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LETTER TO THE EDITOR

Transport coefficients of the Anderson model

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Abstract. The transport coefficients of the Anderson model require knowledge of both the temperature and frequency dependence of the single-particle spectral densities and consequently have proven difficult quantities to calculate. Here we show how these quantities can be calculated via an extension of Wilson's numerical renormalization group method. Accurate results are obtained in all parameter regimes and for the full range of temperatures of interest ranging from the high-temperature perturbative regime $T \gg T_K$, through the cross-over region $T \approx T_K$, and into the low-temperature strong coupling regime $T \ll T_K$. The Fermi liquid relations for the T^2 coefficient of the resistivity and the linear coefficient of the thermopower are satisfied to a high degree of accuracy. The techniques used here provide a new highly accurate approach to strongly correlated electrons in high dimensions.

In this Letter we present accurate new results for the transport coefficients of the Anderson model obtained by using the numerical renormalization group method [1]. The Anderson model has been used extensively to interpret the properties of magnetic impurities in simple metals, certain aspects of heavy fermion behaviour [2] and the low-temperature transport through a quantum dot [3]. Recently this model has also become important for an understanding of the properties of correlated electrons on a lattice in high dimensions. The electron self-energy becomes local in infinite dimensions [4,5] and the problem reduces to that of an impurity [6]. In particular the solution of the $d = \infty$ Hubbard model has been shown to reduce to the solution of an Anderson impurity model with a hybridization function, $\Delta(\omega)$, determined by a self-consistency requirement [7–9]. The self-consistency condition is straightforward to handle and the difficult part of the problem has remained the calculation of the dynamics of the underlying impurity problem, and more specifically of the impurity single-particle spectral densities. This is just the problem which one encounters in attempting to calculate the transport coefficients of the Anderson model which depend sensitively on the temperature and frequency dependence of the single-particle spectral densities $\rho_d(\omega, T)$. An accurate solution of this problem can therefore provide the solution of the $d = \infty$ Hubbard model. Our main interest, then, is the accurate solution of the Anderson model and in particular the calculation of its single-particle spectral densities. The Bethe *ansatz* has been successful in providing exact results on the thermodynamic properties of several models of magnetic impurities including the N-fold degenerate Anderson model [10,11], but the method cannot be used to extract dynamic properties. The latter have been obtained by applying approximate methods. For $N = 2$ perturbation theory in the local Coulomb repulsion, U, has been used [12] whilst for larger N (typically $N \geqslant 6$) the non-crossing approximation (NCA) has been applied to calculate the thermodynamic, transport and dynamic properties [13,14]. The former eventually becomes unreliable for large enough values of U (typically for $U/\pi\Delta \geqslant 2.5$ where Δ is the resonance level width)

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and the latter fails to satisfy some exact Fermi liquid relations at low energies [15]. Recently, Quantum Monte Carlo methods in combination with the maximum entropy principle have also been used to extract dynamic properties [16–18]. These have so far been restricted to the symmetric model and to $U/\pi\Delta \leqslant 3$. They become more inaccurate and time consuming for larger values of U and lower temperatures.

A comprehensive and highly accurate approach to the calculation of dynamic properties of magnetic impurity models has recently been developed, based on an extension of Wilson's numerical renormalization group approach, which overcomes many of the limitations and difficulties of the other approximate schemes. This has led to reliable results valid in all regimes and at both zero [19–24] and finite [25] temperature, and which satisfy all the sum rules and Fermi liquid relations of the Anderson model [20]. With such results for the dynamic properties it becomes possible to calculate the transport coefficients of the Anderson model over the full temperature range of interest. We report here results for the resistivity, and thermopower based on these numerical renormalization group calculations. Results for the Hall coefficient and thermal conductivity have also been calculated and will be presented in a forthcoming publication [26].

