Dissipative Dynamics of a Two-State System, the Kondo Problem, and the Inverse-Square Ising Model

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The dynamics of a two-state system coupled to an Ohmic continuum, the dissipative two-state system, is solved by exploiting its connection to the Kondo problem and the inverse-square Ising model. Such a system is known to possess a zero temperature quantum critical point. In the quantum disordered phase the asymptotic dynamics is *always* an incoherent power-law relaxation. At short times, the system can exhibit damped oscillations only over a limited range of parameters.

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A two-state system, coupled to an environment that renders its dynamics dissipative, is ubiquitous in physics [1]. It defines a prototype that can simulate the behavior of a host of complex and interesting problems. It is, therefore, unfortunate that the dynamics of such a system is still poorly understood, Ref. [1] not withstanding. In the present paper we solve the dynamics at zero temperature. In view of recent developments in the field of high temperature superconductivity, where an analogy to the two-state system is drawn [2,3], the stated problem has acquired a new sense of urgency. The phenomenon in question is the c-axis transport in the normal state of the high temperature superconductors [4].

The connection between the dissipative two-state system and the Kondo problem was recognized by one of us [5]. This led to the realization that such a system possesses a quantum critical point at zero temperature. However, this connection was never fully exploited. Here, we shall show that it is extraordinarily fruitful and leads to a clear physical picture and accurate quantitative results for the dynamics of the system. In a sense, the present paper is the logical conclusion of a line of reasoning begun by Anderson and Yuval [6].

The two-state system coupled to a dissipative environment is defined by the Hamiltonian

$$H_{\rm ts} = -\tfrac{1}{2}\,\Delta\sigma_x + H_{\rm osc} + \tfrac{1}{2}\,\sigma_z \sum_\alpha C_\alpha x_\alpha\,; \qquad (1)$$

throughout the paper we set $\hbar = k_B = 1$. The environment consists of an infinite number of harmonic oscillators and is represented by the Hamiltonian $H_{\rm osc}$. The σ's are the Pauli matrices and $\{x_\alpha\}$ are the coordinates of the oscillators. The spectral density, $J(\omega)$, of the environment is given by

$$J(\omega) = \frac{\pi}{2}\sum_\alpha (C_\alpha^2/m_\alpha\omega_\alpha)\,\delta(\omega - \omega_\alpha), \qquad (2)$$

where m_α and ω_α are the masses and the frequencies, and $\{C_\alpha\}$ the coupling strengths. We shall consider the Ohmic bath, for which $J(\omega) = 2\pi\alpha\omega$, for $\omega < \omega_c$, and $J(\omega) = 0$ for $\omega \geq \omega_c$. The partition function has the well-known Coulomb gas form [7]:

$$Z_{\rm ts} = \sum_{n=0}^{\infty}\left(\frac{\Delta\tau_c}{2}\right)^{2n}\int_0^\beta \frac{d\tau_{2n}}{\tau_c}\cdots\int_0^{\tau_2-\tau_c}\frac{d\tau_1}{\tau_c} \times \exp\Bigg[2\alpha\sum_{i<j}(-1)^{i+j} \times \ln\left|\frac{\beta}{\pi\tau_c}\sin\frac{\pi(\tau_j-\tau_i)}{\beta}\right|\Bigg]. \qquad (3)$$

In this expression we have neglected as irrelevant the interactions between the charges that fall off as $(1/\tau)^x$, $x \geq 1$. To model an actual physical system, including all its high energy details, one needs not only the discarded terms, but also an infinite number of operators beyond those kept in Eq. (1). The neglected terms do not affect the low energy behavior and are, in any case, beyond the scope of the present paper.

Consider the inverse-square Ising model [6] with the set of spins, $\{S_i\}$, located on N lattice sites of a one-dimensional lattice of length L; $L = Na$, where a is the lattice spacing. For this model, and for the Ohmic two-state system, some rigorous mathematical results are now available [8]. The Hamiltonian, H_I, is

$$H_I = -\frac{J_{NN}}{2}\sum_i S_i S_{i+1} - \frac{J_{LR}}{2}\sum_{i<j}\frac{(\pi/N)^2 S_i S_j}{\sin^2[\pi(j-i)/N]}, \qquad (4)$$

where J_{LR} is assumed to be positive, while J_{NN} is allowed to have any sign. By a transformation, the partition function of the Ising model, Z_I, can be cast into the same Coulomb gas language [6]. The charges are the kinks in the Ising model. This Ising model is thus a particular regularization of the Coulomb gas model.

