Spectral Densities of the Symmetric Anderson Model

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The spectral density of the single-impurity Anderson model is calculated by a combination of quantum Monte Carlo method to provide data on the Matsubara Green's function, the maximum-entropy method of image reconstruction to invert numerically the spectral representation, and perturbation theory to provide informative default models. The Kondo central peak of the spectral density is shown to be a universal function of ω/T_K and T/T_K at low frequencies, where T_K is the Kondo temperature. The higher-frequency side peaks are nonuniversal. With decreasing T/T_K the Kondo peak grows as the screened local moment disappears.

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The single-impurity Anderson model[1] was invented nearly thirty years ago to describe dilute magnetic impurities in metallic hosts. Its importance has grown with current research on strongly correlated electronic systems including mixed valent, Kondo, and heavy-fermion phenomena. In recent years considerable progress in understanding the model has been achieved using nonperturbative methods such as the Bethe ansatz,[2] the renormalization group,[3] and quantum Monte Carlo (QMC).[4] Nevertheless, many properties of the model have remained elusive such as the spectral density of the impurity state, which is essential for comparison with spectroscopic and transport measurements. The spectral density has been calculated reliably by perturbative methods only for large orbital degeneracy[5] or for expansion parameters below the range of most physical interest.[6] It cannot be obtained with the Bethe ansatz, has been obtained only at zero temperature by the renormalization-group method,[7] and is extremely difficult to calculate reliably from QMC.[8,9]

In this Letter we report significant progress in obtaining the spectral density of the nondegenerate symmetric single-impurity Anderson model from QMC data. Our approach[10] is to regard the analytic continuation of Matsubara Green's-function data from imaginary time to real time as an image reconstruction problem, and to use the well-established maximum-entropy (ME) method.[11] The spectral density is obtained reliably over the entire range of model parameters accessible by the QMC method with data having much larger statistical error than required by other proposed analytic continuation methods.[8,9,12] For ratios of Coulomb interaction to hybridization width greater than π, we report that the $\omega=0$ peak of the spectral density (Abrikosov-Suhl resonance or Kondo peak) is a universal function of ω/T_K and T/T_K, where T_K is the Kondo temperature. We compare our results to a commonly used perturbation theory[6] for the spectral density, which does not exhibit universal Kondo behavior at least to second order. Moreover, our successful procedure for calculating the spectral density is a general method applicable to a wide variety of quantum simulations.

The Anderson model consists of a half-filled conduction band interacting via a matrix element V with an impurity site. There is a Coulomb energy U for two electrons on the same impurity. For the symmetric case the impurity energy is equal to the Fermi energy. Taking the bandwidth to infinity leaves only two relevant parameters: U and the hybridization width $\Gamma=N(0)\pi V^2$, where $N(0)$ is the conduction-band density of states at the Fermi energy. We expect an impurity spectral density $A(\omega)$, with Lorentzian side peaks centered at $\omega=\pm U/2$ of width Γ, and a central Kondo peak at $\omega=0$ of width on the order of T_K.

$A(\omega)$ is to be obtained from the impurity Matsubara Green's function $G(\tau)$ calculated by QMC. $G(\tau)$ is periodic in $0<\tau<\beta$, where $\beta=1/T$. To generate data on $G(\tau)$, we use the algorithm of Hirsch and Fye.[13] This algorithm is particularly stable at low temperatures when the electron-electron Coulomb interaction U is restricted to a few sites. In such cases the simulations can be performed without stabilization methods, and for the symmetric Anderson model the "sign problem" that plagues other fermion simulations is absent. We obtain $G_i\equiv G(\tau_i)$ for a discrete set of imaginary-time values τ_i. The spacing between the τ_i, $\Delta\tau$, must be kept sufficiently small ($\Delta\tau^2\Gamma U\lesssim 0.19$) to minimize systematic Trotter breakup errors. We made no attempt to remove this error by extrapolation to $\Delta\tau=0$. 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. The G_i are coarse-grained averages of the QMC data[14] to remove correlations in Monte Carlo time. To approach the conditions of Gaussian distributed data, we had to use about 100 bins, each with about 1000 measurements. This binning was accompanied by tests for how Gaussian the data were. A detailed description of these procedures will be given elsewhere.[15]

To use an image-reconstruction method to determine $A(\omega)$, it is also essential to estimate the statistical errors[10] on the G_i embodied in the covariance matrix $C_{ij} \equiv \langle G_i G_j \rangle - \langle G_i \rangle \langle G_j \rangle$. Although all prior approaches[8,9] to calculating spectral functions have assumed that the G_i are statistically independent (**C** is diagonal), we find that the covariance matrix is dense. To a first approximation, all the elements of **C** are of comparable magnitude except where they are required to be small by the symmetry of the model. The eigenvalues of **C** vary over 4 to 6 orders of magnitude.