Our starting point is the non-degenerate ($N = 2$) Anderson model

$$H = \sum_{\sigma} \epsilon_d c^{\dagger}_{d\sigma} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} (V_{k\sigma} c^{\dagger}_{k\sigma} c_{d\sigma} + \text{HC}) + \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma}. \tag{1}$$

This can be re-cast in the form of a linear chain model which may then be iteratively diagonalized. The Lanczos algorithm is applied to $H_c = \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma}$ with starting vector $c^{\dagger}_{0\sigma}|\text{vac}\rangle = \frac{1}{V}\sum_k V_k c^{\dagger}_{k\sigma}|\text{vac}\rangle$ where $V = \sqrt{\sum_k |V_k|^2}$ so that the conduction electron part of H is reduced to a semi-infinite linear chain with site 0 coupled to the impurity via a hybridization term of strength V [1, 19]:

$$H = \sum_{\sigma} \epsilon_d c^{\dagger}_{d\sigma} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} (c^{\dagger}_{0\sigma} c_{d\sigma} + \text{HC}) + \sum_{n=0,\sigma}^{\infty} \epsilon_n c^{\dagger}_{n\sigma} c_{n\sigma} + \sum_{n=0,\sigma}^{\infty} \lambda_n (c^{\dagger}_{n+1\sigma} c_{n\sigma} + c^{\dagger}_{n\sigma} c_{n+1\sigma}) \tag{2}$$

The parameters $\{\epsilon_n, \lambda_n\}, n = 0, 1, \ldots$ reflect the form of the hybridization function $\Delta(\omega) = \pi \sum_k |V_k|^2 \delta(\omega - \epsilon_k)$. In the present case of the magnetic impurity problem we are primarily interested in low-energies where $\Delta(\omega)$ may be taken to be a slowly varying function of ω which can be approximated by a constant Δ. In this case, and by replacing the continuum of conduction electron states in $(-D, D)$ by a discrete set $\pm D\Lambda^{-n}, n = 0, 1, \ldots, \Lambda > 1$, a discrete approximation to H can be obtained with parameters $\lambda_n \sim D\Lambda^{-n/2}, n \gg 1$ [1] (the ϵ_n are zero for a half-filled symmetric band). For the impurity model corresponding to the $d = \infty$ Hubbard model, the frequency dependence of $\Delta(\omega)$ is important and leads to a different set of parameters λ_n. The model has to be solved repeatedly in this case to obtain a self-consistent $\Delta(\omega)$ using the self-consistency requirement in [[7–9].

The discretized Anderson model with $\lambda_n \sim D\Lambda^{-n/2}, n \gg 1$, discussed above, can be iteratively diagonalized to obtain the many-body eigenvalues E^n_p and eigenstates $|p\rangle_n$ on successively lower energy scales $\omega_n \sim D\Lambda^{-n/2}, n = 0, 1, \ldots$ by following the procedure in [1]. The procedure starts with diagonalizing the impurity part $H_0 = \sum_{\sigma} \epsilon_d c^{\dagger}_{d\sigma} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$ and then adding the coupling to the local conduction electron state $V \sum_{\sigma} (c^{\dagger}_{0\sigma} c_{d\sigma} + \text{HC})$. After this one adds successive energy shells $\sum_{\sigma} \lambda_n (c^{\dagger}_{n+1\sigma} c_{n\sigma} + c^{\dagger}_{n\sigma} c_{n+1\sigma}), n = 0, 1, \ldots$ and diagonalizes the resulting Hamiltonian. Since the number of states grows like 4^n

it is in practice only possible to retain the lowest 500 or so states at each stage. This restricts the reliable range of excitations ω to be such that $\omega_n \leqslant \omega \leqslant K\omega_n$, where $K \approx 10$ for $\Lambda \sim 3$. The lower excitations are calculated more reliably in successive iterations, whilst information on the higher excitations is contained in previous iterations. The eigenvalues are used to calculate the partition function at a decreasing sequence of temperatures $T_n = \omega_n/k_B \sim D\Lambda^{-n/2}, n = 0, 1, \ldots$ and from this one extracts the thermodynamic properties [1, 31].

From the eigenvectors $|p\rangle_n$ we recursively evaluate the single-particle matrix elements $M^n_{pp'} = \langle p|c_{d\sigma}|p'\rangle$ which are required for the nth shell Green function $G^n_{d\sigma}(\omega, T)$ and spectral density $\rho^n_d(\omega, T)$,

$$G^n_{d\sigma}(\omega, T) = \langle\langle c_{d\sigma}; c^\dagger_{d\sigma}\rangle\rangle = \frac{1}{Z_n(\beta)} \sum_{pp'} \frac{|M^n_{pp'}|^2(e^{-\beta E^n_p} + e^{-\beta E^n_{p'}})}{\omega - E^n_{p'} + E^n_p} \tag{3}$$

$$\rho^n_d(\omega, T) = \frac{1}{Z_n(\beta)} \sum_{pp'} |M^n_{pp'}|^2(e^{-\beta E^n_p} + e^{-\beta E^n_{p'}})\delta(\omega - E^n_{p'} + E^n_p). \tag{4}$$

