Thermodynamic properties of Kondo insulators

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A family of heavy-fermion materials that exhibits semiconducting-like properties has recently been discovered. A typical representative of this family is the system $Ce_3Bi_4Pt_3$. Behavior similar to these rare-earth materials has also been observed in the compound FeSi. Using a two-band model and treating the electronic correlations beyond the mean-field level, we calculate the thermodynamic properties of this model for the case of two electrons per unit cell. We find that a hybridization gap appears above a critical value of the mixing term which depends on the ratio between the effective masses of the electrons in the large and narrow bands. The two-band model provides a unified description of the rare-earth and transition-metal-based systems. The results obtained for the temperature-dependent susceptibility are in good qualitative agreement with experimental data.

I. INTRODUCTION

The study of heavy-fermion materials has been an area of intense research in the last decade. These materials present a variety of ground states, namely, superconductor, antiferromagnetic, Fermi liquid, and more recently some of them were found to have an insulating ground state.[1-3] The properties of these materials may be traced to the existence of an unstable *f shell* as generally occurs for metallic systems containing *cerium* or *uranium* atoms. A special situation, which is the one of interest here, is that where the material has one electron in a large, *s*-like, uncorrelated band and also one electron in the narrow band associated with the *f electrons* of the Ce or U atoms. There are two basic models to describe these systems. In the first, known as the Kondo lattice model, one starts with a localized description of the f electrons which couple to the band electrons through an isotropic exchange interaction of strength J. This model for the particular counting of electrons we mentioned above has recently been studied[4] in the one-dimensional case where exact results could be obtained. In particular, it has been shown that in $d=1$ the system is always a spin liquid with exponentially decaying magnetic correlations. Furthermore, it has a charge gap, larger than the spin gap and consequently it is also insulating. The peculiarities of the one-dimensional case, however, make it inappropriate to extend these results to higher dimensions and, in particular, to the real systems we are interested.

II. THE MODEL HAMILTONIAN

The second model, which is the one we adopt, considers a two-band system. One is a large, uncorrelated band associated generally with s electrons and the other a narrow correlated band which describes the electrons in the unstable f shell. These bands hybridize and, in the particular case of two electrons per unit cell, interesting results can be readily obtained. A closely related model has recently been proposed[5,6] which considers an Anderson lattice, i.e., a collection of localized f states with strong intra-atomic interactions hybridized with a conduction band. Our model, which considers instead a narrow band, is readily extended to treat transition-metal-based compounds, like FeSi, which exhibit properties very similar to the rare-earth materials we are examining here.[1] The Hamiltonian describing our system is

$$H=\sum_{i,j,\sigma} t_{ij}^{s} c_{j\sigma}^{\dagger} c_{i\sigma}+\sum_{i,j,\sigma} t_{ij}^{f} f_{j\sigma}^{\dagger} f_{i\sigma}+\frac{U}{2}\sum_{i\sigma} n_{i\sigma}^{f} n_{i-\sigma}^{f} + V\sum_{i\sigma}(c_{i\sigma}^{\dagger} f_{i\sigma}+f_{i\sigma}^{\dagger} c_{i\sigma}) , \quad (1)$$

where $t_{ij}^{s,f}$ gives the hopping probability for electrons in the large, uncorrelated s-like band and in the narrow f or d band which we from now on refer generically as an f band. The $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ create and destroy, respectively, electrons in the wide band and $f_{i\sigma}^{\dagger}$ and $f_{i\sigma}$ are creation and annihilation operators for electrons in the narrow f band. The Coulomb interaction between f electrons in the same site is given by U, V is the mixing term, and $n_{i\sigma}^{f}=f_{i\sigma}^{\dagger} f_{i\sigma}$. We could have also introduced a repulsive interaction U_{sf} between s and f electrons on the same site. Since this is weak compared to U, it can be treated within the Hartree-Fock scheme and would pose no additional difficulty to our problem.

