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DYNAMICS OF THE ANDERSON MODEL FOR DILUTE MAGNETIC ALLOYS: A QUANTUM MONTE CARLO AND MAXIMUM ENTROPY STUDY

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INTRODUCTION

The single-impurity Anderson model¹ was invented nearly thirty years ago to describe dilute magnetic impurities in metallic hosts, including the formation and properties of itinerant local moments in alloys. The model is a prerequisite for the understanding of mixed valent and heavy-fermion phenomena.² A limit of the model is the famous Kondo model³ which describes resistivity minima and saturation. The model is simple to state and its properties are readily measurable in the laboratory.⁴ However, the solution of the model is a difficult many-body problem. In recent years considerable progress in understanding the static properties of the model has been achieved using non-perturbative methods such as the Bethe ansatz,⁵ the renormalization group,⁶ and quantum Monte Carlo (QMC).⁷ Nevertheless, the understanding of the dynamical properties has remained elusive. These include the spectral density of the impurity state, the transport coefficients, and the dynamical magnetic susceptibility. The spectral density has been calculated reliably only for large orbital degeneracy⁸ or for expansion parameters below the range of most physical interest.⁹ It has been obtained only at zero temperature by the renormalization group method,¹⁰ and it is extremely difficult to calculate reliably from QMC.¹¹⁻¹⁵

In this article we describe the results^{16,17} of a new method¹⁸ for calculating the dynamical properties of the Anderson model. QMC¹⁹ generates data about the Matsubara Green's functions in imaginary time. To obtain dynamical properties, one must analytically continue these data to real time. This is an extremely ill-posed inverse problem similar to the inversion of a Laplace transform from incomplete and noisy data. Our method is a general one, applicable to

the calculation of dynamical properties from a wide variety of quantum simulations. We use Bayesian methods of statistical inference to determine the dynamical properties based on both the QMC data and any prior information we may have such as sum rules, symmetry, high frequency limits, etc. This provides a natural means of combining perturbation theory and numerical simulations in order to understand dynamical many-body problems. Specifically we use the well-established maximum entropy (ME) method²⁰ for image reconstruction. We obtain the spectral density and transport coefficients over the entire range of model parameters accessible by QMC, with data having much larger statistical error than required by other proposed analytic continuation methods.^{11–15}

In this article, we focus on the new physics we have learned about the dynamics of the Anderson model using these methods. We shall only outline the calculational methods, referring to other papers for details.

THE ANDERSON AND KONDO MODELS

The properties of a metal with a dilute concentration of magnetic impurities has been an enduring problem in condensed matter physics. Anomalies are found experimentally in the resistivity, thermal conductivity, thermopower, specific heat and magnetic susceptibility. The resistivity anomaly is the best known: as the temperature is lowered the resistivity displays a minimum, then increases, and finally saturates as the temperature goes to zero. The qualitative understanding of this resistivity minimum is well understood in terms of the Kondo Hamiltonian.³ This describes a spin one-half impurity interacting with the conduction electron spins via an antiferromagnetic coupling constant J . As the temperature is lowered toward a characteristic energy scale, T_K , the scattering rate of electrons from the impurity calculated by perturbation theory in J begins to diverge logarithmically. The increasing impurity resistivity overwhelms the decreasing phonon resistivity, and the resistivity begins to rise. The behavior as the temperature approaches zero is infinite in any finite order in perturbation theory, and in general it requires a non-perturbative treatment. The understanding which has developed from renormalization group calculations^{21,22} is that the conduction electrons begin to screen the magnetic impurity. This decreases the effective impurity moment toward zero forming a local singlet composed of the impurity spin and a compensating electron cloud. The resistivity saturates. No theories explain the resistivity behavior over the entire range of interest, $T \ll T_K$, to $T \gg T_K$.

