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Dynamic susceptibility of the Anderson model: A quantum Monte Carlo study

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Using a highly accurate method of analytic continuation, we calculated the dynamic susceptibility and NMR relaxation rate $1/T_1$ of magnetic (Anderson or Kondo) impurities over the *entire* range $T \ll T_K$ to $T \gg T_K$. We find that the susceptibility and NMR relaxation rate are universal functions when properly scaled and that the NMR relaxation rate is directly proportional to the universal Kondo resistivity.

The properties of a metal with a dilute concentration of magnetic impurities has been an enduring problem in condensed-matter physics. The spin-$\frac{1}{2}$ Anderson impurity model is a paradigm for this problem. The model describes the formation, and more importantly, the screening of the magnetic moments.[1] At high temperatures, this screening is inhibited by thermal fluctuations; however, as the temperature is lowered below the Kondo temperature T_K, a screening cloud forms that strongly affects the magnetic, thermodynamic, and transport properties of the system.

In this paper, we provide a calculation of the dynamic magnetic susceptibility and NMR relaxation rate for the symmetric spin-$\frac{1}{2}$ single-impurity Anderson model. As shown in Fig. 1, the dynamic susceptibility $\chi''(\omega)$ develops a narrow peak of width $\approx T_K$ as the temperature is lowered. The width of this peak increases monotonically with temperature, as shown in the inset. In Fig. 3, we demonstrate that the shape of this peak is universal, since it depends only upon the ratio T/T_K.

In Fig. 4, we present our most startling result. Here, we plot the NMR relaxation rate versus T/T_K for various values of the model parameters and demonstrate that is universal. The solid line is a fit to our previously published results for the resistivity ratio $\rho(T)/\rho(0)$. We find, to the accuracy of our Monte Carlo procedure, that the two functions are identical when plotted as a function of T/T_K.

We model the impurities with an infinite bandwidth symmetric Anderson model that is characterized by a hybridization width $\Gamma = \pi N(0) V^2$ [where V is the hybridization matrix element, and $N(0)$ is the density of states at the Fermi surface] and an on-site repulsion U. The Hamiltonian for this model is

$$H = \sum_{k,\sigma} \varepsilon_k C^\dagger_{k,\sigma} C_{k,\sigma} + V \sum_{k,\sigma} (C^\dagger_{k,\sigma} d_\sigma + d^\dagger_\sigma C_{k,\sigma}) + \varepsilon_d \sum_\sigma n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} . \tag{1}$$

In the symmetric limit, $\varepsilon_d = -U/2$. The Kondo temperature T_K is a function of U and Γ, and is determined empirically.[2,3] In the limit $U \gg \Gamma$, a spin-$\frac{1}{2}$ magnetic moment forms on the impurity orbital which couples antiferromagnetically to the conduction electrons with an exchange $J = -8\Gamma/\pi N(0) U$. In this paper, we are primarily interested in the dynamic susceptibility $\chi''(\omega)$ of the Anderson model. It is defined through the following two relations:

$$\chi(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''(\omega) e^{-\tau\omega}}{1 - e^{-\beta\omega}} , \tag{2}$$

$$\chi(\tau) = 2 \int_0^\beta d\tau \langle d^\dagger_\downarrow(\tau) d_\uparrow(\tau) d^\dagger_\uparrow(0) d_\downarrow(0) \rangle . \tag{3}$$

For reasons which will become clear below, we chose to work with the function $f(\omega)$, which is related to $\chi''(\omega)$ through the relation

$$f(\omega) = \frac{\pi \chi''(\omega) T_K}{2\omega \chi(T)} , \tag{4}$$

where $\chi(T)$ is the static susceptibility.