If it were not for the Coulomb term, the Hamiltonian above could be exactly diagonalized giving rise to two hybrid bands. However, the many-body term due to the strong interaction U makes this a difficult problem for which an approximation must be introduced. In this paper we shall extend for the two-band problem the so-called Hubbard-I approximation[7] which goes beyond the mean-field level. It is very appropriate for the problem studied here where the systems we are describing have in-

sulating ground states and no long-range magnetic order. We shall employ the equation of motion method[8] and for this purpose we introduce initially two Green's functions, namely, $G_{ij}^{ff}(t)=\langle\langle f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle$ and $G_{ij}^{ss}(t)=\langle\langle c_{i\sigma};c_{j\sigma}^{\dagger}\rangle\rangle$ which describe the propagation of electrons in the f and in the large s band, respectively. The frequency-dependent Green's function $\langle\langle f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}$ given by the Fourier transform of $G_{ij}^{ff}(t)$ obeys the following equation of motion:

$$\omega\langle\langle f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}=\frac{1}{2\pi}\delta_{ij}+\sum_{l}t_{il}^{f}\langle\langle f_{l\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}+V\langle\langle c_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}+U\langle\langle n_{i-\sigma}^{f}f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}\ . \tag{2}$$

Then when writing the equation of motion for this Green's function, new propagators are generated due to both the mixing term and the Coulomb interaction. Within the Hartree-Fock approximation, we would interfere at this point decoupling the newly generated Green's function $\langle\langle n_{i-\sigma}^{f}f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}$ which appears due to the many-body interaction. In this paper, we proceed beyond Hartree-Fock and write the equations of motion for the new propagators

$$\omega\langle\langle c_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}=\sum_{l}t_{il}^{s}\langle\langle c_{l\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}+V\langle\langle f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega} \tag{3}$$

and

$$(\omega-U)\langle\langle n_{i-\sigma}^{f}f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}=\frac{1}{2\pi}\langle n_{-\sigma}^{f}\rangle\delta_{ij}+\sum_{l}t_{il}^{f}\langle\langle n_{i-\sigma}^{f}f_{l\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}+V\langle\langle n_{i-\sigma}^{f}c_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}\ . \tag{4}$$

In the equation above we used the following approximations for the propagators:

$$\langle\langle(f_{i-\sigma}^{\dagger}f_{l-\sigma}-f_{l-\sigma}^{\dagger}f_{i-\sigma})f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}\approx\langle f_{i-\sigma}^{\dagger}f_{l-\sigma}-f_{l-\sigma}^{\dagger}f_{i-\sigma}\rangle\langle\langle f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}=0$$

and

$$\langle\langle(f_{i-\sigma}^{\dagger}c_{i-\sigma}-c_{i-\sigma}^{\dagger}f_{i-\sigma})f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}\approx\langle f_{i-\sigma}^{\dagger}c_{i-\sigma}-c_{i-\sigma}^{\dagger}f_{i-\sigma}\rangle\langle\langle f_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}=0\ .$$

The last equalities follow from translational symmetry. We also introduce the following decouplings:

$$\langle\langle n_{i-\sigma}^{f}f_{l\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}\approx\langle n_{-\sigma}^{f}\rangle\langle\langle f_{l\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}$$

and

$$\langle\langle n_{i-\sigma}^{f}c_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}\approx\langle n_{-\sigma}^{f}\rangle\langle\langle c_{i\sigma};f_{j\sigma}^{\dagger}\rangle\rangle_{\omega}\ ,$$

where we used $\langle n_{i-\sigma}^{f}\rangle=\langle n_{-\sigma}^{f}\rangle$ due to translation invariance. We then obtain a closed system of equations which, after Fourier transforming in space, can be solved. Taking the limit $U\rightarrow\infty$ we finally find, for the f-electron propagator,