The Anderson model¹ is a more general description of magnetic impurities in metallic alloys, which includes the possibility of charge fluctuations (changes in the number of electrons) on the impurity. The model consists of a half-filled conduction band interacting with an impurity via a hybridization matrix element V . The Hamiltonian can be written

$$\hat{H} = \sum_{\sigma} e_d \hat{d}_{\sigma}^{\dagger} \hat{d}_{\sigma} + \sum_{k\sigma} e_k \hat{a}_{k\sigma}^{\dagger} \hat{a}_{k\sigma} + \sum_{k\sigma} V (\hat{a}_{k\sigma}^{\dagger} \hat{d}_{\sigma} + \hat{d}_{\sigma}^{\dagger} \hat{a}_{k\sigma}) + U (\hat{n}_{\uparrow} - 1/2) (\hat{n}_{\downarrow} - 1/2) \quad (1)$$

Here, $\hat{d}_{\sigma}$ is an annihilation operator for an electron on the impurity, $\hat{a}_{k\sigma}$ is an annihilation operator for a conduction electron of energy e_k and spin σ , and $\hat{n}_{\sigma} = \hat{d}_{\sigma}^{\dagger} \hat{d}_{\sigma}$ is the number operator for a spin σ electron on the impurity site. There is a Coulomb energy U for two electrons to be on the same impurity. In the limit of large U charge fluctuations on the impurity are suppressed, and the Anderson model should reduce to the Kondo model in a way to be discussed further below. No essential physics is lost by limiting our discussion of the Anderson model to the infinite conduc-

tion bandwidth limit in which only the conduction band density of states at the Fermi level, $N(0)$, is important. Our calculations will also be restricted to the symmetric Anderson model in which the impurity energy, e_d , is taken to zero.

To develop our expectations for the single electron excitations of this model, we consider some limits. First, if the hybridization is taken to zero, the energy levels of the impurity are $E = 0$ for one electron on the impurity and $E = U/2$ for zero or two electrons on the impurity. We, therefore, expect single-electron excitations at $\omega = \pm U/2$. If now we turn on the hybridization, we expect these excitations to be Lorentzian broadened by a hybridization width $\Gamma = N(0)\pi V^2$. The limit of large U provides another energy scale for single particle excitations. Then, a Schrieffer-Wolf transformation²³ of the Anderson model yields the Kondo Hamiltonian with antiferromagnetic coupling constant, $J = -8\Gamma/\pi N(0)U$. Using high temperature perturbation theory in J , Haldane²⁴ has calculated that the Kondo temperature is given by $T_K^H \approx 0.515\Gamma\sqrt{u}\exp(-\pi^2 u/8)$, where $u \equiv U/\pi\Gamma$. By particle-hole symmetry we expect single particle excitations centered at $\omega = 0$ of width comparable to T_K .

These excitations are to be observed in the impurity single-particle spectral function, $A(\omega)$, which is related to the impurity retarded Green's function by

$$G_d^{ret}(\omega) = \int_0^\infty dt e^{i\omega t} \frac{1}{2} \sum_\sigma \langle [\hat{d}_\sigma(t), \hat{d}_\sigma^\dagger(0)]_+ \rangle = \int_{-\infty}^\infty d\omega' \frac{A(\omega')}{\omega - \omega' + i\epsilon} \quad (2)$$

The spectral function is positive definite, and the integral of it over ω is normalized to one.

While, in general, transport coefficients depend on two-particle Green's functions, Bickers *et al.*⁸ have shown that in the dilute impurity limit for the Anderson model the single-particle spectral function may be related directly to the transport coefficients. The resistivity is given by

$$\frac{\rho(0)}{\rho(T)} = -\frac{1}{\pi\Gamma} \int_{-\infty}^\infty d\omega \frac{\partial f}{\partial \omega} A^{-1}(\omega) \quad , \quad (3)$$

where $f(\omega)$ is the Fermi function. The electronic thermal conductivity is given by

$$\frac{\kappa(T)}{T} = -\left(\frac{\kappa(T)}{T}\right)_{T=0} \frac{3}{\pi^3 \Gamma T^2} \int_{-\infty}^\infty d\omega \omega^2 \frac{\partial f}{\partial \omega} A^{-1}(\omega) \quad . \quad (4)$$