Previous attempts to calculate the dynamic susceptibility of this model have met with limited success. Using high-temperature perturbation theory, Spencer and Doniach found a Kondo-like logarithmic term in the dynamic susceptibility.[4] This term leads to a $\ln(T)$ dependence of the NMR relaxation rate for $T > T_K$.[5] The approximation of Nagaoka[6] and Suhl[6] yielded inconclusive results for the static susceptibility.[7] To our knowledge, this approximation has not been applied to the calculation of the dynamic susceptibility. The virtual bound-state approximation has been applied to this model by Salomaa.[8] This result may be written as a complicated expression of digamma and trigamma functions, and thus will not be reproduced here. It is sufficient to say that the result is a function of ω, T, and Γ_K, where Γ_K is an arbitrary parameter. However, this result is only exact in the $U = 0$ limit in which $\Gamma_K = \Gamma$. The $1/N$ approximation has been applied to the asymmetric Anderson model in the limit as $U \rightarrow \infty$.[9] This approximation becomes exact as the orbital degeneracy N of the impurity becomes large; however, for finite N, low temperatures, or (more importantly) low frequencies, the approximation breaks down. For this reason, the NMR rate (corresponding to the zero-frequency limit of the dynamic susceptibility) could not be calculated accurately. The dynamic susceptibility has also been calculated using perturbation theory in $u=U/(\pi\Gamma)$.[10] This approximation, however, is uncontrolled for large u.

Finally, there are several exact results for the Anderson model's dynamic susceptibility. First, by applying the Friedel sum rule, Shiba[11] was able to determine the $\omega=0$ and $T \ll T_K$ limit of the dynamic susceptibility. In our case, since $\lim_{T\to 0}\chi(T)=[(\pi/2)^2 T_K]^{-1}$,

$$\lim_{T\to 0} f(0)=1\,. \tag{5}$$

By standard perturbation-theory techniques, one may show that in the high-frequency limit ($\omega \gg U/2$)

$$\lim_{\omega\to\infty} f(\omega)=\frac{\pi T_K \Gamma}{\chi(T)}\frac{1}{\omega^3}\,. \tag{6}$$

In addition, the NMR relation rate $1/T_1$ due to the Kondo scattering of conduction electrons is[11]

$$\frac{1}{T_1 T}=A\frac{2\chi(T)}{\pi T_K}f(0)\,. \tag{7}$$

where A is a constant composed of the g factor of the impurity nucleus, the nuclear Bohr magneton, and the coupling between the nuclear spin and the d- electron spin.

To calculate the dynamic susceptibility of the Anderson model, we employed a combination of quantum Monte Carlo and maximum entropy methods. The Monte Carlo was used to generate the two-particle Green's function $\chi(\tau)$ as a function of imaginary time, and the maximum entropy method was used to analytically continue this result to produce the dynamic susceptibility.

Our Monte Carlo calculations are based upon an algorithm developed by Hirsch and Fye.[12] The problem is cast into a discrete path integral formalism in imaginary time τ_l, where $\tau_l=l\Delta\tau$, $\Delta\tau=\beta/L$, β is the inverse temperature, and L is the number of imaginary-time slices. In order to minimize systematic discretization errors, we took $\Delta\tau^2\Gamma U<0.20$ and studied β values as large as 100. A detailed discussion of the treatment of the statistical error appears in Ref. 13.

Analytic continuation of this data [deconvolution of Eq. (2)] was accomplished with the maximum entropy method.[13-15] Here we find the $f(\omega)$ which maximizes the constrained entropy $\alpha S-L$. L is a least-squares measure which determines how well $f(\omega)$ reproduces the Monte Carlo data, and the entropy S is given by

$$S[f,m]=\int d\omega\{f(\omega)-m(\omega)-f(\omega)\ln[f(\omega)/m(\omega)]\}\,. \tag{8}$$

The function $m(\omega)$ serves as a default model for our results. It is our assumed answer in the absence of Monte Carlo data. In most applications of maximum entropy, the parameter α is set by maximizing its posterior probability, the probability obtained after marginalizing over all possible images $f(\omega)$. However, in this case, we also chose to marginalize over all possible values of the Lagrange parameter α. In doing so, we obtain the posterior probability given the data and model $P[D,m]$.[13,14]

We chose the result of Salomaa for the default model $m(\omega)$. The parameter Γ_K was chosen to maximize $P[D,m]$, which causes $m(\omega)\approx f(\omega)$ for small ω. However, our results are independent of variations of Γ_K from this optimal value by as much as a factor of 2. When chosen this way, Γ_K is a roughly universal function of T/T_K. It increases monotonically with increasing T/T_K. At low temperatures, we find $\Gamma_K \approx (\pi/2)T_K$.[16] With this low-temperature limit, the default model satisfies the Shiba sum rule, so that $\lim_{T\to 0} m(0)=1$. We found that this default model produced a larger $P[D,m]$ than a default model constructed from the moments of the distribution $f(\omega)$, which is often used for problems of this type.[17]

With this method, we were able to calculate $f(\omega)$ over a wide range of model parameters and temperatures. At sufficiently high temperatures, the dynamic susceptibility displays deviations from universality. For a given value of u, these deviations occur at roughly the same temperatures at which the static susceptibility $\chi(T)$ deviates from universality.[1] However, in this manuscript we will only report results which are in the universal regime.