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

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

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 $A(\omega)$ all of which fit the data within statistical errors, and small errors in the data can lead to very large changes in $A(\omega)$. ME[10,11] approaches such inverse problems using probability theory. We infer the most probable $A(\omega)$ (termed the *image*) and estimate its reliability, based on both the QMC data and any prior information we have about $A(\omega)$. The data are embodied in a χ^2 measure for the quality of fit. The prior information about the positive and additive nature of $A(\omega)$ is embodied in an entropy functional S. The image is obtained by maximizing $\alpha S - \chi^2/2$ as a function of $A(\omega)$. The scalar α is a statistical regularization parameter which is calculated from the data by statistical inference arguments.[16]

The Shannon-Jaynes entropy functional is

$$S = \int_{-\infty}^{\infty} d\omega \left[A(\omega) - m(\omega) - A(\omega) \ln\left(\frac{A(\omega)}{m(\omega)} \right) \right], \qquad (2)$$

whose form is a unique consequence of the axioms of logical statistical inference.[16] 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. In practice, we used for an informative $m(\omega)$ the prediction of Horvatic, Sokcevic, and Zlatic[6] for $A(\omega)$ which involves a calculation of the self-energy by self-consistent second-order perturbation theory starting from a Hartree-Fock basis.

The generalization of the χ^2 measure to covariant data is[10]

$$\chi^2 \equiv \sum_{ij} (G_i - F_i) C_{ij}^{-1} (G_j - F_j)\,, \qquad (3)$$

where F_i is the fit to G_i which would be generated by a given choice of $A(\omega)$ via Eq. (1). Since **C** is a symmetric positive-definite matrix, we can decompose it by $\mathbf{C} = \mathbf{O}^T \cdot \mathbf{D} \cdot \mathbf{O}$, where the diagonal matrix **D** has as its elements the eigenvalues of **C**, and **O** is an orthonormal matrix. Applying **O** to a discretized version of Eq. (1), we transform the inversion problem to a new data space in which the data are statistically independent and the errors are given by the square roots of the elements of **D**. This permits the use of existing robustly tested ME image-reconstruction algorithms[17] which have been designed for Gaussian-independent data.

For most of our measurements, the systematic errors associated with the finite value of $\Delta\tau$ were estimated to be typically $<0.5\%$, and the QMC statistical errors were typically $<0.3\%$. The internal consistency of classic ME[16] enables the calculation of a statistical error rescaling, which can compensate for a failure of the data to achieve a Gaussian distribution. For most of our runs the errors were rescaled upward by less than 20%, meaning that the covariance matrix and the data were consistent with a Gaussian distribution. In cases where the error rescaling was larger, there was significant kurtosis in the distributions of the G_i. The error rescaling could usually be reduced to less than 20% by decreasing $\Delta\tau$, implying a greater consistency with a Gaussian distribution.

To describe our results for the symmetric Anderson model, we find it convenient to reexpress the parameters U and Γ in terms of the expansion parameter of the perturbation theory of Horvatic, Sokcevic, and Zlatic, $u = U/\pi\Gamma$, and the Kondo temperature T_K. We take as T_K the Haldane[18] high-temperature perturbation-theory expression multiplied by a correction $(1+1/2u)$ found numerically;[19] i.e.,

$$T_K = (1+1/2u) 0.515 \Gamma \sqrt{u} \exp(-\pi^2 u/8)\,.$$

We scale energies by Γ and plot the image as $\pi\Gamma A(\omega)$.

Figure 1 shows typical results. The $A(\omega)$ obtained from the QMC data using ME is labeled QMC-ME. The prediction of Horvatic, Sokcevic, and Zlatic for $A(\omega)$ 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 which preserves the zeroth-moment sum rule on $A(\omega)$. In general, we find that QMC-ME and H agree for $u \lesssim 1.2$, but 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. We were able to calculate up to $u = 3.5$ before running into Trotter breakup limitations. In prin-

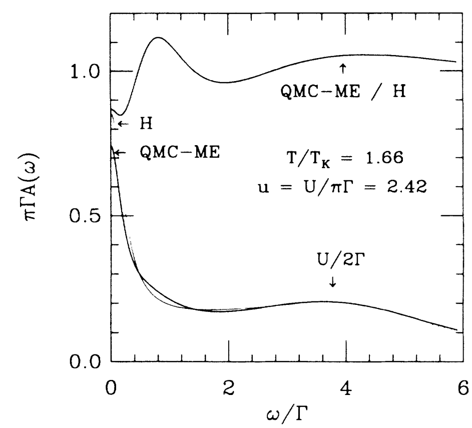

FIG. 1. QMC-ME labels the quantum Monte Carlo and maximum-entropy results for the spectral density of the symmetric Anderson model for the parameters indicated. H is the prediction of the self-consistent second-order perturbation theory of Horvatic, Sokcevic, and Zlatic for the self-energy. QMC-ME/H labels the ratio of the two calculations.