$$G_{k\sigma}^{ff}(\omega)=\frac{(1-\langle n_{-\sigma}^{f}\rangle)(\omega-\epsilon_{k}^{s})}{2\pi\{[\omega-\epsilon_{k}^{f}(1-\langle n_{-\sigma}^{f}\rangle)](\omega-\epsilon_{k}^{s})-V^{2}(1-\langle n_{-\sigma}^{f}\rangle)\}}\ , \tag{5}$$

we also get for the s-electron propagator

$$G_{k\sigma}^{ss}(\omega)=\frac{\omega-\epsilon_{k}^{f}(1-\langle n_{-\sigma}^{f}\rangle)}{2\pi\{[\omega-\epsilon_{k}^{f}(1-\langle n_{-\sigma}^{f}\rangle)](\omega-\epsilon_{k}^{s})-V^{2}(1-\langle n_{-\sigma}^{f}\rangle)\}}\ . \tag{6}$$

We can see from the above equations that the main role of the interactions is to renormalize the mixing term V^2 and the f-electron propagator through the contraction factor $(1-\langle n_{-\sigma}^{f}\rangle)$. The effective mass m_f defined by $\epsilon_k^f=\hbar^2k^2/2m_f$ is also renormalized. Incidentally the contraction factor obtained here is different from the one which arises using the slave boson[5,6] or Gutzwiller[9] approaches where it is given by $(1-\langle n^{f}\rangle)$ with $\langle n^{f}\rangle=\sum_{\sigma}\langle n_{\sigma}^{f}\rangle$.

Since we are interested in paramagnetic solutions $\langle n_{-\sigma}^{f}\rangle=\langle n_{\sigma}^{f}\rangle$. Due to a special symmetry of the bands we shall consider here and the fact that we have one electron f per unit cell, the largest value these averages can assume is $\frac{1}{2}$. In this case the contraction factor is given by $(1-\langle n_{-\sigma}^{f}\rangle)=\frac{1}{2}$ and the effective hybridization remains finite at all temperatures.

The new excitations of the system are given by the poles of the propagators, that is they are obtained from the equation

$$(\omega-\epsilon_{k}^{s})(\omega-\tilde{\epsilon}_{k\sigma}^{f})-V^{2}(1-\langle n_{-\sigma}^{f}\rangle)=0\ , \tag{7}$$

where

$$\tilde{\epsilon}_{k\sigma}^{f}=\epsilon_{k}^{f}(1-\langle n_{-\sigma}^{f}\rangle)\ .$$

The equation above has the following roots:

$$\omega_{1,2}(k)=\tfrac{1}{2}\{\epsilon_{k}^{s}+\tilde{\epsilon}_{k\sigma}^{f}\pm\sqrt{(\epsilon_{k}^{s}-\tilde{\epsilon}_{k\sigma}^{f})^{2}+4V^{2}(1-\langle n_{-\sigma}^{f}\rangle)}\}\ . \tag{8}$$

The propagators can also be written in terms of simple fractions as

$$G_{k\sigma}^{ff}(\omega)=\frac{1}{2\pi}\left[\frac{A_{1}^{f}(k)}{\omega-\omega_{1}(k)}-\frac{A_{2}^{f}(k)}{\omega-\omega_{2}(k)}\right], \tag{9}$$

where

$$A_{i}^{f}(k)=\frac{f_{k}^{f}[\omega_{i}(k)]}{\omega_{1}(k)-\omega_{2}(k)}$$

and

$$f_k^f(\omega)=(1-\langle n_{-\sigma}^f\rangle)(\omega-\epsilon_k^s)\ . \tag{10}$$

