Transport coefficients for the Anderson model

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(Received 10 February 1993)

We have calculated the temperature-dependent electrical resistivity and thermal conductivity for the nondegenerate Anderson model of the magnetic-impurity system. Our calculation is based on Yamada's perturbative Green's-function solution and the Doniach-Sunjic prediction for the universal Kondo peak. We obtain results that are in quantitative agreement with the available quantum Monte Carlo data.

The Anderson model[1] has been employed in the investigation of many physical phenomena. For example, it has been applied to the magnetic-impurity problem,[2] heavy-fermion and mixed-valence phenomena,[3] and chemisorption theory.[4] The model has become an important tool in the understanding of strongly correlated electron systems. Many properties of the model have been precisely analyzed using the Bethe-ansatz[5] (BA) and renormalization-group[6] (RG) methods. Thus, the Anderson model also serves as a useful testing ground for alternative solution schemes.[7,8] The Hamiltonian for the single-impurity Anderson model[1] is given by

$$H=\sum_{k,\sigma} E_{k\sigma}c^{\dagger}_{k\sigma}c_{k\sigma} +\sum_{\sigma}(E_{d\sigma}c^{\dagger}_{d\sigma}c_{d\sigma}+\tfrac{1}{2}Uc^{\dagger}_{d\sigma}c_{d\sigma}c^{\dagger}_{d\bar{\sigma}}c_{d\bar{\sigma}}) +\sum_{k,\sigma}(V_{dk}c^{\dagger}_{d\sigma}c_{k\sigma}+V_{kd}c^{\dagger}_{k\sigma}c_{d\sigma}) , \tag{1}$$

where the operators $c^{\dagger}_{k\sigma}$ and $c_{k\sigma}$ create and destroy electrons in the metal states with energy $E_{k\bar{\sigma}}$, respectively, and the operators $c^{\dagger}_{d\sigma}$ and $c_{d\sigma}$ create and destroy electrons on the impurity atom with energy $E_{d\sigma}$ or $E_{d\sigma}+U$, respectively. The electron spin is denoted by σ ($\bar{\sigma}=-\sigma$). In this paper, we consider the symmetric ($E_{d\sigma}=-U/2$) limit of the Anderson model with an infinite bandwidth. For this case, the relevant parameters are the temperature T, the correlation energy U, and the hybridization width $\Delta=\pi N\langle |V_{dk}|^2\rangle_{\rm av}$, where N is the density of states at the Fermi energy.

The purpose of this paper is to present a calculation of the temperature-dependent electrical resistivity $R(T)$ and thermal conductivity $\kappa(T)$ for the full range of values of T/T_K, where T_K is the characteristic scaling temperature commonly referred to in the literature as the "Kondo temperature." It is an interesting fact that, in the wake of the understanding generated by the BA and RG analyses, a quantitatively correct calculation of these quantities for the single-impurity Anderson model seems to have been quite difficult to obtain. A notable early success is the perturbative calculation of $R(T)$ vs T/Δ by Yamada.[9] The recent quantum Monte Carlo calculation[10] may be viewed with some skepticism, because it is not obvious from the data presented that it accounts for the effects of charge fluctuations. The charge fluctuations are an essential feature of the Anderson model. Their effects are most pronounced at $T\geq\Delta$ ($k_B=1$) and disappear in the Kondo limit ($u=U/\pi\Delta\gg 1$). The effect on the resistivity $R(T)$ is to suppress its decrease as the temperature increases above T_K (see Figs. 1 and 2). The effect on $\kappa(T)$ is less obvious, but it is clear that the quantum Monte Carlo data[10] are inconclusive for $T>T_K$.

The transport coefficients are given by the formulas derived from Boltzmann's transport equation.[11] The resistivity $R(T)$ for the Anderson model is determined by

$$\frac{R(0)}{R(T)}=-\int_{-\infty}^{\infty}\frac{\partial f(E)}{\partial E}(\Delta\pi\rho_{d\sigma}(E))^{-1}dE , \tag{2}$$

where $f(E)=\{\exp(\beta E)+1\}^{-1}$, $\beta=1/T$, and the spectral density function $\rho_{d\sigma}$ is

$$\rho_{d\sigma}(E)=\frac{[\Delta-{\rm Im}\Sigma_{d\sigma}(E)]}{[E-{\rm Re}\Sigma_{d\sigma}(E)]^2+[\Delta-{\rm Im}\Sigma_{d\sigma}(E)]^2} . \tag{3}$$