The evolution of the dynamic susceptibility as a function of T/T_K for fixed $u=U/(\pi\Gamma)=1.5$ is shown in Fig. 1. As the temperature is lowered toward T_K, $f(\omega)$ develops a Kondo-like peak centered at $\omega=0$. The evolution of the half width at half maximum of the $f(\omega)$ as a function of T/T_K is shown in the inset. Contrary to results obtained with the $1/N$ expansion[9] this plot does not display a minimum at $T\approx T_K$. Rather, the half width increases monotonically. This discrepancy is probably due to the difference in orbital degeneracy between the two calculations (as was surmised from experimental evidence[18]). The solid line in the inset demonstrates that the half width varies as $(T/T_K)^{1/2}$ for $T \gg T_K$ as found in the $1/N$ approximation.[9] However, we find that to an excellent ap-

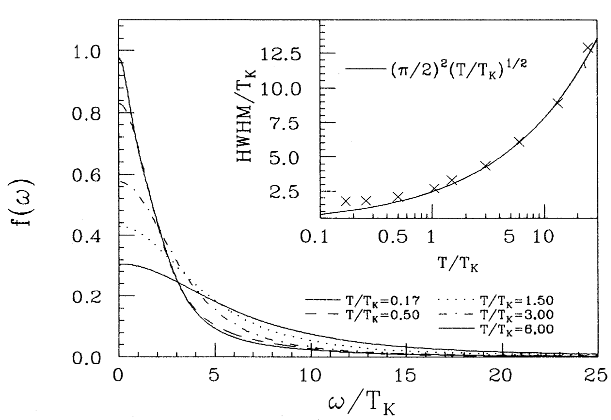

FIG. 1. $f(\omega)=[\pi T_K/2\chi(T)][\chi''(\omega)/\omega]$ plotted vs ω/T_K for various values of T/T_K when $u=1.5$. The peak is sharpest at low temperatures and broadens as the temperature is raised. The half width of the peak is plotted in the inset. Note that it increases monotonically and is proportional to $(T/T_K)^{1/2}$ when $T/T_K \gg 1$.

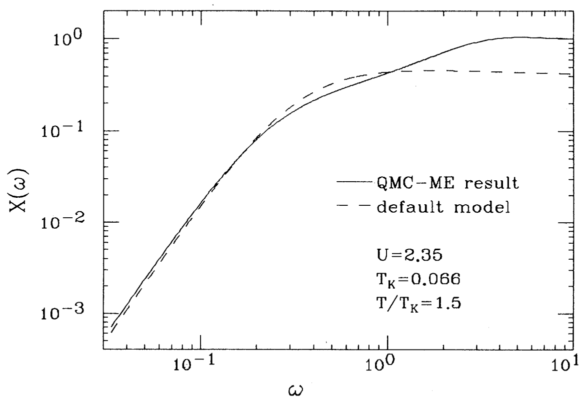

FIG. 2. $X(\omega)=w^3 f(\omega)/[\pi T_K \Gamma/\chi(T)]$ plotted vs ω when $U=2.35$, $\Gamma=0.5$, and $T/T_K=1.5$ (solid line), and the correspondingly normalized default model (dashed line) with $\Gamma_K=2.08$. Note the small additional feature beginning at $\omega \approx U/2$.