For the s electron we find

$$G_{k\sigma}^{ss}(\omega)=\frac{1}{2\pi}\left[\frac{A_1^s(k)}{\omega-\omega_1(k)}-\frac{A_2^s(k)}{\omega-\omega_2(k)}\right], \tag{11}$$

where

$$A_i^s(k)=\frac{f_k^s[\omega_i(k)]}{\omega_1(k)-\omega_2(k)}$$

and

$$f_k^s(\omega)=\omega-\tilde{\epsilon}_{k\sigma}^f\ . \tag{12}$$

The next step to calculate the density of states of the hybrid bands is to obtain the quantities $\langle n_{k\sigma}^s\rangle$ and $\langle n_{k\sigma}^f\rangle$. These can be found from the discontinuity of the respective Green's functions along the real axis,[8] i.e., $\langle n_{k\sigma}^{s,f}\rangle=\mathcal{F}_\omega[G_k^{s,f}(\omega)]$, where

$$\mathcal{F}_\omega[G_k^{s,f}(\omega)]=i\lim_{\eta\to 0}[G_k^{s,f}(\omega+i\eta)-G_k^{s,f}(\omega-i\eta)]\ . \tag{13}$$

In the case of f electrons we obtain

$$\mathcal{F}_\omega[G_k^{ff}(\omega)]=\left|\frac{f_k^f(\omega)}{\omega-\omega_2(k)}\right|\delta[\omega-\omega_1(k)] + \left|\frac{f_k^f(\omega)}{\omega-\omega_1(k)}\right|\delta[\omega-\omega_2(k)]$$

and a similar equation for $\langle n_{k\sigma}^s\rangle$ by substituting $f_k^s(\omega)$ for $f_k^f(\omega)$. Using the properties of the δ functions we obtain the expressions for the density of states $n^s(\omega)$ and $n^f(\omega)$ in the following form:

$$n_\sigma^{s,f}(\omega)=\sum_k|f_k^{s,f}|\delta\{[\omega-\omega_1(k)][\omega-\omega_2(k)]\}\ . \tag{14}$$

III. THE HOMOTHETIC BANDS MODEL

In order to obtain explicit results for the density of states we introduce a model of homothetic bands[10] which consists in taking

$$\epsilon_k^s=\epsilon_k\ ,$$

$$\tilde{\epsilon}_{k\sigma}^f=\alpha\epsilon_k+\beta\ .$$

The quantity α may be interpreted as taking into account the different effective masses of the f and s electrons, i.e., $(m_s/m_f^*)=\alpha$. We have included in the parameter α the renormalization of the f-electron mass due to the contraction factor $(1-\langle n_{-\sigma}^f\rangle)$ arising from the Coulomb repulsion between electrons of opposite spins in the same site. The quantity β gives the shift of the f band with respect to the large s band and also includes the contraction factor. Introducing two new functions $g_1(\omega)$ and $g_2(\omega)$ through the following equation,

$$[\omega-\omega_1(k)][\omega-\omega_2(k)]=\alpha[g_1(\omega)-\epsilon_k][g_2(\omega)-\epsilon_k]\ , \tag{15}$$

we get, in terms of these new functions, the s and f contributions to the density of states of the new hybrid bands. For the f contribution to the first hybrid band we find

$$n_{\sigma 1}^f(\omega)=\frac{|f^f[\omega,g_1(\omega)]|}{\alpha|g_1(\omega)-g_2(\omega)|}\sum_k\delta[g_1(\omega)-\epsilon_k]\ , \tag{16}$$

and for the second

$$n_{\sigma 2}^f(\omega)=\frac{|f^f[\omega,g_2(\omega)]|}{\alpha|g_1(\omega)-g_2(\omega)|}\sum_k\delta[g_2(\omega)-\epsilon_k]\ . \tag{17}$$

For the s density of states we get

$$n_{\sigma 1}^s(\omega)=\frac{|f^s[\omega,g_1(\omega)]|}{\alpha|g_1(\omega)-g_2(\omega)|}\sum_k\delta[g_1(\omega)-\epsilon_k] \tag{18}$$

and

$$n_{\sigma 2}^s(\omega)=\frac{|f^s[\omega,g_2(\omega)]|}{\alpha|g_1(\omega)-g_2(\omega)|}\sum_k\delta[g_2(\omega)-\epsilon_k]\ . \tag{19}$$