The quantity $\Sigma_{d\sigma}(E)$ is the retarded self-energy correction for the symmetric Anderson model. For simplicity we consider only the second-order self-energy correction,[12,13] which should give correct results for the transport coefficients at sufficiently small u. The second-order correction may be expressed as

$$\Sigma_{d\sigma}(\omega)=\frac{U^2}{2\pi}\int_{-\infty}^{\infty}dE\{\tanh(\beta E/2)\,{\rm Im}G(E)\chi'(\omega-E)+\coth(\beta E/2)\,{\rm Im}\chi'(E)G(\omega-E)\} , \tag{4}$$

where $G(\omega)=\{\omega+i\Delta\}^{-1}$ is the Hartree-Fock Green's-function solution for the symmetric Anderson model, and $\chi'(E)$ is given by[13]

$$\chi'(E)=\frac{2\Delta}{E(E+2i\Delta)}\{\Psi(z_1)-\Psi(z_2)\} , \tag{5}$$

where $z_1=(1+\Delta/\pi T)/2$, $z_2=z_1-iE/2\pi T$, and Ψ is the digamma function. For the thermal conductivity $\kappa(T)$ we have

$$\frac{\kappa(T)/T}{[\kappa(T)/T]_0}=\frac{-3}{(\pi T)^2}\int_{-\infty}^{\infty}\frac{\partial f(E)}{\partial E}E^2(\Delta\pi\rho_{d\sigma}(E))^{-1}dE . \tag{6}$$

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The bracket $[\cdots]_0$ denotes the $T=0$ value of the enclosed quantity.

Using Eq. (4), we have calculated the transport coefficients as functions of T/T_K and u for the range of values $0.1 \le T/T_K \le 100$ and $u \le 2.0$. For $u \gg 1.0$ (the Kondo limit), we use the Doniach-Sunjic[14] prediction for the universal Kondo peak $A_d(\omega)$ of the spectral density function:

$$A_d(\omega) = \mathrm{Re}\sqrt{i\Gamma_K/(\omega+i\Gamma_K)}/\pi\Delta \ . \tag{7}$$

The parameter Γ_K is determined by comparing the Taylor-series expansions of $A_d(\omega)$ and $\rho_{d\sigma}(\omega)$ about $\omega=0$ at $T=0$. According to Yamada,[12] for small ω and $T=0$,

$$\rho_{d\sigma}(\omega) \cong \{1-3(\tilde{\chi}_a\omega)^2/8\}/\pi\Delta \ , \tag{8}$$

where $\tilde{\chi}_a$ is the reduced spin susceptibility[5,15] at $T=0$ and $u \gg 1$:

$$\tilde{\chi}_a = \left[\frac{\pi}{2u}\right]^{1/2} \exp\{\pi^2 u/8 - 1/2u\} \ . \tag{9}$$

The comparison gives $\Gamma_K = (\tilde{\chi}_a)^{-1}$. According to the BA and RG analyses, for sufficiently low temperatures the thermodynamic functions and transport coefficients are universal functions of T/T_K. For any given temperature, the transition to this scaling regime is not a sharp one but occurs gradually as u increases. For our calculation we use a definition for T_K that is based on Yamada's[9] low-temperature expression for $R(T)$:

$$R(T) = R(0)\left\{1 - \frac{\pi^2}{3}\left[\frac{T}{\Delta}\right]^2 \left(\tfrac{3}{4}[\tilde{\chi}_S^2 + \tilde{\chi}_C^2] - \tfrac{1}{2}\tilde{\chi}_S\tilde{\chi}_C\right)\right\} \ . \tag{10}$$

The equations for the reduced spin susceptibility $\tilde{\chi}_S$ and charge susceptibility $\tilde{\chi}_C$ (Refs. 5 and 15) at $T=0$ and arbitrary u are

$$\tilde{\chi}_S = \left[\frac{2}{\pi u}\right]^{1/2} \exp\{\pi^2 u/8\} \times \int_0^\infty \exp\{-x^2/2u\} \frac{\cos(\pi x/2)}{1-x^2} dx \ , \tag{11}$$

$$\tilde{\chi}_C = \left[\frac{2}{\pi u}\right]^{1/2} \exp\{-\pi^2 u/8\} \times \int_0^\infty \exp\{-x^2/2u\} \frac{\cosh(\pi x/2)}{1+x^2} dx \ . \tag{12}$$

Comparing Eq. (10) with the Fermi-liquid theory[16] result $R(T) = R(0)[1-(T/T_K)^2]$ gives

$$T_K = \frac{\Delta}{\pi}\left(\tfrac{1}{4}[\tilde{\chi}_S^2 + \tilde{\chi}_C^2] - \tfrac{1}{6}\tilde{\chi}_S\tilde{\chi}_C\right)^{-1/2} \ . \tag{13}$$