Here $Z_n(\beta)$ is the partition function for the nth cluster† or energy shell. In evaluating $\rho^n_d(\omega, T)$ the delta functions are replaced by Gaussians having widths α_n of order ω_n appropriate to the cluster size. At $T = 0$ the spectral density is evaluated at excitations $\omega \approx \omega_n$ using the nth cluster. At finite temperature $k_BT > 0$, and when $\omega \approx \omega_n$ becomes of order k_BT excited states not contained in the nth cluster become important. In this case we use a smaller cluster (containing information about the higher excited states) to evaluate the spectral densities at energies ω such that $\omega \leqslant k_BT$. Results for the spectral densities $\rho_d(\omega, T)$ are shown in figure 1 and figure 2 for various temperatures.

The Friedel sum rule $\rho_d(\omega = \epsilon_F, T = 0) = (1/\pi\Delta)\sin^2(\pi n_d/2)$ and Shiba relation for the dynamic susceptibility [34] are satisfied to within a few percent in all parameter regimes [19, 20, 35].

The calculation of transport properties is straightforward once accurate results for the temperature and frequency dependence of the spectral densities are obtained. The resistivity $\rho(T)$ and thermopower $S(T)$ are given in terms of the integrals

$$L_{ml} = -C \int_{-\infty}^{+\infty} \frac{\partial f(\omega)}{\partial \omega} \tau^l(\omega)\omega^m d\omega \tag{5}$$

by

$$\rho(T) = 1/e^2L_{01} \tag{6}$$

$$S(T) = -(1/eT)(L_{11}/L_{01}) \tag{7}$$

where the relaxation time $\tau(\omega, T)$ is given in terms of the local d-electron Green function by $\tau(\omega, T)^{-1} = 2\pi|V|^2\rho_d(\omega, T)$, and e is the electronic charge. There are two exact Fermi liquid relations for the transport coefficients. The first is for the coefficient of the T^2 term in the low-temperature resistivity [27, 28]. For $T \ll T_K$ and in the Kondo regime we have

$$\rho(T) = \rho(0)\left\{1 - c\,(T/T_K)^2\right\} \tag{8}$$

where $c = \pi^4/16 = 6.088$, and T_K is defined by

$$k_BT_K = U(\Delta/2U)^{1/2}e^{\pi\epsilon_d(\epsilon_d+U)/2\Delta U}. \tag{9}$$

Results for the resistivity are shown in figure 3 for $U/\pi\Delta = 4$ and for several values of the local level position ranging from the Kondo regime ($\epsilon_d/\Delta = -(U/2\Delta), -4, -3, -2$) to

† The term *cluster* is suggested by the notation, although the calculations described here are in k-space [1]

