Transport coefficients of dilute magnetic alloys: A quantum Monte Carlo study

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Using a new, highly accurate, method of analytic continuation, we provide the first quantitatively correct calculation of the resistivity and thermal conductivity of dilute spin-$\frac{1}{2}$ magnetic (Anderson and Kondo) alloys over the *entire* range of interest $T \ll T_K$ to $T \gg T_K$. We find that our results are consistent with previous approximate theories in their regions of applicability. Our results are the first calculation of transport for any strongly correlated electronic many-body system obtained by direct analytic continuation of Monte Carlo data.

The properties of a metal with a dilute concentration of magnetic impurities has been an enduring problem in condensed-matter physics, and the spin-$\frac{1}{2}$ Anderson impurity model is the central paradigm for this and related strongly correlated electronic and magnetic systems. As such, it has been studied for over 30 years in a variety of contexts. In this paper we provide the first qualitatively correct calculation of the transport coefficients of a dilute system of Anderson impurities embedded in a metallic host. Experimentally, anomalies are found in the transport of such systems. The anomaly in the resistivity is the best known: as the temperature is lowered the resistivity displays a minimum, then increases, and finally saturates as $T \to 0$. Qualitatively, this resistivity minimum is well understood. As the temperature is lowered toward a characteristic energy scale T_K, the scattering rate of electrons from the magnetic impurities diverges logarithmically. As the temperature is lowered further, the conduction electrons begin to screen the magnetic impurity, forming a local singlet, and the resistivity saturates. Few theories explain this behavior qualitatively over the entire range of interest and none are quantitatively correct.

In this paper we provide the first quantitatively correct calculation of transport for the spin-$\frac{1}{2}$ Anderson model. Our calculation encompasses the *entire* range of interest $T \ll T_K$ to $T \gg T_K$, including the crossover regime $T \approx T_K$. Our results are consistent with previous approximate results in their regions of validity when their adjustable parameters are set by our results. Thus, our results may serve as benchmarks for these approximations. In addition, we believe that these are the first calculations of transport by direct analytic continuation of quantum Monte Carlo data for any strongly correlated electronic many-body system. Thus, another feature of this work is that it demonstrates that such calculations are feasible.

We assume that a small finite concentration of uncorrelated magnetic impurities are embedded in a metallic host. We model the impurities with an infinite-bandwidth symmetric Anderson model which 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 Kondo temperature T_K is a function of U and Γ. 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 Fig. 1 we fitted our results for the static susceptibility to the numerical renormalization-group results of Krishnamurthy *et al.*[1] This fit allows us to determine T_K. The transport coefficients are universal functions of T/T_K for sufficiently large $u = U/\pi\Gamma$ and low T/T_K. This universality is reflected in the resistivity, as shown in Fig. 2 where $\rho(T=1.5T_K)/\rho(T=0)$ saturates to a universal constant as u is increased. In Fig. 3, the resistivity is plotted as a function of T/T_K, and is compared with previous approximate results. Results for the thermal conductivity are shown in Fig. 4.

There have been many theoretical attempts to solve the Kondo transport problem, of which we will mention a few. Kondo,[2] using a high-temperature expansion to third order in J, was able to describe the resistivity minimum, but not the low-temperature saturation. Hamann,[3] using a third-order (in J) self-consistent approach due to Nagaoka and Suhl,[4] found the result

$$\rho(T) = \frac{\rho(T=0)}{2} \times \left[1 - \frac{\ln(T/T_{KN})}{\{[\ln(T/T_{KN})]^2 + \pi^2 S(S+1)\}^{1/2}} \right] . \quad (1)$$

This result qualitatively describes the resistivity for all temperatures; however, it is only quantitatively correct at high temperatures $T > T_K$. Nozières[5] argued that, at low temperatures $T \ll T_K$, the Kondo impurity system becomes a Fermi liquid, so that