For $u > 2$, $\tilde{\chi}_C$ becomes relatively small so that $T_K \approx 2\Delta/\pi\tilde{\chi}_S$. At very large u, $\tilde{\chi}_S \approx \tilde{\chi}_a$. We note that the RG definition[6] $T_K = 2\pi\Delta(0.103)/\tilde{\chi}_S$ differs from Eq. (13) by only a small percentage for all values of u. Since the Kondo peak is universal, and because for temperatures arbitrarily close to zero and u arbitrarily large the factor $\partial f(E)/\partial E$ in Eqs. (2) and (6) samples $\rho_{d\sigma}(E)^{-1}$ only near $E=0$, replacing $\rho_{d\sigma}$ by A_d in Eqs. (2) and (6) gives an accurate account of $R(T)$ and $\kappa(T)$ in the Kondo limit ($u \gg 1$).

The results of our calculation are shown in Figs. 1 and 2. We expect that for $u \ge 1$ the transport coefficients for the Anderson model at sufficiently low temperatures will exhibit the universal behavior predicted by the BA (Ref. 5) and RG (Ref. 6) theories, and, therefore, will be independent of u when plotted as functions of T/T_K for sufficiently large u. As the temperature increases the universality gives way to the effects of charge fluctuations. For very large u the charge fluctuations disappear and the system has reached the Kondo limit. These

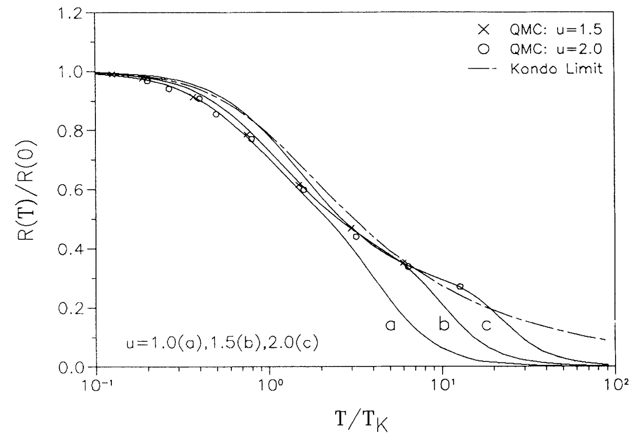

FIG. 1. $R(T)/R(0)$ vs T/T_K for several values of u. The solid curves were obtained using Eq. (4). The shoulder at $T/T_K > 1$ is the result of charge fluctuations. For the Kondo limit ($u \gg 1$), we use the Doniach-Sunjic prediction of Eq. (7) (with $\Gamma_K = \tilde{\chi}_a^{-1}$) for the spectral density function. Also shown is the quantum Monte Carlo calculation (QMC) of Ref. 10.

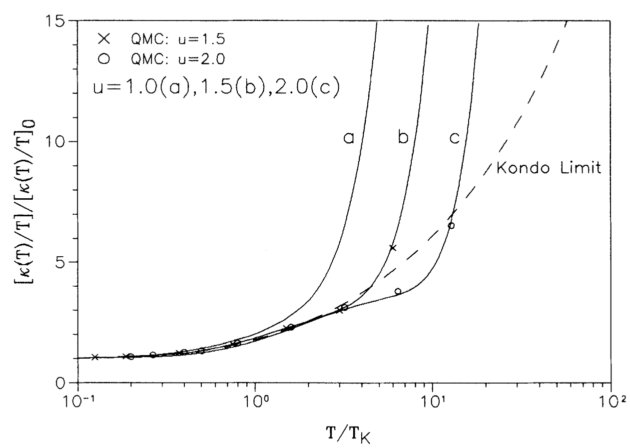

FIG. 2. $[\kappa(T)/T]/[\kappa(T)/T]_0$ vs T/T_K for several values of u. The solid curves were obtained using Eq. (4). For the Kondo limit ($u \gg 1$), we use the Doniach-Sunjic prediction of Eq. (7) (with $\Gamma_K = \tilde{\chi}_a^{-1}$) for the spectral density function. Also shown is the QMC of Ref. 10.