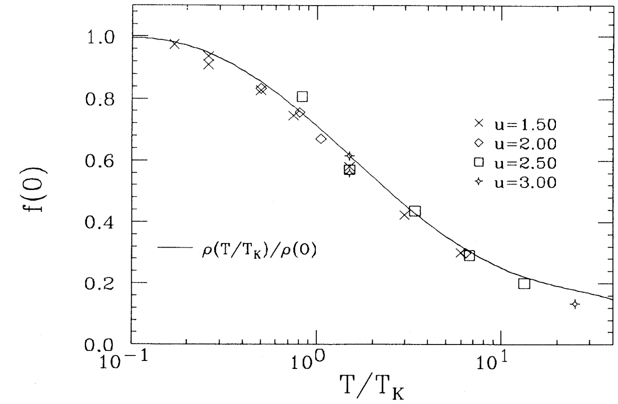

FIG. 4. $f(0)$ for various values of u plotted vs T/T_K. The solid line is a fit to our previously published resistivity data (Ref. 2).

proximation, the prefactor of this dependence is the Wilson number $\pi^2/4$ (determined exactly by the Bethe ansatz[19]) which describes the relation between the high- and low-temperature energy scales of the Kondo problem.

In addition to the low-frequency peak, the data also displayed a very small secondary feature beginning around $\omega=U/2$. This is demonstrated in Fig. 2. Here, $X(\omega)=w^3 f(\omega)/[\pi T_K \Gamma/\chi(T)]$ is plotted versus ω. Asymptotically, $X(\omega)\sim 1$, as predicted from perturbation theory. Because this secondary feature is small, its existence is most likely of little experimental relevance. Its presence in our results, on the other hand, demonstrates the remarkable resolution of our method: small features are not lost in the statistical noise.

With our choice of normalization, $f(\omega/T_K)$ is also a universal function, as shown in Fig. 3 where f is plotted versus ω/T_K for several values of u and fixed $T/T_K=1.5$. All these curves roughly coincide indicating universality. Universality of $f(w)$ results in the observed universality of $\chi(T)=\int d\omega \chi''(\omega)/(\pi\omega)$.

As shown in Fig. 4, the low-frequency intercept $f(0)$, which is related to the NMR relaxation rate [Eq. (7)], is

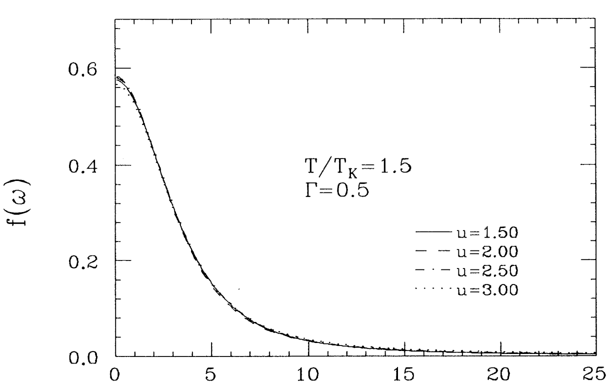

FIG. 3. $f(\omega)$ vs ω for various values of u when $T/T_K=1.5$ and $\Gamma=0.5$.

universal for all T/T_K calculated. Universality is indicated by the fact that the data for different values of u overlap to form a single curve. The data for $T \approx T_K$ is roughly log linear, as predicted by Walker.[5] As discussed in a previous publication,[13] it is not possible to accurately determine the error bar for a single point in a continuous distribution like $f(\omega)$. However, error bars due to statistical sources are roughly determined by the spread of the data. The solid line in Fig. 4 is a fit to the universal resistivity $\rho(T)/\rho(0)$ determined earlier.[2] The coincidence of the two data sets is our most surprising result.

Our result is surprising given the different nature of the two results when explored diagrammatically. However, this result does have a physical basis. Spin-flip scattering from the impurity is the primary source of resistivity of the conduction electrons. It is also the mechanism which relaxes the nuclear moment. Thus, both the NMR relaxation rate and the resistivity are in some sense a measure of the spin-flip scattering rate from the impurity. Hence, one might expect them to be qualitatively similar. It is the quantitative similarity which is surprising.

In conclusion, we have demonstrated that the dynamic susceptibility of the Anderson model, when properly scaled, is a universal function of ω/T_K and T/T_K. Consequently, the scaled NMR relaxation rate is a universal function of T/T_K. Surprisingly, we find that the scaled NMR rate is identical to the universal Kondo resistivity for a dilute magnetic alloy. This correspondence could be explored with NMR experiments. The predicted universal shape of the dynamic susceptibility as a function of ω can, in principle, be explored by inelastic neutron-scattering experiments. In the dilute impurity limit, the dynamic structure function measured in neutron scattering is proportional to the produce of the ω-dependent dynamic susceptibility calculated here with the squares of the momentum-dependent atomic form factors.

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