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Symmetric Anderson impurity model with a narrow band

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The single-channel Anderson impurity model is a standard model for the description of magnetic impurities in metallic systems. Usually, the bandwidth represents the largest energy scale of the problem. In this paper, we analyze the limit of a *narrow* band, which is relevant for the Mott-Hubbard transition in infinite dimensions. For the symmetric model we discuss two different effects. (i) The impurity contribution to the density of states at the Fermi surface always turns out to be negative in such systems. This leads to a new crossover in the thermodynamic quantities that we investigate using the numerical renormalization group. (ii) Using the Lanczos method, we calculate the impurity spectral function and demonstrate the breakdown of the skeleton expansion on an intermediate energy scale. Luttinger's theorem, as an example of the local Fermi liquid property of the model, is shown to still be valid. [S0163-1829(99)50420-7]

I. INTRODUCTION

The single-channel Anderson impurity model[1] is commonly used to describe the physics of a magnetic impurity in a conducting host and exhibits different types of behavior, such as mixed valency and the Kondo effect. Usually, the case of a flat band is of interest, where the conduction electron bandwidth represents the largest energy scale in the problem. For this particular case, the model has been solved using the Bethe ansatz,[2] which enables one to calculate static properties, e.g., the impurity susceptibility and the specific heat. A numerical solution of the problem has been given by Krishna-Murthy *et al.*[3]

In the context of the Hubbard model in high dimensions[4] (''dynamical mean field theory''), the physics of the correlated lattice system is described by a single Anderson impurity interacting with a bath whose properties are determined in a self-consistent way.[5] The bath is characterized by a hybridization strength of the order of the bandwidth and a nonconstant density of states. For this case, no exact results exist and one either has to rely on analytical approximations (which are, however, not available in the whole parameter space) or numerical means.

In this paper, we numerically solve the Anderson impurity model in the extreme limit, where the bandwidth is much smaller than the hybridization (*narrow-band* systems). In the context of the Mott-Hubbard transition in high dimensions, such models are self-consistently generated in one possible transition scenario.[6] By analyzing the narrow-band limit (without the additional complications caused by the $d\to\infty$ self-consistency condition), we will establish two characteristic features of Anderson impurity models that to some extent will also hold for intermediate situations. (i) The impurity density of states $\rho_d(\omega)$ and the change in the density of states of the total system due to the impurity $\Delta\rho(\omega)$ show a very different behavior, since the conduction electrons react to the presence of the impurity. This is in contrast to the flat-band case where $\rho_d(\omega)=\Delta\rho(\omega)$ always. It leads to an interesting crossover in the thermodynamic impurity properties of the system when the interaction is turned on. (ii) The skeleton expansion, which plays an important role in deriving properties of the interacting system, breaks down on intermediate energy scales. This has important implications for the Mott-Hubbard transition in $d=\infty$, as will be explained below.

II. DENSITY OF STATES

The Hamiltonian of the symmetric model is given by

$$H=\sum_{\mathbf{k},\mu}\epsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\mu}c_{\mathbf{k}\mu}+\sum_{\mathbf{k},\mu}\left(V_{\mathbf{k}d}c^{\dagger}_{\mathbf{k}\mu}d_{\mu}+V^{*}_{\mathbf{k}d}d^{\dagger}_{\mu}c_{\mathbf{k}\mu}\right)+U\left(d^{\dagger}_{\uparrow}d_{\uparrow}-\frac{1}{2}\right)\left(d^{\dagger}_{\downarrow}d_{\downarrow}-\frac{1}{2}\right), \tag{1}$$

with $c_{\mathbf{k}}$ the conduction electrons and d the impurity orbital. In the following, we will restrict ourselves to scalar $k's$, implying—if necessary—a reduction to s waves in the conduction band. The impurity density of states (DOS) is defined by

$$\rho_d(\omega)=-\frac{1}{\pi}\mathrm{Im}\,G_{dd}(\omega^{+}), \tag{2}$$

where G_{dd} is the retarded zero-temperature Green's function of the impurity orbital. On the other hand, the total change of the density of states due to the introduction of the impurity into the conduction band is given by

$$\Delta\rho(\omega)=-\frac{1}{\pi}\mathrm{Im}\left\{\sum_{k}G_{kk}(\omega^{+})+G_{dd}(\omega^{+})\right\}+\frac{1}{\pi}\mathrm{Im}\sum_{k}G^{(0)}_{kk}(\omega^{+}), \tag{3}$$

where $G^{(0)}$ refers to the Green's function of the conduction electrons without the impurity. Using the equations of motion for $G_{kk'}$ and G_{dk}, one finds

$$\Delta\rho(\omega)=-\frac{1}{\pi}\mathrm{Im}\left\{G_{dd}(\omega^{+})\left(1-\frac{\partial}{\partial\omega}\sum_{k}\frac{V_k^2}{\omega^{+}-\epsilon_k}\right)\right\}. \tag{4}$$