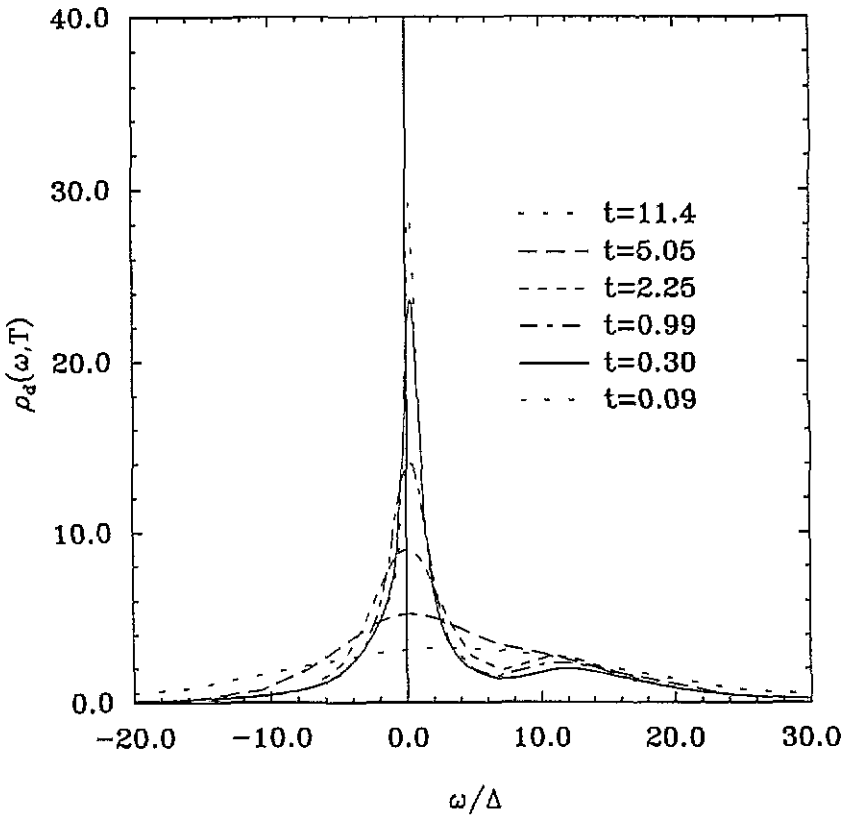

Figure 1. The spectral density $\rho_d(\omega, T)$ in the mixed valent regime $\epsilon_d/\Delta = -1$ for several values of the reduced temperature $t = T/T_K$ and for $U/\pi\Delta = 4$. Note that Δ is a more appropriate energy scale in this regime than T_K. For the present parameters $T_K = 0.59\Delta$.

the mixed valent regime ($\epsilon_d/\Delta = -1, 0$) and the empty orbital regime ($\epsilon_d/\Delta = +1$). For high temperatures $T \gg T_K$, as described elsewhere [25], the resistivity is well described by the Hamann result [36]. In the Fermi liquid regime $T \ll T_K$ the inset in figure 3 shows the expected T^2 behaviour. In the Kondo regime the values of the T^2 coefficient extracted from a least squares fit in the region $0 \leqslant T \leqslant 0.1T_K$ are 5.7, 5.8, 6.4 and 6.6 in going from the symmetric case to $\epsilon_d = -2\Delta$. These values agree to within 8% of the exact result $c = 6.088$. Quantum Monte Carlo results for the symmetric case for $U/\pi\Delta \leqslant 3$ give the T^2 coefficient to within 19% of the exact result [18]. The current approach which is not restricted to very low or very high temperatures also gives accurate results for the resistivity in the cross-over region $T \sim T_K$ [25]. The $T = 0$ resistivity $\rho(0)$ satisfies $\rho(0) \sim \sin^2(\pi n_d/2)$ in accordance with the Friedel sum rule for the single-particle spectral density [26].

A second Fermi liquid relation relates the linear coefficient of the thermopower to the local level occupancy, $n_d(T = 0)$, and the linear coefficient of specific heat, γ, [29, 30]

$$\lim_{T\to 0} \{eS(T)/\gamma T\} = \pi \cot(\pi n_d(0)/2). \tag{10}$$

This is a much more difficult Fermi liquid relation to satisfy, because the local level occupancy $n_d(0)$ is obtained by integrating the single-particle spectral density up to the Fermi level, the linear coefficient of specific heat is obtained as a second derivative $-\lim_{T\to 0}\{\partial^2 F(T)/\partial T^2\}$ of the Free energy and $\lim_{T\to 0}\{S(T)/T\}$ involves evaluating