To discuss their scaling properties, we first remove an arbitrary energy scale by dividing all energies by Γ , and then we discuss a *scaled spectral function* $\pi\Gamma A(\omega)$. If U is sufficiently large compared to T such that there are no significant charge fluctuations on the impurity site, we expect that the only energy scale at low ω is the Kondo temperature, T_K . We refer to a lack of dependence on U as *universality*. For example, for U large enough that the static magnetic susceptibility of the Anderson model depends only on T/T_K , we say that the susceptibility is a universal function of T/T_K . We expect the scaled spectral function to depend only on ω/T_K and T/T_K for ω small compared with U . At sufficiently low temperatures the Fermi factor, $\partial f/\partial \omega$, in the transport coefficients ensures that only the low frequency part of the scaled spectral function

contributes. Therefore the transport coefficients can also be expected to be universal functions of T/T_K . At sufficiently high temperatures the Fermi factor will mix in the high frequency peaks at $\omega = \pm U/2$ resulting in non-universal behavior of the transport coefficients.

Not only do we wish to calculate this universal behavior in the Kondo limit at large U , but we also wish to study the approach to universality in the Anderson model with increasing U . Horvatic *et al.*⁹ have developed a perturbation expansion for the spectral function with u as the small parameter. While this expansion is in principle absolutely convergent, in practice only a few diagrams in the expansion are calculated. The available results correspond to self-consistent second order perturbation theory for the self-energy starting from a Hartree-Fock basis. We expect their results to be valid at small u , and to become increasingly poor at large u . While they recover the main features of the spectral function discussed above, the $\omega = 0$ peak in their spectral function does not scale with T_K , nor are the transport coefficients calculated using their spectral functions in Eqs. (3) and (4) universal functions. A critical question we wish to address is how high must u be in order for Kondo universality to apply

The Kondo limit leads to several expectations for the spectral functions and transport coefficients. The detailed shape of the spectral function at zero temperature has been predicted by Doniach and Sunjic²⁵ by exploiting the analogy between the Kondo model and the X-ray edge singularity problem. They predicted the form

$$\pi\Gamma A(\omega)_{T=0} = \text{Re} \sqrt{\frac{i\Gamma_K}{\omega + i\Gamma_K}}, \quad (5)$$

although they did not predict the value of Γ_K . At zero temperature, the Friedel sum rule requires the scaled spectral function to equal 1.0 at $\omega = 0$.

Wilson²² carried out a famous numerical renormalization group study of the Kondo model. The model considered by Wilson had a finite conduction bandwidth that provided a natural cutoff to the calculations, and his expressions for T_K depended on this cutoff. However, his universal results are straightforwardly mapped onto the infinite bandwidth limit studied here. He defined a low temperature energy scale, T_K^L , by $T_K^L \chi(0) = \mu_B^2$, where $\chi(T)$ is the magnetic susceptibility. He found that $T_K^L = 2.5 T_K^H$, where T_K^H is the Kondo temperature predicted by high temperature perturbation theory and 2.5 is referred to as the *Wilson number*. We expect a similar relation for the Anderson model with something like T_K^H playing the role of T_K^L . The precise mapping of the Kondo model onto the Anderson model is discussed further in the results section.

Based on Wilson's study, Nozieres²⁶ predicted that at low temperatures the resistivity would show Fermi liquid behavior with

$$\lim_{T \ll T_K} \frac{\rho(T)}{\rho(0)} = 1 - \alpha \left(\frac{T}{T_K^H} \right)^2. \quad (6)$$

Nozieres suggested that α is determined by the Wilson number to have the value 1.03.

At temperatures high enough to apply perturbation theory in J , the resistivity is expected

to be given by the Hamann–Nagaoka–Suhl expression²⁷

$$\text{for } T \gtrsim T_K^N \quad \frac{\rho(T)}{\rho(0)} = \frac{1}{2} \left[1 - \frac{\ln T/T_K^N}{\sqrt{\ln^2 T/T_K^N + 3\pi^2/4}} \right] \quad (7)$$

Here T_K^N is the “Nagaoka” Kondo temperature defined by where the resistivity goes through one-half its peak value.