Therefore, the total change in the DOS can be expressed as a function of the impurity Green's function. We introduce the notation

$$\sum_k \frac{V_k^2}{\omega^+ - \epsilon_k} = \Lambda(\omega) - i\Delta(\omega), \tag{5}$$

where $\Delta(\omega)$ is the hybridization function and the real part is given by the principal value integral $\Lambda(\omega) = \mathcal{P}\int (d\epsilon/\pi)\{[\Delta(\epsilon)]/(\omega-\epsilon)\}$. Now we can express $\Delta\rho(\omega)$ in terms of the impurity density of states and write

$$\Delta\rho(\omega) = \rho_d(\omega)\left(1 - \frac{\partial\Lambda}{\partial\omega}\right) - \frac{\partial\Delta}{\partial\omega}\mathcal{P}\int \frac{d\epsilon}{\pi}\frac{\rho_d(\epsilon)}{\omega-\epsilon}. \tag{6}$$

We define the *narrow-band* limit by the property

$$\left.\frac{\partial\Lambda(\omega)}{\partial\omega}\right|_{\omega=\epsilon_F} \gg 1, \tag{7}$$

leading to a negative coefficient multiplying the first term in Eq. (6) at the Fermi energy.

We will study one exemplary realization of a *narrow-band* system with a constant hybridization function $\Delta(\omega) = \Delta$ and conduction-band energies extending from $-D$ to D (we set $\epsilon_F = 0$ in the following). This leads to

$$\left.\frac{\partial\Lambda(\omega)}{\partial\omega}\right|_{\omega=0} = \frac{2\Delta}{\pi D} \tag{8}$$

and hence the *narrow-band* limit is defined by $\Delta \gg D$. However, the main conclusions in the following analysis hold equally for other realizations of narrow-band systems (7) as well, in particular, even for systems without band edges at all.

We notice that for our model the second term of Eq. (6) vanishes inside the conduction band. Luttinger's theorem[7,8] for the symmetric Anderson model, which we will later verify numerically for the narrow-band case as well, ensures the ''pinning'' of the impurity spectral function at the Fermi energy at its noninteracting value

$$\rho_d(0) = \frac{1}{\pi\Delta}. \tag{9}$$

Therefore, the first term in Eq. (6) gives a negative contribution,

$$\Delta\rho(0) = \frac{1}{\pi\Delta}\left(1 - \frac{2\Delta}{\pi D}\right), \tag{10}$$

at the Fermi energy. In the following, we discuss the relationship of $\Delta\rho(\omega)$ to thermodynamic properties of the model.

III. CALCULATION OF THE IMPURITY SUSCEPTIBILITY

In noninteracting fermionic models, the total density of states at the Fermi energy determines thermodynamic properties such as the static susceptibility χ. Introducing an impurity into the system induces a change in χ proportional to $\Delta\rho(0)$. For the narrow-band Anderson systems analyzed here, one therefore expects a negative impurity contribution to the susceptibility. This is obviously true for $U=0$, where one obtains the usual Pauli susceptibility in dimensionless units ($\mu_B = \hbar = g = 1$):

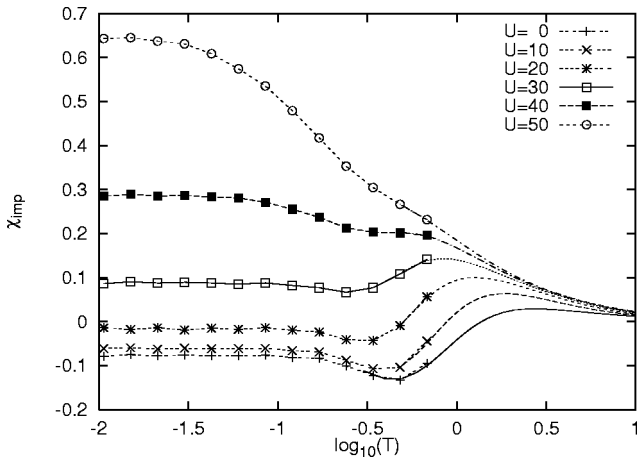

FIG. 1. Impurity susceptibility vs logarithmic temperature at hybridization $\Delta = 10$ and half bandwidth $D = 1$ for different interactions U.

$$\chi_{\rm imp} = \frac{\Delta\rho(0)}{2} = \frac{1}{2\pi\Delta}\left(1 - \frac{2\Delta}{\pi D}\right). \tag{11}$$