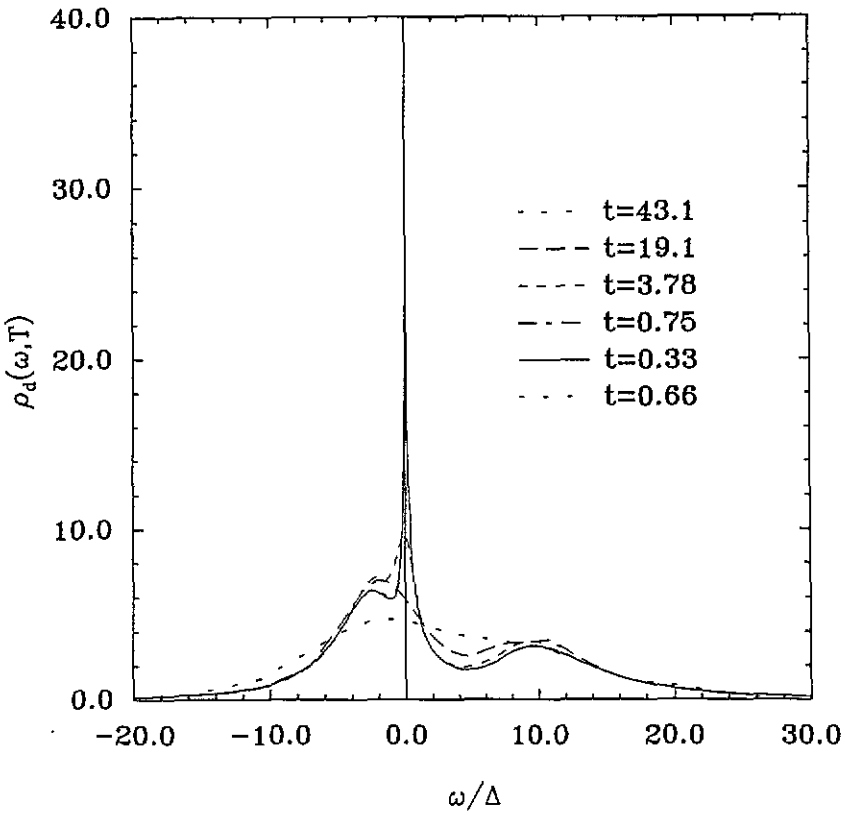

Figure 2. The spectral density $\rho_d(\omega, T)$ in the Kondo regime $\epsilon_d/\Delta = -3$ for several values of the reduced temperature $t = T/T_K$ and for $U/\pi\Delta = 4$.

the transport integrals using the finite T spectral densities $\rho_d(\omega, T)$. All these quantities are evaluated using the numerical renormalization group method and the above relation provides a very severe test of the accuracy of the method.

The thermopower is shown in figure 4 for the mixed valent, empty orbital and Kondo regimes. The sign of the thermopower at low temperatures is determined by the sign of $(\partial\rho(\omega, T)/\partial\omega)_{\omega=0}$ and is always positive for the range of parameters considered. At higher temperatures the behaviour of $S(T)$ is more complicated. However, in the mixed valent and empty orbital regimes the single resonance always lies above the Fermi level (see figure 1), and from equation (7) the thermopower is positive at all temperatures. In the Kondo regime a distinctive maximum appears in the thermopower at $T \approx T_K$. At higher temperatures, the thermopower can become negative and for sufficiently high temperatures positive again. This behaviour is associated with the temperature dependence of the satellite peaks at ϵ_d and $\epsilon_d + U$ (see figure 2). The low-temperature behaviour of the thermopower (inset to figure 4) shows the expected linear in T Fermi liquid behaviour and one can use this to extract $\lim_{T\to 0}\{S(T)/T\}$. By calculating the linear coefficient of specific heat from the free energy and $n_d(T = 0)$ from the spectral densities we can test the Fermi liquid relation (10). This is shown in figure 5. It is seen that $\lim_{T\to 0}\{S(T)/\gamma T\}$ lies within 6% of $\cot(\pi n_d/2)$ in nearly all cases. This agreement is remarkable and shows clearly that the method is capable of giving close to exact results for transport coefficients and finite temperature dynamic properties in addition to the $T = 0$ dynamics and the thermodynamics. We have not made any of the sophisticated corrections [31] to improve on the thermodynamics and