One goal of our calculations is to verify these predictions and to determine the parameters Γ_K , α , and T_K^N along with their relation to T_K^H . In addition, we wish to obtain the universal curves over the entire range from $T \ll T_K$ to $T \gg T_K$, and to observe the breakdown of universality for the transport coefficients at small u and large T .

QUANTUM MONTE CARLO AND MAXIMUM ENTROPY

In our approach, the spectral function is to be obtained by statistical inference from QMC data on the impurity Matsubara Green’s function in imaginary time, $G(\tau)$. The QMC algorithms have been described in detail elsewhere.^{7,28} The basics of the maximum entropy analysis of these data has also been published elsewhere,¹⁸ and the details of the application to the Anderson model will be described in forthcoming publications.^{29,30} Although the focus of the present article is on the physics results we have obtained, we will briefly sketch the novel elements of our calculational approach.

$G(\tau)$ is defined by

$$G(\tau) = \frac{1}{2} \sum_{\sigma} \langle T_{\tau} [\hat{d}_{\sigma}(\tau) \hat{d}_{\sigma}^{\dagger}(0)] \rangle \quad (8)$$

This is periodic in $0 < \tau < \beta$, where $\beta = 1/T$. To generate data on $G(\tau)$, we use the QMC algorithm of Hirsch and Fye.²⁸ We obtain $G_i = G(\tau_i)$ for a discrete set of imaginary time values, τ_i . The spacing between the τ_i , $\Delta\tau$, must be kept sufficiently small ($\Delta\tau^2 \Gamma U < 0.2$) to minimize systematic *Trotter* breakup errors in the formulation of the QMC procedure. The computational time required for the calculation scales as $(\Delta\tau/\beta)^{-3}$. These two potentially conflicting requirements limit the range of U , Γ and β which can be realistically calculated by QMC. Our calculations were limited to $u < 3.5$ and $T/T_K > 0.1$.

To extract the spectral function from $G(\tau)$ data, we must invert the spectral representation

$$G(\tau) = \int_{-\infty}^{\infty} d\omega A(\omega) \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} \quad (9)$$

This is similar to a Laplace transform. The numerical inversion of such transforms is *extremely ill-posed* when the data are noisy and incomplete; that is, there exists an infinite set of spectral functions all of which fit the data within statistical errors, and small errors in the data can lead to very large changes in the spectral function. MaxEnt^{20,31,32} approaches such inverse problems

using probability theory. We infer the most probable spectral function (termed the *image*) and estimate its reliability, based on both the QMC data and any prior information we may have about the spectral function before we obtained the data. The prior information may include sum rules, symmetry, high frequency limits, etc. It is embodied in an entropy functional. The data are embodied in a chi-squared measure for the quality of fit.

The Shannon-Jaynes entropy functional is

$$S = \int_{-\infty}^{\infty} d\omega \left[A(\omega) - m(\omega) - A(\omega) \log \left(\frac{A(\omega)}{m(\omega)} \right) \right], \quad (10)$$

whose form is a unique consequence of the axioms of logical statistical inference.³¹ The quantity $m(\omega)$ is termed the *default model*, as it is the spectral density the method would return in the absence of any data. Choosing a good default model has benefits similar to a variance reduction technique. The choice should be based on the prior information we have about the spectral function before we obtain the QMC data. The transform, Eq. (9), contains the most information about the many-body effects at low frequency, but it is insensitive to the high frequency behavior of the spectral function. In practice, for an informative default model we used the Horvatic *et al.* perturbation theory prediction,⁹ which can be expected to be reliable at high frequencies.

The method requires an estimate of the statistical errors¹⁸ for the G_i , which is embodied in a covariance matrix. Although all prior approaches¹¹⁻¹⁵ to calculating spectral functions from QMC data have assumed that the G_i are statistically independent and the covariance matrix is diagonal (or worse, they ignored the errors), we find that the covariance matrix is dense. The eigenvalues vary over 4 to 6 orders of magnitude. The generalization of the chi-square measure to covariant data is¹⁸

$$\chi^2 \equiv \sum_{ij} (G_i - F_i) C_{ij}^{-1} (G_j - F_j), \quad (11)$$

where the F_i is the fit to G_i which would be generated by a given choice of spectral function in Eq. (9), and C is the covariance matrix of the G_i .