In order to determine whether this also holds for the interacting case, we have calculated χ using the numerical renormalization group method with discretization parameter $\Lambda = 2$ following Krishna-Murthy *et al.*[3] At high temperatures, complete diagonalization of the logarithmically discretized five-site model yields essentially exact results (continuous lines), as no low-energy information is needed in that case. The results for fixed hybridization $\Delta = 10$ and half bandwidth $D = 1$ are shown in Fig. 1. At large T, the almost free orbital leads to $\chi_{\rm imp} = 1/8T$. Upon lowering the temperature, we find a characteristic dependence on the value of the interaction. For $U \lesssim 2\Delta$ we see a crossover to a negative $\chi_{\rm imp}$, which is due to the loss of spectral weight at low frequencies as a consequence of hybridization. After a characteristic minimum at finite temperature, the susceptibility saturates at a negative value as $T \to 0$. For $U \gtrsim 2\Delta$, we recover the usual positive $\chi_{\rm imp}$, which is strongly enhanced at large U/Δ by the Kondo effect, defining a new exponentially small energy scale T_K.

In spite of these different types of behavior (depending on the interaction strength), the impurity contribution to the density of states at the Fermi energy is negative (10) for *any* U. We therefore conclude that only in the weakly interacting case, $\Delta\rho(\epsilon_F)$ yields the thermodynamic properties of the model. In the strong-coupling regime, the susceptibility enhancement is determined by the many-body resonance in $\rho_d(\omega)$ which—similarly to the wide-band case—has to be interpreted as a quasiparticle peak with a large effective mass. The low-temperature behavior of the system for strong correlations is governed by many-particle excitations that are not contained in $\Delta\rho(\omega)$ and, in fact, completely predominate over the reduction in the single-particle DOS $\Delta\rho(\epsilon_F) < 0$.

IV. SPECTRAL DENSITY AND SKELETON EXPANSION

Next, we discuss the spectral density of narrow-band Anderson systems. We calculate the impurity orbital Green's function at zero temperature using the Lanczos method as implemented by Krauth.[5] We fix the values of the interaction U and the hybridization Δ and then successively reduce the bandwidth, thus taking the limit $D\to 0$. For each set of parameters we calculate the spectral function ρ_d, using an Anderson star with $11+1$ sites. For not too large U/Δ the spectral density is found to be only weakly dependent on the number of sites.

In the limit of small bandwidth at any finite value of the ratio U/Δ, we find a three-peak structure consisting of the atomic levels at $\omega=\pm U/2$ containing almost the full spectral weight and a central quasiparticle peak of width $\sim D$. Apart from numerical broadening effects, there is no spectral weight between the peaks. This gives rise to resonances in the imaginary part of the self-energy, which can be seen in the following way:[9,10] As a consequence of Dyson's equation, for values of ω inside the gap (where spectral function and hybridization vanish) the self-energy $\Sigma(\omega^+)=K(\omega)-iJ(\omega)$ is given by

$$\Sigma(\omega^+)=\omega-\Lambda(\omega)-\frac{1}{\Gamma(\omega)-i0^+}, \tag{12}$$

where we have defined $\Gamma(\omega)\equiv\mathcal{P}\int d\epsilon\{[\rho_d(\epsilon)]/(\omega-\epsilon)\}$. The imaginary part of the self-energy therefore has the form

$$J(\omega)=\pi\delta[\Gamma(\omega)]. \tag{13}$$

For the spectral density found here, $\Gamma(\omega)$ has zeros at energies $\epsilon\sim\pm\sqrt{D}$ and this leads to δ functions in $J(\omega)$ inside the gap as shown above.

As argued previously,[9] these resonances are incompatible with the skeleton expansion, i.e., the self-consistent perturbation theory in U. Within this expansion, the full propagator $G_{dd}(\omega)$ is inserted into every diagram contributing to $J(\omega)$. As $G_{dd}(\omega)$ possesses spectral weight only on the small energy scale $D\ll\sqrt{D}$, there is no possibility of generating the resonances at $\pm\sqrt{D}$. We therefore conclude that in our model, already at small but finite bandwidth D the skeleton expansion breaks down at energies of the order $\sqrt{D}$ (strictly speaking $\sim\sqrt{\Delta D}$, but note that here we have chosen $\Delta=1$ dimensionless).

As a measure of the convergence of the expansion at lower energies, we take the Fermi liquid properties of the Anderson model, especially the pinning of the density of states at its noninteracting value (9). This is equivalent to the vanishing of the imaginary part of the self-energy at the Fermi level. This property has been proven for a general class of systems by Luttinger[7] using the skeleton expansion to all orders. A proof for the (flat-band) Anderson model within unrenormalized perturbation theory was given by Yamada.[11] In order to verify the pinning, we focus on the central peak of ρ_d and compare different, not too strong interactions at constant broadening. The pinning of $\rho_d(0)$ in the limit $D\to 0$ is evident from Fig. 2. At even larger interactions (not shown here), a narrow Kondo resonance develops inside the band, which cannot be resolved well on a small cluster. From the above, though, we do not expect deviations from Luttinger's theorem for any interaction.