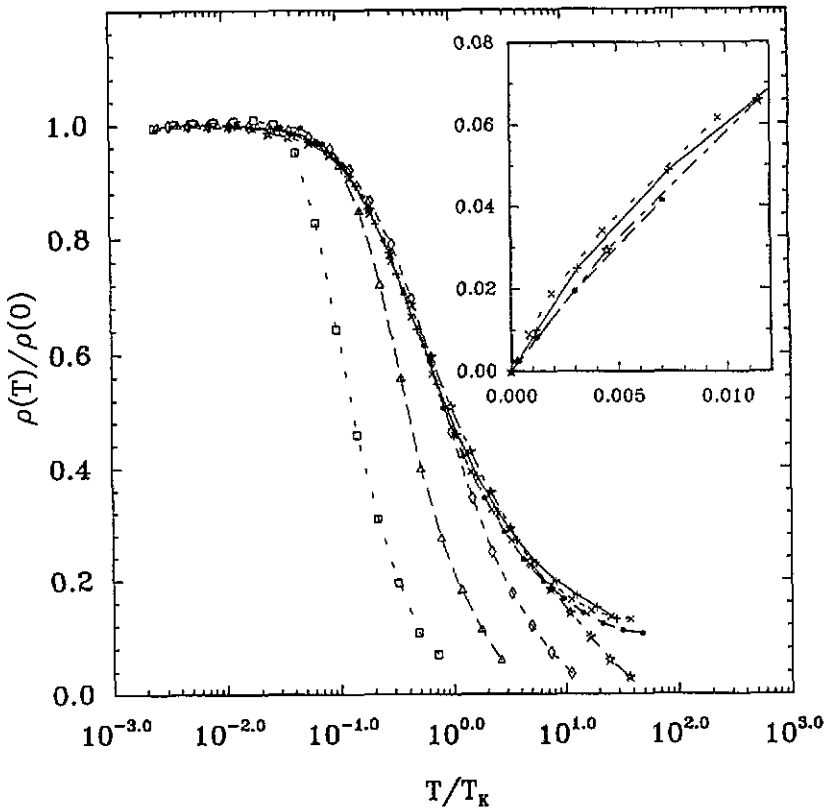

Figure 3. The scaled resistivity $\rho(T)/\rho(0)$ over the full temperature range in various regimes and for $U/\pi\Delta = 4$, $\epsilon_d/\Delta = 1$ (□), $\epsilon_d/\Delta = 0$ (△), $\epsilon_d/\Delta = -1$ (◇), $\epsilon_d/\Delta = -2$ (⋆), $\epsilon_d/\Delta = -3$ (+), $\epsilon_d/\Delta = -4$ (×) and the symmetric case (•). It should be noted that a more appropriate energy scale in the mixed valent and empty orbital regimes is Δ. The inset is for $(1 - (\rho(T)/\rho(0)))$ versus $(T/T_K)^2$ and shows the T^2 Fermi liquid behaviour for $T \ll T_K$ in the Kondo regime.

only the even energy shell spectral densities have been utilized, hence there is scope for improvement. The characteristic peak at $T \approx T_K$ in the thermopower in the Kondo regime is often referred to as the giant thermopower. This peak can become very large, although to see this one needs to keep n_d fixed and approach the Kondo regime by increasing U. In our calculations ϵ_d was varied to approach the symmetric case for which the thermopower is zero as can be seen by setting $n_d = 1$ in equation (10). From equation (10) it is clear that keeping n_d fixed and increasing U leads to an exponential increase in the thermopower since $\gamma \sim 1/T_K \sim e^{\alpha U}, \alpha > 0$ thus giving a giant thermopower in the Kondo limit. The vanishing of the thermopower for half-filling is an artifact of the simplified model used here which neglects the non-resonant scattering of conduction electrons as discussed in [32]. An extension of the present calculations to include non-resonant scattering, leads to enhanced thermopowers for half-filled systems and describes the qualitative behaviour of the thermopower of concentrated Kondo compounds [33].

In this letter we have presented new results for the thermopower and resistivity of the Anderson model over the full temperature range of interest and in several parameter regimes by using the numerical renormalization group approach. The Fermi liquid relation for the linear coefficient of the thermopower is satisfied with remarkable accuracy, as is