The image is obtained by maximizing $\alpha S - \chi^2/2$ as a functional of the spectral function. The scalar α is a statistical regularization parameter which is calculated from the data by Bayesian statistical inference arguments.³¹ One may also say that the entropy is maximized subject to the constraint that the spectral function fit the data with Lagrange multiplier $1/\alpha$. This procedure is implemented using a commercial maximum entropy code.³³ An important feature of the maximum entropy method is full error propagation. It allows us to calculate the errors on any quantity formed by integrating over the spectral function, such as the transport coefficients.

RESULTS

Since a focus of our effort will be studying Kondo universality, we must first establish the mapping of the T_K of the Anderson model onto the T_K of the Kondo model. The Haldane expression²⁴ for the T_K of the Anderson model was obtained in a large u limit. There may be corrections to the Haldane result, T_K^H , at the modest u achievable with QMC. We¹⁷ calculate this correction numerically from the static magnetic susceptibility. Krishnamurthy *et al.*⁶ obtained universal magnetic susceptibility curves of the Kondo model from a numerical renormalization group cal-

culatation. The solid line in Fig. 1 shows their results for the screened local moment, $T\chi(T)/g^2$, plotted versus $\ln(T/T_K)$. From our calculations we obtain the magnetic susceptibility of the Anderson model at various u , as also shown in Fig. 1 plotted versus $\ln(T/T_K^H)$. By shifting the T_K scale, the Anderson model results can be made to overlap the Kondo model results. The inset in Fig. 1 shows the ratio of the shifted T_K to T_K^H plotted versus $1/u$. One sees that these data may be fit by a straight line, $T_K/T_K^H = 1 + 1/2u$. We use this to define the T_K of the Anderson model.

Fig. 1 $T\chi(T)/g^2$ (symbols) vs. $\ln(T/T_K^H)$ (lower scale) for various values of $u \equiv U/\pi \Gamma$. The solid line is the numerical renormalization group result of Krishnamurthy *et al.* vs. $\ln(T/T_K)$ (upper scale). The correction to $T_K^H = 0.515 \Gamma \sqrt{u} \exp(-\pi^2 u/8)$, for each value of u , may be determined by scaling T_K^H until the data fit the renormalization group 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.* The solid line in the inset is $T_K/T_K^H = (1 + 1/2u)$.

Figure 2 shows typical results¹⁶ for the scaled spectral function $\pi \Gamma A(\omega)$. The spectral function obtained from the QMC data using maximum entropy is labeled QMC-ME. The perturbation theory prediction of Horvatic *et al.*⁹ is labeled H. The ratio of the two results is labeled QMC-ME / H. While the H prediction has the qualitatively correct structure, the QMC-ME Kondo peak is depressed and broadened compared to H and the $U/2$ peaks are slightly enhanced. This preserves the sum rule on the spectral function. In general, we find that QMC-ME and H agree for $u < 1.2$. However, with increasing u the QMC-ME Kondo peak becomes increasingly depressed and broadened compared to H, and the QMC-ME $U/2$ peaks become increasingly enhanced compared to H. In principle, higher order terms in the Horvatic *et al.* expansion may be calculated which would improve the agreement with the QMC data at higher u . In practice, this has not yet been carried out. Nevertheless, second order perturbation theory for the self-energy has provided a very good default model for the MaxEnt method. Images obtained with a flat (or ignorant) default model have much larger errors. Our spectral densities are obtained from data having more than ten times the statistical error required by direct methods for analytic continuation, such as simple Padé approaches.^{13,15} The difference is that MaxEnt fits the data only within

Fig. 2 QMC-ME labels the quantum Monte Carlo and maximum-entropy results for the spectral density of the symmetric Anderson model for the parameters indicated. H is the prediction of the self-consistent second-order perturbation theory of Horvatic *et al.* for the self-energy QMC-ME/H labels the ratio of the two calculations.

