion of a σ^+ (σ^-) acts to change the allowed configurations to those requiring two consecutive positive (negative) charges about the insertion point. The finite fugacity of other charges translates this into an effective charge insertion for distances long compared to the Kondo scale, and this insertion of an extra charge cannot be screened since plus and minus charges are required to alternate away from

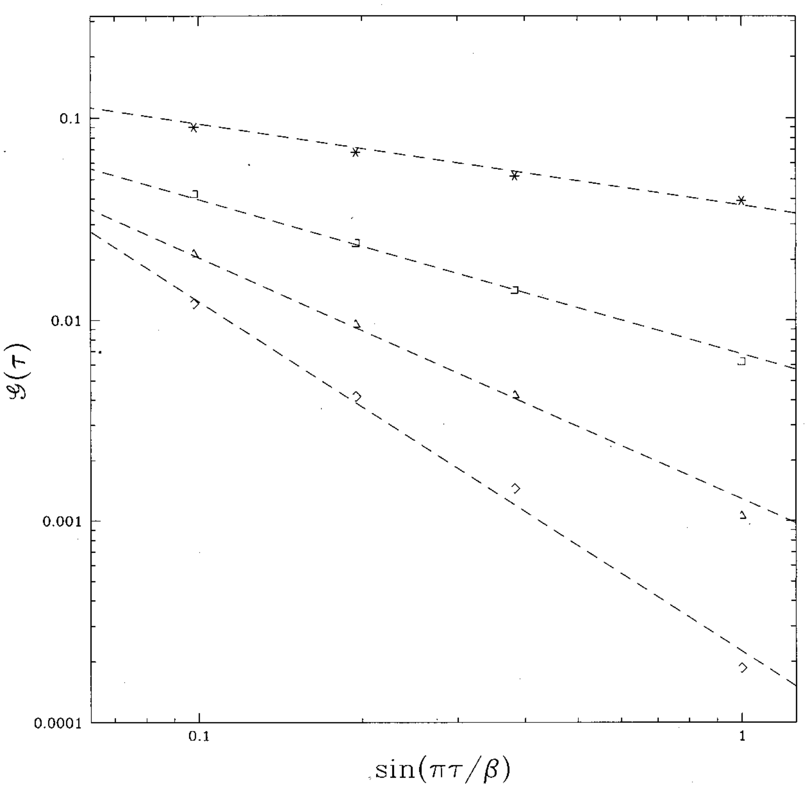

FIG. 2. A log-log plot of $\mathcal{G}(\tau)$ versus $\sin(\pi\tau/\beta)$ for $N=\beta=256$. * correspond to $\alpha=0.2$, $T_K\sim0.70$; □ to $\alpha=0.4$, $T_K\sim0.66$; △ to $\alpha=0.6$, $T_K\sim0.62$; and ◇ to $\alpha=0.8$, $T_K\sim0.62$. Dashed lines are guides to the eye with slopes of 0.4, 0.8, 1.2, and 1.6, the expected behaviors if $\mathcal{G}(\tau)\propto\sin^{-2\alpha}(\pi\tau/\beta)$.

insertions. Therefore, at long distances, G behaves as the charge insertion correlator with unrenormalized α.

While all α correspond to different fixed points, there is an important distinction between $\alpha<\frac{1}{2}$ and $\alpha>\frac{1}{2}$. For $0<\alpha<\frac{1}{2}$, the long-imaginary-time behavior of $\mathcal{G}$ dominates the low-frequency behavior and a continuation from Matsubara frequencies to real frequencies will give a low-frequency singularity in $G_{\mathrm{ret}}(\omega)\sim|\omega|^{-1+2\alpha}e^{i(\pi/2)(1-2\alpha)\mathrm{sgn}(\omega)}$. Since the spectral function diverges at low frequencies, we know that $G(t)\sim F(t)\sim t^{-2\alpha}$, with the prefactor in F vanishing as $\alpha\rightarrow\frac{1}{2}$ [15]. Throughout this region, the susceptibility of the systems with respect to a perturbation coupling to σ^x:

$$\chi_{\mathrm{coh}}=\int_0^\infty dt[\sigma^x(t),\sigma^x(0)], \tag{9}$$

is *divergent*; the system is enormously sensitive to any small perturbation that tends to induce coherence as defined by finite off-diagonal elements in the density matrix. Conversely, for $\frac{1}{2}<\alpha<1$, χ_{coh} is finite because of the rapid decay of the correlation functions of σ^x, and this sensitivity is absent.