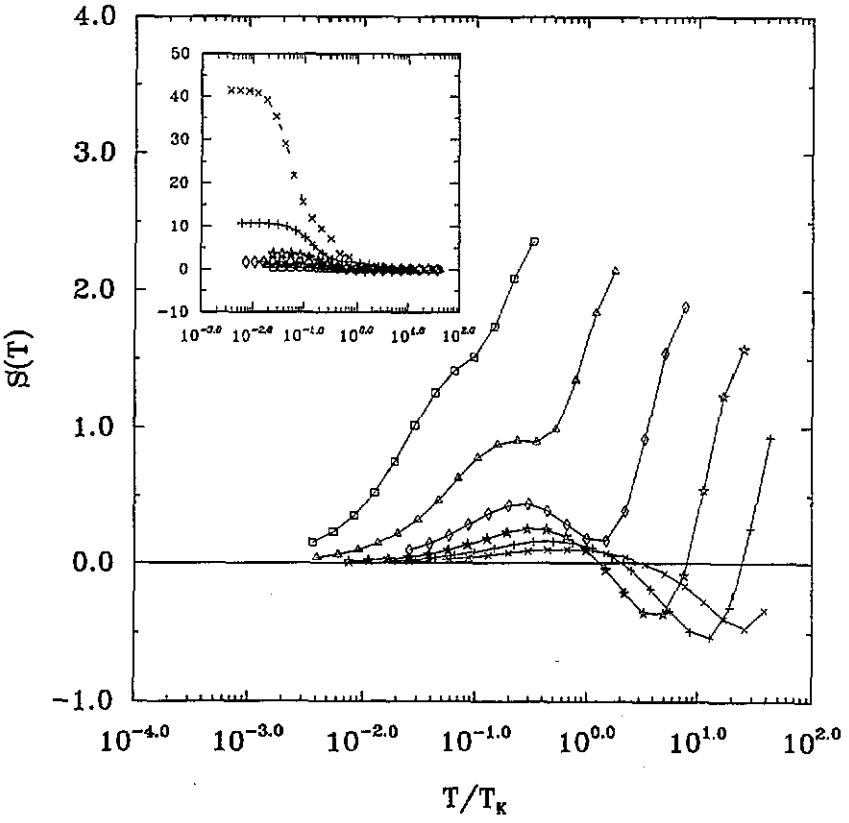

Figure 4. The thermopower $S(T)$ over the full temperature range in various regimes and for $U/\pi\Delta = 4$ $\epsilon_d/\Delta = +1$ (□), $\epsilon_d/\Delta = 0$ (△), $\epsilon_d/\Delta = -1$ (◇), $\epsilon_d/\Delta = -2$ (⋆), $\epsilon_d/\Delta = -3$ (+), $\epsilon_d/\Delta = -4$ (×). The inset is for $S(T)T_K/T$ versus T/T_K and shows the linear in T Fermi liquid behaviour for $T \ll T_K$.

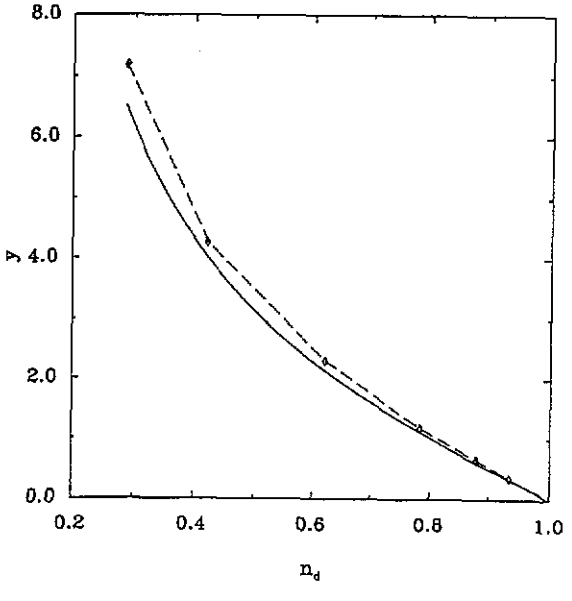

Figure 5. $\lim_{T\to 0}\{S(T)/\gamma T\}$ (dashed line with diamonds) and $\cot(\pi n_d/2)$ (solid line) versus n_d for the various parameter sets ranging from Kondo to mixed valent and empty orbital behaviour. The two curves lie within 6% of each other in all cases, except for the empty orbital case $\epsilon_d/\Delta = +1$ where the error is 10%.

that for the T^2 coefficient of the resistivity. The Hall coefficient, thermal conductivity and finite temperature dynamic susceptibilities have also been calculated and will be presented elsewhere [26, 35]. Our results are in contrast to NCA calculations [13, 14] which violate Fermi liquid relations at low energies, and to perturbation in U calculations which, although accurate, eventually break down for $U/\pi\Delta \geqslant 2.5$ [12]. We are able to treat a much wider range of regimes than the Monte Carlo approach [18] which has so far only been applied to the symmetric case where the thermopower is zero and which often builds in the sum rules which constitute independent tests within our approach. The techniques presented here for extracting the spectral densities of the Anderson model provide a new highly accurate approach to the $d = \infty$ Hubbard model.

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