The fugacity, y, of the kinks is given by $y \approx e^{-\beta_I J_{NN} - \beta_I J_{LR}(1+\gamma)}$, where γ is Euler's constant. Here, y plays the role of $\Delta\tau_c/2$ and $\beta_I J_{LR}$ the role of α. The parameter τ_c maps to the lattice spacing of the Ising model and β/τ_c to N. The quantity β_I is the inverse temperature of the Ising model.

Finally, consider the anisotropic spin-half Kondo Hamiltonian, where the spin-spin coupling in the z

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direction is denoted by $J_{\|}$ and that in the x-y plane by $J_{\perp}$. The partition function for the Kondo impurity can also be cast in the Coulomb gas language [7], using the same assumptions with respect to the low energy behavior. Now, $J_{\perp}\rho$ plays the role of $\Delta\tau_c$ and $1 - J_{\|}\rho$ plays the role of α, where ρ is the density of states; the high energy cutoff is given by $1/\rho$.

The dynamical information is contained in the correlation function $C(t) = \mathrm{Re}\langle\sigma_z(t)\,\sigma_z(0)\rangle$. At finite temperature, the average is the equilibrium average, defined by the total Hamiltonian; at $T = 0$, it is the ground state average. Here, $\sigma_z(t)$ is the Heisenberg operator at time t. By contrast, in Ref. [1] a quantity called $P(t)$ is defined. It is the conditional average $\langle\sigma_z(t)\rangle$, where σ_z is known to be $+1$ at $t = 0$ and the oscillators adjusted to this state of the spin. Although the evolution for $t > 0$ is determined by the full Hamiltonian, the average is taken with respect to the *initial* state. For most applications, this correlation function is not relevant, as the initial state is orthogonal to the true ground state. As time evolves this initial state will dissolve into the exact ground state. Thus, $P(t)$ expresses the equilibration at initial times.

Consider the special value of α, $\alpha = 1/2$, at which the Hamiltonian can be diagonalized exactly. It can be shown [9] that $P(t) = e^{-2\lambda t}$, where $\lambda = \pi\Delta^2/4\omega_c$. In contrast, $C(t) = [(2\lambda/\pi)\int_0^\infty d\epsilon\, e^{-i\epsilon t}/(\epsilon^2 + \lambda^2)]^2$. Asymptotically, $C(t) \sim 4/\pi^2\lambda^2 t^2$, reflecting the critical nature of the Ohmic heat bath. In Ref. [1], extensive use was made of an approximation called "the noninteracting blip approximation." Within this approximation, it was found that $P(t) = C(t)$ and $P(t) = e^{-2\lambda t}$, and therefore, within this approximation, $C(t)$ must be $e^{-2\lambda t}$, which is incorrect. The logical conclusion is that the noninteracting blip approximation fails, at least at $\alpha = 1/2$. Below, we shall see that this approximation is, strictly speaking, incorrect almost everywhere in the parameter space.

We calculate $C(t)$, or equivalently its spectral representation. To do this, we exploit the equivalences described earlier and consider the inverse-square Ising model. First, the imaginary time correlation function, $C(\tau)$, is obtained from Monte Carlo simulations of the inverse-square Ising model [10]. The number of sweeps through the lattice was chosen to be 8×10^6, of which 10^6 sweeps were used to equilibrate the system. Next, the Fourier transform $C(\omega_n)$ at the Matsubara frequencies, $\omega_n = 2\pi n/\beta$, was obtained: $C(\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau}C(\tau)$. Finally, the Padé approximant method of Vidberg and Serene [11] was used to analytically continue to the real axis. This method was also briefly, but successfully, considered by Hirsch [12] in a similar problem.

First, we address the definition of correlation length in the inverse-square Ising model. The correlation length in the Ising model translates to the Kondo temperature, T_K, of the Kondo problem. It is a theorem [13] that the spin-spin correlation function cannot fall off *faster* than the interaction, in this case $\propto |i - j|^{-2}$. From conformal field theory [14], the asymptotic decay of the imaginary time spin-spin correlation function in the Kondo problem is rigorously known to be $(1/\tau)^2$; at finite β, this is $[\pi/\beta \sin(\pi\tau/\beta)]^2$. Our numerical calculation, described below, precisely confirms this result, constituting an excellent check of the numerical methods. Therefore, in the absence of an exponential decay, the conventional definition of the correlation length does not apply. We note, however, that the asymptotic inverse-square decay changes to a slower decay at shorter length scales. The crossover scale can be defined to be the correlation length, ξ_c. This definition is similar to the Josephson definition of the correlation length in the ordered phase of the isotropic Heisenberg ferromagnet [15]. There, the Goldstone behavior in the *ordered* phase is strictly enforced by symmetry [16]. The Josephson length separates the short distance critical behavior from the long distance Goldstone behavior.