We believe that the disappearance of the divergent susceptibility may be interpreted as a ‘‘transition’’ from degeneracy to nondegeneracy in the action of Δ, as has been previously suggested [16]. To understand this, consider the meaning of σ^+ (σ^-) in the XCL language. The Hilbert space of the system is spanned by the $\Delta=0$ eigenstates, which consist of two towers of oscillator eigenstates ($|A_i\rangle$ and $|B_i\rangle$). The towers are distinguished by the value of σ^z, but are otherwise identical ($|A_i\rangle=\sigma^+|B_i\rangle$). At finite Δ and for $\alpha<1$, the ground state is a complicated superposition of these states $[|\Psi_0\rangle=\Sigma_i(\lambda_i^a|A_i\rangle+\lambda_i^b|B_i\rangle)]$ with equal weight coming from each tower $(\Sigma_i|\lambda_i^a|^2=\Sigma_i|\lambda_i^b|^2=\frac{1}{2})$. σ^x converts the λ_i^b's into the λ_i^a's (and vice versa), probing the phase relationship between the λ^a's and the λ^b's. The vanishing of $\langle\sigma^+\rangle$ implies that the phases of the λ^a's and the λ^b's are, on average, completely uncorrelated in the ground state. This might appear natural since, away from $\alpha=0$, the matrix elements of the Δ term in the Hamiltonian connecting $|A_i\rangle$ and $|B_i\rangle$ vanish in the $\Delta=0$ ground state due to an orthogonality catastrophe. However, consider the spectral function in the $\Delta=0$ ground state for $e^{i\Omega}$:

$$\begin{aligned}\rho_\Delta(\omega)&=\sum_m |\langle m|e^{i\Omega}|\mathrm{g.s.}\rangle|^2\delta(\omega-E_m)\\&=\Gamma^{-1}(2\alpha)\theta_+(\omega)\omega^{-1+2\alpha}\omega_c^{-2\alpha}\exp(-\omega/\omega_c).\end{aligned} \tag{10}$$

For small α the spectral function is strongly peaked about small energy. The phases of the λ_i^a associated with various low-lying states $|A_i\rangle$ should therefore be weakly correlated with the phases of a large number of λ_j^b that represent states nearly degenerate in energy. The dephasing of these states resulting from their energy difference with respect to the $\Delta=0$ Hamiltonian is very slow and, since the phases of each of these λ_j^b should be correlated with the phases of a large number of λ_k^a, which again represent states nearly degenerate in energy (and nearly degenerate with $|A_i\rangle$), there should be an increasingly strong tendency for the phases of the λ^a's and the λ^b's to correlate in the limit of small α. It is this near degeneracy of the perturbation theory in Δ that underlies the very slow decay of the σ^x correlations in time and the diverging susceptibility to coherence χ_{coh}. As we tune α up from 0, we move away from the case where Δ couples completely or even nearly degenerate states, until at $\alpha=\frac{1}{2}$, the spectral function ρ_Δ is completely flat, perturbation theory in Δ is nondegenerate, and $\chi_{\rm coh}$ is finite.

Since evolution of the effects of Δ in the XCL from degenerate to nondegenerate is not merely quantitative but has qualitative changes in the long-time behavior of the system associated with it, it is natural to conjecture that these changes underly the evolution from coherence to incoherence of the TLS model. In fact, the near degeneracy with respect to the $\Delta=0$ Hamiltonian of the states connected by Δ is also exactly what is required to allow quantum interference to be observable as oscillations in $P(t)$ [16] and the oscillations in $P(t)$ vanish at $\alpha=\frac{1}{2}$ [2], precisely the point where the susceptibility to ''coherence'' became finite.