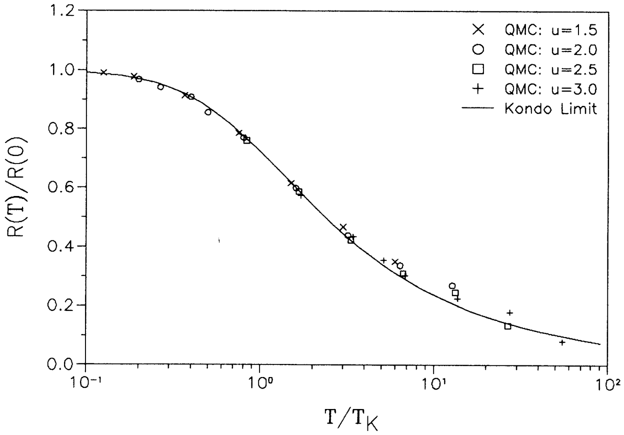

FIG. 3. $R(T)/R(0)$ vs T/T_K. The QMC of Ref. 10 is compared to the Kondo limit calculation using the Doniach-Sunjic equation (7) with $\Gamma_K = 1.2T_K$.

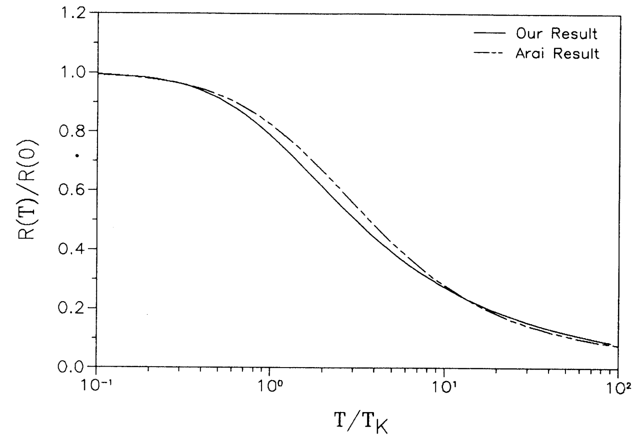

FIG. 4. $R(T)/R(0)$ vs T/T_K for the Arai formula [Eq. (14)] and our Kondo limit calculation using the Doniach-Sunjic equation (7) with $\Gamma_K = \tilde{\chi}_a^{-1}$.

trends are clearly shown in Figs. 1 and 2. On comparing the universality of $R(T)$ and $\kappa(T)$, it is clear that $R(T)$ is a universal function for a larger range of values of T/T_K. Also in Figs. 1 and 2, we give a comparison of our results with the quantum Monte Carlo calculation of Jarrel *et al.*[10] *The second-order perturbative and quantum Monte Carlo calculations are in quantitative agreement* for $u < 2$. This is strikingly true for $\kappa(T)$, which appears to be quite insensitive to the detail shape of the spectral density function. However, there are not enough quantum Monte Carlo data for a detailed comparison at $T/T_K > 1$ where the charge fluctuation effects are most pronounced. We have found that $\Gamma_K \approx 1.2T_K$ gives an excellent fit (see Fig. 3) of our Kondo limit calculation to the Monte Carlo data.[10]

Finally, we mention the work of Arai.[17] Using a nonperturbative solution scheme[8] for the impurity Green's function for the Anderson model, he derived an equation for $R(T)$ which is valid in the Kondo limit:

$$\frac{R(T)}{R(0)} = \{1 + (\pi^2/3)[\alpha(T)]^{-2}\}^{-1} , \tag{14}$$

where $\alpha(T)$ is a universal function of T/T_K and is given by the solution of

$$[\alpha(T) - T_L/T] \ln\{[1+\alpha(T)^2]^{1/2} T/T_L\} - \pi \ln 2 = 0 , \tag{15}$$

where $T_L = T_K/0.624$. The function $\alpha(T)$ is multivalued for $T/T_K < 0.676$. However, once these values are sorted out, Eq. (14) is at least qualitatively correct for the full range of T/T_K. Figure 4 shows a plot of Eq. (14) and our Kondo limit calculation of $R(T)$. Comparing the low-temperature expansion of Eq. (14) with the Fermi-liquid theory[16] formula $R(T) = R(0)[1 - (T/T_K)^2]$ yields $T_L = \pi T_K/\sqrt{3}$, which gives an even poorer agreement between the two results for $T/T_K \sim 1$.

In summary, we have calculated the temperature-dependent electrical resistivity and thermal conductivity for the symmetric Anderson model by using the results of Yamada's[9] perturbation theory and the Doniach-Sunjic[14] prediction for the Kondo peak. We also observed that the second-order perturbative calculation is in quantitative agreement with the recent quantum Monte Carlo calculation.[10] Thus, our results supplemented by the quantum Monte Carlo data give the complete picture of the electrical resistivity and thermal conductivity for the symmetric Anderson model.

We would like to thank Professor Mark Jarrel for sending us the Monte Carlo data of Ref. 10. This research was supported in part by the National Science Foundation through the Clark Atlanta University Center for Theoretical Studies of Physical Systems.

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