Fig. 3 Study of the Kondo scaling of the spectral density at fixed $T/T_K = 1.5$ and for the values of $u \equiv U/\pi\Gamma$ indicated. QMC-ME labels the quantum Monte Carlo and maximum entropy results. They are universal functions of ω/T_K (independent of u) for ω/T_K less than 20, and they are nonuniversal for larger ω/T_K in the vicinity of the $\omega = U/2$ peaks. Inset: Average of $\pi\Gamma A(\omega)$ for $\omega/T_K < 20$ plotted vs. u . H labels the predictions of Horvatic *et al.* for the same values of u , with higher $\pi\Gamma A(0)$ corresponding to larger u . The H theory is distinctly non-universal.

statistical error, whereas the direct methods fit the data exactly and, therefore, propagate statistical noise into the spectral density.

As discussed above, there is only a single low energy scale in the problem, T_K . Therefore we expect that at low frequencies the Kondo peak should scale with T_K and be independent of u . Figure 3 shows our most striking results.¹⁶ Here the QMC-ME spectral functions are plotted against ω / T_K at fixed $T / T_K = 1.5$ and for a variety of u . The semilog scale emphasizes the behavior at low frequencies. One can see that the QMC-ME spectral density is approximately universal (independent of u) for $\omega / T_K \lesssim 20$, although the high frequency behavior around the $U/2$ peak is non-universal. While MaxEnt does not provide error estimates at individual ω / T_K points, it does provide error estimates on integrals of the spectral function. The insert in Fig. 3 shows that the average of $\pi \Gamma A(\omega)$ for $\omega / T_K \lesssim 20$ is universal for $u > 1.25$ within statistical error. We have repeated such calculations at a variety of T / T_K and for a variety of integrated quantities to verify the universal behavior. In contrast, the H predictions are distinctly non-universal in the same frequency range. Only for $u \lesssim 1.25$ where both H and QMC-ME agree within statistical errors is QMC-ME non-universal. It is remarkable that the H prediction appears to be tangent to the universal behavior at $u \approx 1.2$. At larger u the Lorentzian broadened $|\omega| = U/2$ peaks are distinct from the Kondo peak, whereas at smaller u the two peaks are merged.

Figure 4 shows¹⁶ the evolution of the universal Kondo peak as a function of T/T_K at fixed $u = 2.0$. At $T/T_K \gtrsim 10$ the Kondo peak is absent. With decreasing T/T_K the Kondo peak grows and narrows until at $T/T_K \lesssim 0.2$ the height of the central peak has almost approached the Freidel sum rule value of 1.0. The insert in Fig. 3 shows the screened local moment calculated by QMC, $T\chi(T)/g^2$, plotted versus T/T_K for $u = 2.0$. The growth of the Kondo peak with decreasing T/T_K is correlated with the screening of the impurity local moment by the conduction electrons. Plotted as the dashed line labeled DS in this figure is the Doniach-Sunjić²⁵ prediction for the shape of the Kondo peak at zero temperature. We find that a best fit to the $T/T_K = 0.2$ QMC-ME curve is obtained with $\Gamma_K = 2.5 T_K$, which is remarkably the Wilson number²² for the Kondo problem. The Doniach-Sunjić formula also agrees with zero temperature numerical renormalization group calculations.¹⁰

For sufficiently large u and low temperatures, we find that the transport coefficients are universal functions of T/T_K . This is demonstrated for the resistivity¹⁷ in Fig. 5, where the resistivity ratio, $\rho(T)/\rho(0)$, is plotted vs. u for $T/T_K = 1.5$. 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 Horvatic *et al.* perturbation theory prediction contains to rise monotonically. We wish to emphasize that the error bars on our resistivity come from our estimates of the covariance matrix of the QMC calculation, and the errors are propagated by our maximum entropy image reconstruction code into integrals over the spectral function. We found that these estimates were reproducible when the QMC calculation was repeated with a different random number seed. The increasing error bars with increasing u are due to two factors: 1) the perturbation theory when used as a default model diverges from the QMC data with increasing u ; and 2) the QMC calculation becomes more difficult with increasing u due to the Trotter breakup limitation discussed earlier. The error estimates are much larger when uninformative default models are used, making it more difficult to prove universality. In Figure 6 the resistivities are plotted versus $\ln(T/T_K)$ for several values of u . One can see that these define a universal resistivity curve (independent of u) over the desired range from $T \ll T_K$ to $T \gg T_K$.