$$\rho(T)/\rho(0) = 1 - \alpha (T/T_K)^2 ,$$

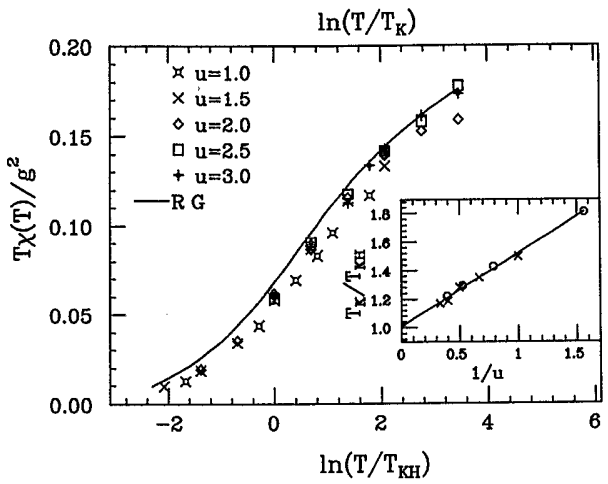

FIG. 1. $T\chi(T)/g^2$ (symbols) vs $\ln(T/T_{KH})$ (lower scale) for various values of $u=U/\pi\Gamma$. The solid line is the numerical renormalization-group result of Krishnamurthy *et al.* vs $\ln(T/T_K)$ (upper scale). The correction to $T_{KH}=0.364(2\Gamma U/\pi)^{1/2}e^{-\pi U/8\Gamma}$, for each value of u, may be determined by scaling T_{KH} until the data fits the Krishnamurthy result. For each $1/u$, this correction term is plotted in the inset where the crosses are our results, and the open circles are the results of Hirsch *et al.* (Ref. 8). In the inset, the solid line is the result $T_K/T_{KH}=(1+1/2u)$.

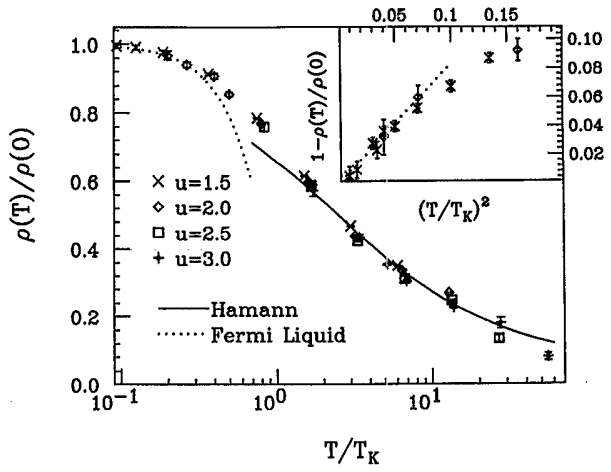

FIG. 3. $\rho(T)/\rho(0)$ vs T/T_K for different values of u. The solid line is from the self-consistent high-temperature calculation of Hamaan *et al.* (Ref. 3), Eq. (1). It is fit to our results by varying T_{KN} so that the curves agree when $\rho(T_{KN})/\rho(0)=0.5$. As expected, this result fails at low temperatures. The dotted line is the Fermi-liquid result of Nozières (Ref. 5) $\rho(T)/\rho(0)=1-\alpha(T/T_K)^2$, with $\alpha=0.83\pm0.06$ determined from a fit to the data as shown in the inset. The resistivity is roughly logarithmic for $0.5<T/T_K<4.0$.

and the thermal conductivity $\kappa(T)=\gamma T$. Using a $1/N$ perturbation theory in the total degeneracy N of the magnetic impurity, Bickers *et al.*[6] calculated all the thermodynamic and transport properties in the limit of infinite U (no particle-hole symmetry is possible in such a limit) and large N. Finally, Horvatić *et al.*,[7] using a self-consistent approach to second order in U, calculated the single-particle spectrum and the transport coefficients for the Anderson impurity.

Our calculations are based upon a Monte Carlo algorithm developed by Hirsch and Fye.[8] The problem is cast into a discrete path-integral formalism in imaginary time τ_l, where $\tau_l=l\,\Delta\tau$, $\Delta\tau=\beta/L$, and L is the number of time slices. In order to minimize systematic discretization errors, we took $(\Delta\tau)^2\Gamma U<0.19$, and studied β values as large as 200, $2<U<6$, and $0.3<\Gamma<0.6$. Larger values of β were avoided since the computer time required by the algorithm scales like L^3. For measurements of the impurity single-particle Greens function $G(\tau)$, the systematic errors associated with the finite value of $\Delta\tau$ were estimated to be typically $<0.5\%$, and the statistical errors were typically $<0.3\%$.