Now, one can describe the Kondo crossover in terms of finite size scaling [10] of the inverse-square Ising model. The susceptibility of the Kondo problem, χ_K, is related to the susceptibility of the Ising model by $T_I\chi_I/N = \chi_K/\tau_c$. For $Na < \xi_c$, $T > T_K$, the system appears ordered and $T_I\chi_I/N = \langle M^2\rangle \sim N^2/N = N$ [17]. In other words, $\chi_K \sim 1/T$, because $1/N \propto T$. However, for $Na > \xi_c$, the Ising model appears disordered. By a random walk argument, $T_I\chi_I/N = \langle M^2\rangle \sim N/N = 1$. Thus χ_K saturates as $T \rightarrow 0$. As we approach the phase transition of the Ising model, ξ_c grows and T_K decreases. The finite size scaling is demonstrated in Fig. 1, where

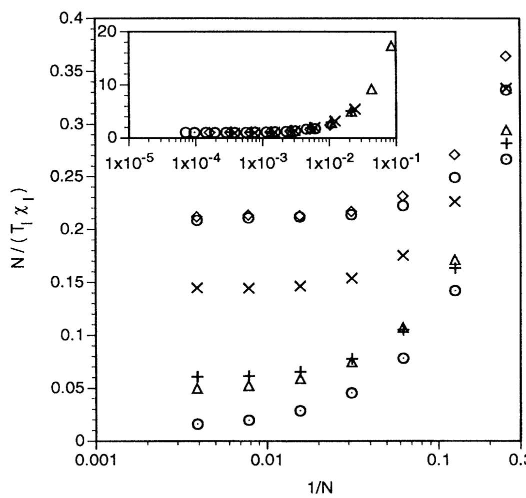

FIG. 1. $N/T_I\chi_I = \tau_c/\chi_K = \tau_c/\chi_{ts}$ as a function of $1/N = \tau_c/\beta$. ⊙: $\beta_I J_{NN} = 1.0$, $\beta_I J_{LR} = 0.7$; △: $\beta_I J_{NN} = 0.5$, $\beta_I J_{LR} = 0.7$; +: $\beta_I J_{NN} = 1.0$, $\beta_I J_{LR} = 0.5$; ×: $\beta_I J_{NN} = 0.5$, $\beta_I J_{LR} = 0.5$; ○: $\beta_I J_{NN} = 1.0$, $\beta_I J_{LR} = 0.2$; and ◇: $\beta_I J_{NN} = 0.5$, $\beta_I J_{LR} = 0.4$. The inset shows the data collapse onto a universal scaling curve.

we show the data collapse of χ_K onto an universal scaling curve.

As mentioned earlier, the Padé approximant method is used to analytically continue $C(\omega_n)$ from the positive Matsubara frequencies to the real axis. The imaginary part is the response function $\chi''(\omega) = \frac{1}{2}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\langle[\sigma_z(t), \sigma(0)]\rangle$, which is a real and odd function of ω. The spectral function $S(\omega) = \chi''(\omega)/\omega$ is therefore determined, as is the spin-spin correlation function. The number of Matsubara points used in constructing the Padé approximants was 129. The most important aspect is the accuracy of the data for the imaginary time correlation function.

For $\alpha = 0$, $S(\omega)$ is a sum of two δ functions at $\omega = \pm\Delta$, which we shall call the "quasiparticle" behavior, signifying the coherent oscillations of the two-state system. For finite, but small α, one may expect these peaks to survive. This is not always the case. In the Ising picture, and in the limit of vanishing J_{NN} (large Δ) and small J_{LR} (small α), $\langle S_i S_j\rangle$ is entirely determined by the inverse-square part of the Ising model. In this limit, $C(\omega_n)$, analytically continued to real frequency ω, has an imaginary part that is proportional to $|\omega|$, as $\omega \rightarrow 0$. The resulting $S(\omega)$ is broad and centered at $\omega = 0$, and the quasiparticle picture is destroyed. As J_{NN} is increased, J_{LR} remaining small, the J_{NN} term can force the spins to be correlated over the correlation length of the nearest neighbor Ising model, as there are no restrictions on the slowness of the decay of the correlations. Therefore, the dynamics at short times can show quasiparticle behavior and the spectral function can exhibit quasiparticle peaks. That the spectral function must be finite at $\omega = 0$ follows from the rigorous inverse-square decay of the correlation function. In turn, asymptotically, $C(t) \sim 1/t^2$. The damped oscillation can be present at shorter times, depending on the parameters. The noninteracting blip approximation [1] incorrectly produces a power law decaying slower than $1/t^2$, proportional to $1/t^{2(1-\alpha)}$ for $\alpha \neq 1/2$. The numerical results confirming the above picture are shown in Fig. 2.