Nozières²⁶ has provided an asymptotic prediction of Fermi liquid behavior for the resis-

Fig. 4. QMC-ME labels the quantum Monte Carlo and maximum entropy results for fixed $u = 2.0$ and varying T/T_K as indicated. The Kondo peak is approximately independent of u for $\omega/T_K < 20$. DS labels the Doniach-Sunjić expression, Eq. (5), for the zero temperature shape of the Kondo peak. We find a best fit for $\Gamma_K = 2.5T_K$. Inset: Screened local moment, $T\chi(T)/g^2$, plotted vs. T/T_K .

Fig. 5 The resistivity ratio $\rho(T)/\rho(0)$ vs. $u \equiv U/\pi\Gamma$ when $T/T_K = 1.5$. The open circles are from the perturbation theory of Horvatic *et al.* For $u < 1.2$ there was no significant difference between the perturbation theory and the Monte Carlo results. Universality of the Monte Carlo data is indicated by the fact that for $u > 1.5$ the value of the ratio saturates to a constant within MaxEnt statistical errors, whereas the perturbation theory continues to rise monotonically.

tivity as T/T_K goes to zero given by Eq. (6) with $\alpha = 1.03$. Since at $T \ll T_K$ the resistivity ratio is very close to one and the QMC calculation is approaching the Trotter limit, it is difficult to determine the difference between the resistivity ratio and one reliably. The dotted line in Fig. 6 is the Fermi liquid result, Eq. (6), with α an adjustable parameter. We found a best fit for $(T/T_K)^2 < 0.1$ of $\alpha = 0.83 \pm 0.06$. The quoted error reflects only statistical sources of error, but there is also a potential for systematic error. A subtle point of the maximum entropy method is a built-in bias toward the default model of approximately one standard deviation. The default model was the Horvatic *et al.* perturbation theory which had a larger resistivity ratio than the QMC-ME calculation (Alternatively, it had a smaller α , although Horvatic *et al.* calculation does not show Kondo universality). For $(T/T_K)^2 < 0.1$ the Nozières prediction is approximately one standard deviation above the QMC-ME results for all data points. We conclude that our QMC-ME results are consistent with Nozières prediction within one standard deviation.

The solid line in Fig. 6 is the Hamann *et al.* prediction, Eq. (7) obtained by fitting the data for $T > T_K$ by adjusting T_K^N so that the curves agree when $\rho(T_K^N)/\rho(0) = 0.5$. This is consistent with how T_K^N is defined in Hamann-Nagaoka-Suhl theory. We find $T_K^N/T_K = 2.5$, which is remarkably again the Wilson number for the Kondo problem. Our results agree well with Eq. (7) at high temperatures, but they diverge for $T < T_K$. However, for the highest temperatures simulated the resistivity shows some slight non-universality and the resistivity ratio falls below the Hamann result. In this limit the Anderson model moment is thermally reduced due to occupation of the zero electron and two electron states on the impurity, whereas the moment in Hamann's calculation is fixed at one-half. For finite u and $T \gg T_K$ the impurity moment which scatters the conduction electrons is reduced and hence so is the resistivity.

Figure 7 shows our results¹⁷ for the electronic thermal conductivity. These also exhibit universal Kondo scaling at low T for $u > 1.2$, but there is a breakdown of scaling at large T . Because of the ω^2 term in Eq. (4), the thermal conductivity samples higher frequency behavior of the spectral function than the resistivity. Since the high frequency behavior around the $\omega = \pm U/2$ peaks is non-universal, as the temperature increases the $\partial f/\partial \omega$ factor will result in non-universality at lower temperatures for the thermal conductivity than for the resistivity. Unfortunately, unlike the resistivity, there are no detailed Fermi liquid or high temperature perturbation theory predictions for the thermal conductivity with which to compare our QMC-ME results.