The aim of analytic continuation is to construct the

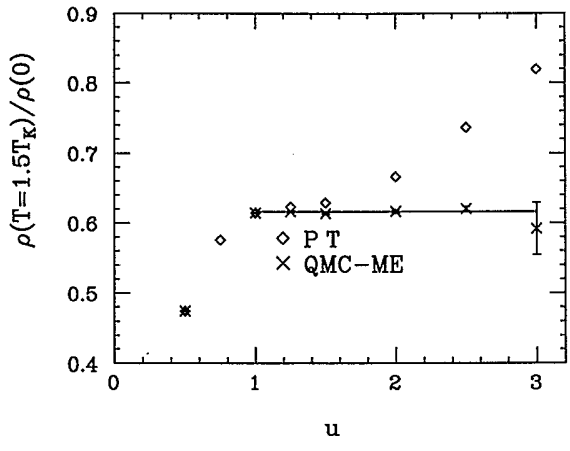

FIG. 2. $\rho(T)/\rho(0)$ vs $u=U/\pi\Gamma$ when $T/T_K=1.5$ and $\Gamma=0.5$. The open diamonds are from the perturbation theory of Horvatic *et al.* (Ref. 7). For $u\leq1.0$ there was no significant difference between the perturbation theory and Monte Carlo results. The universality of the Monte Carlo data is indicated by the fact that, for $u>1.5$, the value of the resistivity saturates to a constant whereas the perturbation-theory result continues to rise monotonically.

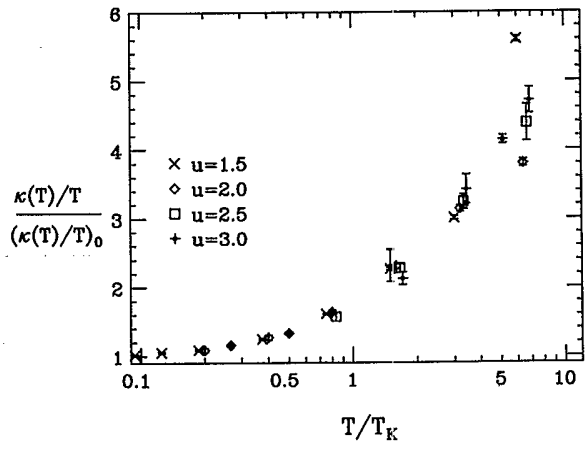

FIG. 4. $[\kappa(T)/T]/(\kappa/T)_{T=0}$ vs T/T_K different values of u. Note that at low temperatures, κ is linear in T, indicative of a Fermi liquid, as argued by Nozières (Ref. 5).

single-particle spectrum $A(\omega)$ from the $G(\tau)$ data. Previous methods employed a least-squares[9] or dynamical[10] approach to find the best smooth function which is consistent with the data. Using the maximum-entropy method,[11–14] we find the $A(\omega)$ which is consistent with the data and has maximum entropy. This method has several advantages. First, it allows $A(\omega)$ to have sharp features if they are consistent with the data. Second, we are able to propagate statistical errors through the method, so that we can provide error bars for the transport coefficients. Third, the maximum-entropy procedure allows us to incorporate perturbation-theory data of Horvatić *et al.*[7] [which we identify as $m(\omega)$] as a default model for $A(\omega)$. Thus, for large ω, where the perturbation theory becomes exact and the Monte Carlo provides no information due to the finite value of $\Delta\tau$, the maximum-entropy algorithm assigns $A(\omega)=m(\omega)$. This feature significantly reduces the calculated error of the transport coefficients. Finally, there are no adjustable parameters.

The transport coefficients may be calculated from $A(\omega)$. The measurements we make are macroscopic, thus, in our calculation, we will average over all possible spacial configurations of a dilute uncorrelated system of impurities. In such a system, as shown by Bickers *et al.*,[6] averaging over the locations of the impurities removes the vertex correction terms from the diagrammatic expansions for the transport coefficients. Thus, the transport depends only upon the single-particle scattering information contained in $A(\omega)$. The resistivity becomes

$$\frac{\rho(0)}{\rho(T)}=-\frac{1}{\pi\Gamma}\int\frac{\partial f}{\partial\omega}A^{-1}(\omega)d\omega\ , \tag{2}$$

while the thermal conductivity is

$$\kappa(T)/T=-(\kappa/T)_0\frac{3}{\pi^3\Gamma T^2}\int\frac{\partial f}{\partial\omega}A^{-1}(\omega)\omega^2 d\omega\ , \tag{3}$$

where $\partial f/\partial\omega$ is the derivative of the Fermi function evaluated at ω. The Lorentz number (not plotted here) is the product $\kappa(T)\rho(T)/T$, and in the symmetric limit the thermopower is zero.

At low temperatures, the factor of $\partial f/\partial\omega$ restricts these integrals to sampling the low-frequency features of $A^{-1}(\omega)$ which are universal for large $u=U/\pi\Gamma$ and small T. However, for higher temperatures or smaller u, the nonuniversal features of $A^{-1}(\omega)$ are sampled. In addition, the large-ω features have larger statistical error, as shown previously by some of the authors.[13] Thus, we expect our results to be more universal for small T and large u. Furthermore, we expect κ, which samples higher ω features, to be less universal and have larger error bars than ρ.