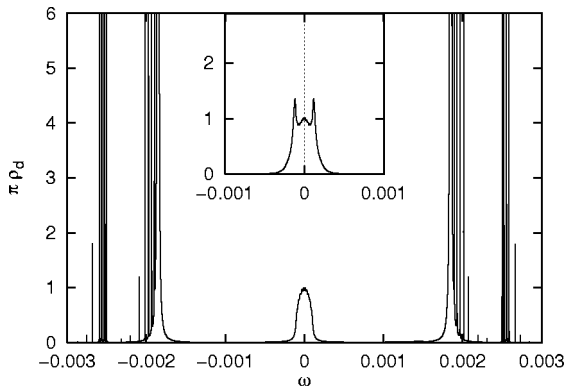

FIG. 2. Central peak in the impurity density of states for different interactions $U=0.2$ and 4.0 (inset), hybridization $\Delta=1.0$, and bandwidth $D=10^{-4}$. We have used a Lorentzian broadening of $b=1.5\times10^{-5}$ at the quasiparticle resonance and $b=5\times10^{-8}$ for the poles at higher frequencies. The atomic levels at $\pm U/2$ carrying most of the spectral weight are not shown. At the Fermi edge, $\pi\rho_d(0)=1.00\pm0.02$ for both values of U.

As can also be seen in Fig. 2, the ''quasiparticle'' resonance in $\rho_d(\omega)$ has an internal structure itself (including bound states outside the band for small U/Δ). In the limit $D\to 0$ this can be described by a scaling function

$$\rho_d(\omega)=f(\omega/D), \tag{14}$$

where f is independent of D. The δ peaks in Fig, 2, dominant at small U, can be understood by approximating the Hamiltonian as a ''zero bandwidth'' Anderson model,[12] where the impurity couples to one single orbital and the hybridization is given by a δ function carrying the integrated weight $\int d\epsilon\Delta(\epsilon)$. The effect of the continuous hybridization band is to generate spectral density close to $\omega=0$ and to create sidebands also visible in Fig. 2. For larger values of U the weight of the bound states decreases (from the zero bandwidth model we expect a decrease $\sim 1/U^2$) and they numerically merge with the continuum at small ω.

For other hybridization functions in the narrow-band limit (7), the main conclusions of the above analysis remain unaffected. A detailed numerical study is, however, difficult due to the limited number of orbitals that can be taken into account using exact diagonalization. For example, in a ''narrow'' band with band tails extending to $\pm\infty$ but $(\partial\Lambda/\partial\omega)|_{\omega=0}\gg 1$, the bound states for $U=0$ become sharp resonances. Likewise, the imaginary part of the self-energy then contains sharp resonances at $\pm O(\sqrt{D})$ instead of δ functions. Still, the resonances contain the same spectral weight as these δ functions and the breakdown of the skeleton expansion occurs in the same manner.[9]

V. CONCLUSION

In this paper we have studied the Anderson impurity model in the narrow-band limit (7) using numerical methods. We have found two features that do not apply to the usual wide-band limit. (i) One observes a crossover in the impurity contribution to the susceptibility: for small interactions, the impurity reduces the total susceptibility; for large interac-

tions the impurity increases it. In fact, the same behavior is also found for the specific heat, although this has not been discussed explicitly here. This crossover is in contrast to the observation that the impurity contribution to the total density of states at the Fermi level is *always* negative. This quantity does, therefore, not determine the thermodynamic properties of the system at large interactions. (ii) Holding U and Δ fixed, the skeleton expansion breaks down for sufficiently small (but still finite) bandwidth D. The breakdown occurs at energies of order $\sqrt{D}$ and larger, while for smaller energies no problems can be found. This shows that this specific breakdown of the skeleton expansion is a generic feature of narrow-band Anderson impurity systems.[13] On the other hand, the skeleton expansion is an essential tool for deriving the locality of the self-energy in the dynamical mean field theory in the Fermi liquid phase.[4,14] Its convergence also provides a sufficient condition for the analytic continuation to the noninteracting Hubbard model. At present, the question of the correct description of the Mott-Hubbard transition in large dimensions is in debate:[9,15,16] While NRG simulations[17,18] at $T=0$ seem to indicate a ''preformed gap,'' no coexistence between metallic and insulating solutions is found in finite-temperature quantum Monte Carlo calculations.[19] In any case, the analysis presented above shows that for the preformed gap scenario [which naturally leads to an effective action governed by a narrow-band system in the sense of Eq. (7)], one has to address the question of whether such systems can be related to the original Hubbard model in large dimensions.

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