Given this, it is natural to ask whether or not the TLS model has a unique fixed point for $0<\alpha<1$ or several different fixed points, some of which exhibit quantum coherence and some of which do not. If one takes the σ^x operator whose correlations distinguished the fixed points of the XCL model and maps it back to the TLS model, it becomes the operator $\frac{1}{2}(\sigma^+ e^{i\Omega}+\mathrm{H.c.})$, so the fact that it exhibits an α-dependent power law in its correlation functions is unsurprising and not necessarily indicative of multiple fixed points. In fact, the behavior is expected based on the description of the physics of the TLS given in [7], where it was argued that the low-lying oscillators (those with energies below what I am calling T_K) are unaffected by the two-state degree of freedom. Further, for the TLS, the off-diagonal elements of the density matrix for the spin of the TLS model have no interesting α dependence since they are finite for finite Δ and any $\alpha<1$. It therefore appears very likely that the TLS problem for $0<\alpha<1$ is described by a single unique fixed point, although the interesting change in the intermediate time properties of $P(t)$ appears intimately connected to the different quantum coherence properties of the different XCL fixed points.

Similarly to the TLS case, for the AKM, the operators that correspond to the σ^x operator of the XCL take the form $\frac{1}{2}(\sigma^+ e^{-i(\sqrt{1-\alpha})\phi(0)}+\mathrm{H.c.})$ and again the α-dependent correlation functions neither require nor suggest multiple fixed points. Thus the results presented here are not in contradiction to previously known results. They do demonstrate the surprising fact that the renormalization-group flows for the XCL model are vertical in (α,Δ) space for $0<\alpha<1$, with Δ growing large, but α as measured by the correlations of σ^x unrenormalized at large scales. This result is of particular interest since a number of problems involving coupled Luttinger liquids have been connected to the AKM because they are analogous to the XCL model. These models may well *not* exhibit a unique fixed point as has commonly been supposed based on that connection.

In conclusion, we have studied the correlation functions of the σ^x operator of the transformed Caldeira-Leggett model defined by Eq. (4) and we find clear evidence for two distinct families of fixed points. The two families are distinguished by the (in)finiteness of a particular susceptibility that is closely connected to the question of the quantum coherence of the σ variable. We identify the transition in behavior between the two regimes as an effective ''transition'' from degenerate to nondegenerate action by the operator Δ and have shown that it is closely connected to the quantum to classical crossover of the Caldeira-Leggett model.

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[10] We are considering different systems as having different fixed points if the asymptotic correlations of the same operator show a different power law in the different systems. This implies the existence of Wilsonian fixed-point Hamiltonians with different parameters for the different systems; however, such Hamiltonians may still be related via a canonical transformation and thus have identical eigenvalues and identical structures among their low-energy states. The differences among such systems are embodied in differences in the matrix elements of operators among the low-energy states. An example of such behavior is given by *XXZ* spin chains, where, for $-J_{xy}<J_z\leqslant J_{xy}$, the effective low-energy theory, after an appropriate canonical transformation, is that of a harmonic fluid, yet, since the correlation exponents of the various spin operators depend on the transformation made and therefore on J_z/J_{xy}, it is conventional to refer to the existence of a fixed line. This line is simply the quantum version of the fixed line in the Kosterlitz-Thouless transition below the transition temperature. Since it is conventional to speak of a line of different fixed points in both cases, we have adopted the same notation here.
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[12] $P(t)$ measures the time dependence of the diagonal elements of this density matrix under a particular set of circumstances and is a less direct probe of quantum coherence. However, it is much more closely related to possible experimental realizations and enjoys other advantages for the TLS model.
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fixed point since the power-law behavior sets in on scales long compared to the Kondo scale. There is no reason to believe that at some much longer scale there is crossover to an α independent behavior, but this cannot be ruled out numerically.

[15] For $\alpha > \frac{1}{2}$, it is difficult to determine the long time behavior of $G(t)$ from the imaginary time result since the long-imaginary-time behavior does not dominate. The most likely behavior is $\sim t^{-2\alpha}$ with a *negative* real part; however, the question requires further study.

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