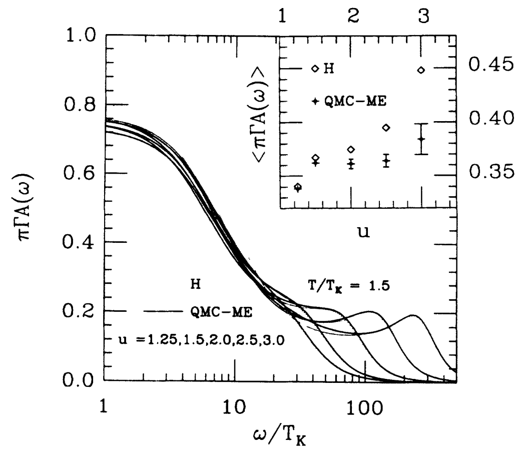

FIG. 2. Study of Kondo scaling of the spectral density at fixed $T/T_K = 1.5$ and for the values of $u = U/\pi\Gamma$ indicated. QMC-ME labels the quantum Monte Carlo and maximum-entropy results. They are universal functions of ω/T_K (independent of u) for ω/T_K less than 20, and they are nonuniversal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

ciple, the perturbation expansion of Horvatic, Sokcevic, and Zlatic in u is absolutely convergent, and higher-order terms 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 ME method. Images obtained with a flat (or ignorant) default model have much larger errors. Our spectral densities are obtained from data having more than 10 times the statistical error required by direct methods for analytic continuation, such as simple Padé approaches.[12] The difference is that ME fits the data only within statistical error, whereas the direct methods fit the data exactly and, therefore, propagate statistical noise into the spectral density.

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 2 shows our most striking results. Here the QMC-ME images $\pi\Gamma A(\omega)$ are plotted against ω/T_K at fixed $T/T_K = 1.5$ and for a variety of u. The semilogarithmic 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 nonuniversal. While ME does not provide error estimates at individual ω/T_K points, it does provide error estimates on integrals of $A(\omega)$. The inset in Fig. 2 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 nonuniversal in the same frequency range. Only for $u \lesssim 1.25$ where both H and QMC-ME agree within statistical errors is QMC-ME nonuniversal. 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 $\omega = \pm U/2$ peaks are distinct from the Kondo peak, whereas at smaller u the two peaks are merged.

Figure 3 shows 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 inset 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-Sunjic[20] prediction for the shape of the Kondo peak at zero temperature. This is given by

$$\pi\Gamma A_{\mathrm{DS}}(\omega) = \mathrm{Re}\sqrt{i\Gamma_K/(\omega + i\Gamma_K)}\,.$$

We find that a best fit to the $T/T_K = 0.2$ QMC-ME curve is obtained with $\Gamma_K = 2.5T_K$, which is remarkably the Wilson ratio[21] for the Kondo problem. Wilson found that $T_K^0 \cong 2.4T_K$, where $T_K^0\chi(0) = \mu_B^2$ and again T_K is the high-temperature perturbation prediction. The

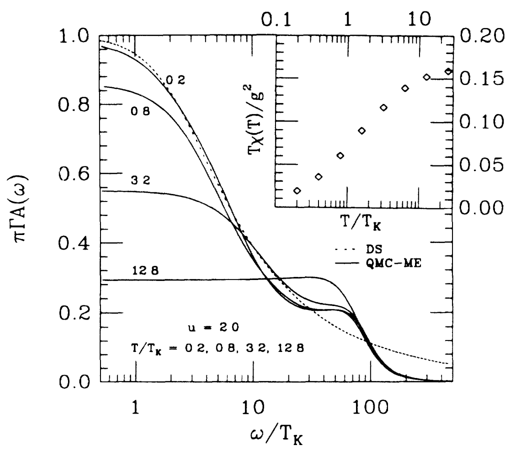

FIG. 3. QMC-ME labels the quantum Monte Carlo and maximum-entropy results for fixed $u=2.0$ and varying T/T_K as indicated. The Kondo peak is approximately independent of u for ω/T_K less than 20. DS labels the Doniach-Sunjic expression for the shape of the Kondo peak at zero temperature. The width in the DS formula is $\Gamma_K=2.5T_K$. Inset: Screened local moment, $T\chi(T)/g^2$, plotted vs T/T_K.

Doniach-Sunjic formula also agrees with zero-temperature numerical renormalization-group calculations.[7]

In conclusion, we have obtained dynamical information for a strongly correlated electronic system by a novel combination of a quantum Monte Carlo method, the maximum-entropy method for image reconstruction, and perturbation theory. We have established that the spectral densities of the symmetric Anderson model are universal functions of ω/T_K and T/T_K at low frequencies. A fit of the Doniach-Sunjic formula to our lowest-temperature results yields the Wilson ratio. The universal behavior of the spectral density at low ω/T_K leads to universal transport coefficients which will be reported in a subsequent paper.[9]

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