Now suppose that we hold J_{NN} sufficiently large such that the spectral function shows quasiparticle peaks for sufficiently small J_{LR}. As J_{LR} is increased, that is, α is increased, the quasiparticle peaks shift towards $\omega = 0$, broadening at the same time; the weight at $\omega = 0$ increases, because the spin susceptibility increases. At $\alpha = \beta_I J_{LR} = \frac{1}{2}$, the quasiparticle peaks disappear entirely, for all J_{NN}. As shown in Fig. 3, the numerical results accurately confirm the analytical result, serving, in addition, as a valuable check on the numerical methods. As α is increased further, critical slowing down sets in and the peak at $\omega = 0$ sharpens. This leads to a δ function below the transition and is due to the long range order present in the inverse-square Ising model. The above picture is confirmed in detail in Fig. 4.

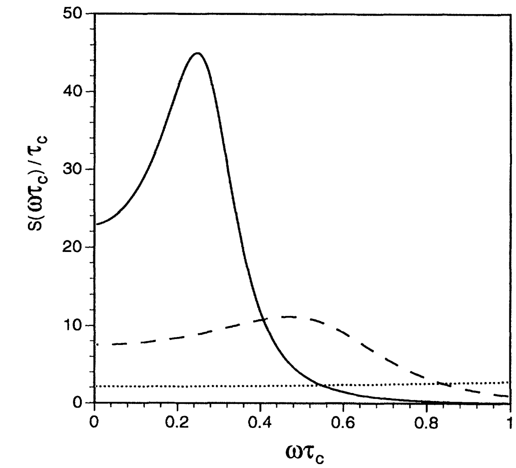

FIG. 2. $S(\omega)$ plotted as a function of ω for $\beta_I J_{LR} = 0.2$; the solid line: $\beta_I J_{NN} = 1.5$; the dashed line: $\beta_I J_{NN} = 1.0$; the dotted line: $\beta_I J_{NN} = 0.5$. $\beta/\tau_c = 256$.

To summarize, in the entire parameter space, the asymptotic behavior of $C(t)$ is incoherent. At shorter times, and for $\alpha < 1/2$, the system can exhibit damped oscillations, or the quasiparticle behavior, if J_{NN} is sufficiently large, that is, if Δ is sufficiently small, *not large*, as one may have naively guessed.

It has been argued [2,3] that the c-axis motion of electrons in high temperature superconductors have broad similarities with the dynamics of a two-state system coupled to a dissipative bath. From the present analysis, it appears that the generic behavior, over almost the entire range of the parameter space, is incoherent, independent of α. Coherent behavior for short times exists only over a limited domain. The weak coupling flow of

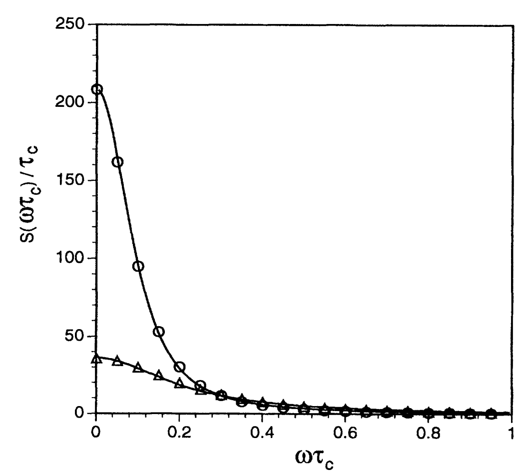

FIG. 3. $S(\omega)$ at $\alpha = 1/2$. The solid lines are the numerical results for $\beta/\tau_c = 256$. The circles ($\beta_I J_{NN} = 1.0$) and triangles ($\beta_I J_{NN} = 0.5$) are plots of exact analytical results at $T = 0$.