CONCLUSIONS AND DISCUSSION

We have verified all of our expectations about the dynamical properties of the symmetric Anderson model. For $u < 1.2$ our results agree with the non-universal behavior of the Horvatic *et al.*⁹ perturbation theory. For $u > 1.2$ we obtain universal Kondo scaling for low frequency properties including the Abrikosov-Suhl peak in the spectral function and for transport coefficients such as the resistivity and electronic thermal conductivity. We find agreement with the Doniach-Sunjic expression²⁵ for the zero-temperature shape of the spectral function and with the Hamann-Nagaoka-Suhl expression²⁷ for the resistivity for $T > T_K$. Our results are within one standard deviation of the Nozières prediction²⁶ for the coefficient α of the $(T/T_K)^2$ term in Fermi liquid expression for the resistivity at $T \ll T_K$. Moreover, we find a remarkable convergence for the numerical parameters of these theories, summarized in the following equation,

Fig. 6 $\rho(T)/\rho(0)$ vs. T/T_K at different values of u . The solid line is from the self-consistent high temperature calculation of Hamann *et al.*, Eq. (7). It is fit to our results by varying T_K^N so that the curves agree when $\rho(T_K^N)/\rho(0) = 0.5$. We find $T_K^N = 2.5 T_K$. As expected, this prediction fails at low temperatures. The dotted line is the Fermi liquid result due to Nozieres, Eq. (6), with a best fit of $\alpha = 0.83 \pm 0.06$. The resistivity is roughly logarithmic for $0.5 < T/T_K < 4.0$.

Fig. 7 Thermal conductivity, $(\kappa(T)/T)/(\kappa(T)/T)_{T=0}$ vs. T/T_K at different values of u . Note that at low temperatures, $\kappa(T)$ is linear in T , indicative of a Fermi liquid, as argued by Nozieres. Universality breaks down at large T/T_K .

$$T_K^N = \Gamma_K = T_K^o = 2.5 \left(1 + \frac{1}{2u} \right) T_K^H = 2.5 T_K \quad (12)$$

Here, T_K^N is the Nagaoka Kondo temperature²⁷ defined by where the resistivity ratio goes through one-half; Γ_K is the width in the Doniach-Sunjić expression²⁵ for the zero temperature spectral function; T_K^o is Wilson's Kondo temperature determined²² by numerical renormalization group calculations; 2.5 is the famous Wilson number; T_K^H is the Haldane Kondo temperature²⁴ determined by high temperature perturbation theory in the impurity-conduction electron spin coupling constant J obtained by a Schrieffer-Wolff transformation²³ of the Anderson model in the large u limit; and, the factor $(1+1/2u)$ is the result of our mapping¹⁷ of the Kondo model onto the Anderson model at finite u by comparing the static magnetic susceptibility of the QMC calculation of the Anderson model to the static magnetic susceptibility of Krishnamurthy *et al.*'s renormalization group study³⁴ of the Kondo model. This remarkable simplicity and convergence certainly deserves an analytic explanation.

Perhaps even more significantly for the long term, we have established a general methodology¹⁶⁻¹⁸ for the *ab initio* calculation of the dynamical properties of many-body systems. This combines quantum Monte Carlo to generate Matsubara Green's functions in imaginary time, the maximum entropy method to solve the extremely ill-posed problem of numerically inverting the spectral representation, and perturbation theory and other forms of prior knowledge to provide informative default models needed to minimize the variance of the maximum entropy results. Our method provides for full error propagation from the raw QMC data all the way to integrated properties of the spectral function, such as the transport coefficients.

The method has already been applied to several other problems in computational condensed matter physics. These include verifying the Haldane conjecture about Heisenberg spin chains,³⁴ calculating gap states in superconductors induced by magnetic impurities,³⁵ and the determining the density of states of the Hubbard models³⁶ which are perhaps relevant to high T_c superconductivity. We are currently applying the method to the calculation of the dynamical magnetic susceptibility of the Anderson model, to the asymmetric Anderson model to better compare with experimental data, and to the X-ray edge singularity problem.

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