An accurate determination of T_K is essential to demonstrate the universality of the transport coefficients. As shown in Fig. 1, we determine the corrections to Haldane's perturbation-theory expression for T_K,

$$T_{KH}=0.364(2\Gamma U/\pi)^{1/2}e^{-\pi U/8\Gamma}$$

(Refs. 1 and 15). This is done by fitting our susceptibility results to the universal susceptibility curve of Krishnamurthy *et al.*[1] obtained from a numerical renormalization-group calculation. We found, to an excellent approximation, that $T_K\approx T_{KH}(1+1/2u)$.

For sufficiently large u and low temperatures, we find that the transport coefficients are universal functions of T/T_K. This is demonstrated for ρ in Fig. 2 where $\rho(T)/\rho(0)$ is plotted versus u when $\Gamma=0.5$ and $T/T_K=1.5$. For our results, universality is indicated by the fact that, for $u>1.5$, the value of the resistivity saturates to a constant whereas the perturbation-theory result continues to rise monotonically.

In Fig. 3 the universal resistivity is plotted versus T/T_K for several values of u. The dotted line is the Fermi-liquid result

$$\rho(T)/\rho(0)=1-\alpha(T/T_K)^2\ ,$$

with $\alpha=0.83$. As shown in the inset to Fig. 3, $\alpha=0.83\pm0.06$ was determined from a fit to our low-T results ($T/T_K<0.25$). The quoted error ±0.06 reflects only statistical sources of error. Since, in this region, $\rho(T)/\rho(0)$ is very close to one, $1-\rho(T)/\rho(0)$ is strongly effected by both systematic and statistical errors. Thus, it was difficult to determine α accurately. At high temperatures $T>T_K$, the Hamann result (the solid line) is fitted to our results by varying T_{KN} in Eq. (1) so that the curves agree when $\rho(T_{KN})/\rho(0)=0.5$. This is consistent with how T_{KN} is defined in the Nagaoka-Suhl theory. We find $T_K/T_{KN}\approx0.4$. Our results agree well with Eq. (1) high temperatures, but diverge for $T<T_K$. However, for the highest temperatures simulated, the resistivity shows some slight nonuniversality in that the data fall below the Hamann result. In this limit the Anderson-model moment is thermally reduced, whereas the moment in Hamann's calculation is fixed. Thus, for finite u and $T\gg T_K$, the impurity moment which scatters the conduction electrons is reduced and hence so is the resistivity.

It is remarkable that the Wilson number often appears when we fit our results to previous results. The Wilson number relates the perturbation-theory value of T_K to the intrinsic Kondo scale T_{K0}, defined such that $\chi(T=0)=\mu^2/T_{K0}$, where μ is the electron spin. Wilson found that $T_K/T_{K0}=0.412$.[16] We find that Eq. (1) fits our results when $T_{KN}\approx T_{K0}$. Previously,[11] we found that, for $T\ll T_K$, the width of Abrikosov-Suhl peak in the impurity spectral density is determined by T_{K0}. Finally, Nozieres asserted that α is uniquely determined by the Wilson number

$$\alpha=(0.412\pi^2/4)^2=1.03\ ,$$

which may be consistent with our result.

In Fig. 4, the universal thermal conductivity $[\kappa(T)/T]/(\kappa/T)_{T=0}$ is plotted versus T/T_K for several values of u. For low temperatures $T/T_K<0.2$, κ is linear in T, indicative of a Fermi liquid. For high temperatures note that κ becomes nonuniversal and the error bars increase much more readily than ρ did.

In summary, using a combination of Monte Carlo

simulation and maximum entropy analytic continuation, we calculated the resistivity and thermal conductivity of dilute magnetic alloys. Our work is the first quantitatively correct calculation of transport for the spin-$\frac{1}{2}$ Anderson impurity over the entire range of interest $T \ll T_K$ to $T \gg T_K$. We find that our results are consistent with previous approximate calculations in their limits of applicability. This work demonstrates that it is possible to accurately calculate the transport coefficients for a strongly correlated many-body system by direct analytic continuation of quantum Monte Carlo data.

Note added in proof. Recently B. Horvatić pointed out to us that our empirically derived formula for T_K, over the range of u considered, always agrees with the exact Bethe-ansatz result [B. Horvatić and V. Zlatić, J. Phys. (Paris) **46**, 1459 (1985)] to within a few percent.

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