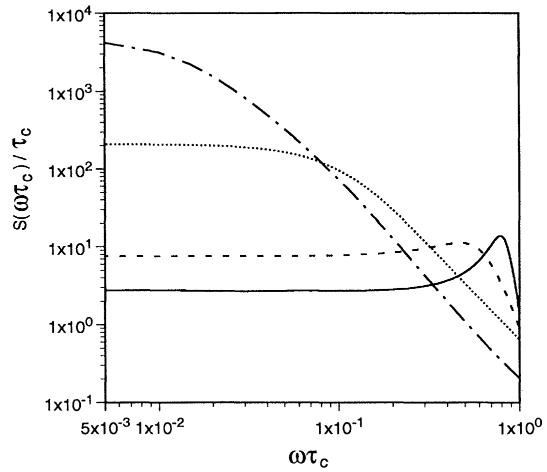

FIG. 4. $S(\omega)$ plotted as a function of ω for $\beta_I J_{NN} = 1.0$; the solid line: $\beta_I J_{LR} = 0.1$; the dashed line: $\beta_I J_{LR} = 0.2$; the dotted line $\beta_I J_{LR} = 0.5$; and the dash-dotted line: $\beta_I J_{LR} = 0.7$. $\beta/\tau_c = 256$.

the renormalization group equations is not particularly revealing with respect to the dynamics of the system [18]. Even when the flows indicate a growth of Δ/ω_c, which is the entire region of the delocalized phase, the dynamics is rigorously incoherent over much of the parameter space. The lack of exponential decay of the correlation function in the disordered phase of the inverse-square Ising model is responsible for the incoherent dynamics of the two-state system. Note, however, that ξ_c is finite and well defined.

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[1] S. Chakravarty and A. J. Leggett, Phys. Rev. Lett. **52**, 5 (1984); A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).
[2] S. Chakravarty and P. W. Anderson, Phys. Rev. Lett. **72**, 3859 (1994).
[3] D. G. Clarke, S. P. Strong, and P. W. Anderson, Phys. Rev. Lett. **72**, 3218 (1994).
[4] K. Tamasaku, Y. Nakamura, and S. Uchida, Phys. Rev. Lett. **69**, 1455 (1992); S. Tajima *et al.,* Phys. Rev. B **48**, 16 164 (1993); S. L. Cooper *et al.,* Phys. Rev. Lett. **70**, 1533 (1993).
[5] S. Chakravarty, Phys. Rev. Lett. **49**, 681 (1982); A. J. Bray and M. A. Moore, Phys. Rev. Lett. **49**, 1546 (1982).
[6] P. W. Anderson and G. Yuval, J. Phys. C **4**, 607 (1971).
[7] P. W. Anderson, G. Yuval, and D. R. Hamann, Phys. Rev. B **1**, 4464 (1970).
[8] J. Z. Imbrie and C. M. Newman, Commun. Math. Phys. **118**, 303 (1988), and references therein. See also H. Spohn, Commun. Math. Phys. **123**, 277 (1989).
[9] See Ref. [7]; see also F. Guniea, V. Hakim, and A. Muramatsu, Phys. Rev. B **32**, 4410 (1985).
[10] An attempt to obtain the thermodynamic properties of a Kondo impurity using the Monte Carlo method was first considered by Schotte and Schotte in the Coulomb gas language: K. D. Schotte and U. Schotte, Phys. Rev. B **4**, 2228 (1971). In contrast to the present method, it involves simulation in the grand canonical ensemble, a technically more difficult problem.
[11] H. J. Vidberg and J. Serene, J. Low Temp. Phys. **29**, 179 (1977).
[12] J. E. Hirsch, in *Quantum Monte Carlo Methods in Equilibrium and Nonequilibrium Systems,* edited by M. Suzuki (Springer, New York, 1987).
[13] R. B. Griffith, J. Math. Phys. (N.Y.) **8**, 478 (1987).
[14] The result follows from conformal field theory of A. W. W. Ludwig and I. Affleck, Nucl. Phys. **B428 [FS]**, 545 (1994). We thank A. W. W. Ludwig for drawing our attention to this fact. It has also been argued by M. Sassetti and U. Weiss, Phys. Rev. B **41**, 5383 (1990), and R. Egger and C. H. Mak, Phys. Rev. B **50**, 15 210 (1994).
[15] B. D. Josephson, Phys. Lett. **21**, 608 (1966).
[16] We feel, but are unable to prove, that a strict hidden symmetry in the present problem is responsible for the inverse-square decay.
[17] This argument would be more subtle, if the magnetization vanished continuously at the transition of the inverse-square Ising model. It is much stronger here, because the magnetization is known to have a discontinuity at the transition [6,8]; see also D. J. Thouless, Phys. Rev. **187**, 732 (1969). We thank L. Chayes for an interesting conversation.
[18] P. W. Anderson, Phys. Rev. Lett. **67**, 3844 (1991).