Now it remains to find the functions $g_{1,2}(\omega)$ which can be obtained from Eq. (15), we get

$$g_{1,2}(\omega)=\frac{1}{2\alpha}\{(1+\alpha)\omega-\tfrac{1}{2}\Delta(1-\alpha) \pm\sqrt{[(1-\alpha)\omega-\tfrac{1}{2}\Delta(1-\alpha)]^2+4\alpha\tilde{V}^2}\}\ , \tag{20}$$

where $\tilde{V}^2=V^2(1-\langle n_{-\sigma}^f\rangle)$. Δ is the width of the large-s band and appears in the above equation because the parameter β, which determines the position of the f band, was fixed by the condition that the center of this f band coincides with that of the large band at the energy $\Delta/2$ for $V=0$. For symmetric bands this arrangement is particularly useful since when the hybridization is turned on and is sufficiently strong, we obtain two symmetric hybrid bands, separated by a gap, which can accommodate each one exactly two electrons. Then, in the case of two electrons per unit cell that we are considering, the Fermi level sits in the middle of the gap and it can be easily shown that it does not shift with temperature. Furthermore, for symmetric hybrid bands the factors $\langle n_\sigma^f\rangle$ are temperature independent implying that this is also the case for the parameters α and β. Since the total number of f electrons, $n_f=1$, we get $\langle n_\sigma^f\rangle=\frac{1}{2}$, for paramagnetic solutions and the contraction factor is given by $(1-\langle n_{-\sigma}^f\rangle)=\frac{1}{2}$ independent of temperature.

The equation for the gap can be obtained from the difference in energy between the top of the first hybrid band and the bottom of the second. We find

$$\Delta_G=\left[\frac{\Delta^2(1-\alpha)^2}{4}+4\tilde{V}^2\right]^{1/2}-(1+\alpha)\frac{\Delta}{2}\ . \tag{21}$$

Consequently, for a two-band system the opening of a hy-

bridization gap, contrary to what occurs for the Anderson lattice model, requires a critical value of the hybridization which is given by

$$\tilde{V}_c = \frac{\Delta}{2}\sqrt{\alpha} \ . \tag{22}$$

For transition-metal compounds where the ratio $\alpha_d = (m_s/m_d)$ is larger than that for rare-earth system $\alpha_f = (m_s/m_f^*)$, a larger value of the hybridization is required to open a gap. In Fig. 1 we show the gap, given by Eq. (21) as a function of V for different values of α. A comparison of the magnitude of the critical hybridization parameter with the usual values of the hybridization for Ce and U systems and for transition metals, shows that V_c is sufficiently large to make the phenomenon of hybridization gaps rather unusual specially in transition-metal-based compounds where α_d is not such a small number. Note that the many-body contraction factor, which renormalizes both $\tilde{V}^2$ and α, cancels out in Eq. (22). Consequently, whenever the interacting system is insulating the same holds for the noninteracting one ($U=0$) in agreement with Luttinger's theorem.

In Fig. 2 we show the total density of states of our system obtained from Eqs. (16)–(19). We start with two normalized square bands of width Δ and $\alpha\Delta$ representing the large conduction band and the narrow band, respectively. When the hybridization is turned on and for $V > V_c$ we obtain two new hybrid bands separated by a gap. The bands are symmetric and the Fermi level rests at the middle of the gap. The lower band accommodates the two electrons per unit cell. As mentioned before the Fermi level turns out to be temperature independent in the case of symmetric bands. Using this band structure we can calculate the thermodynamic properties of the system. The susceptibility is shown in Fig. 3 for different values of the ratio of effective masses α and of the effective mixing $\tilde{V}$. They show the same qualitative behavior of the experimental data and in particular that for FeSi where the susceptibility actually goes to zero exponentially after subtracting a tail due to paramagnetic impurities.[1] Other thermodynamic quantities can be readily obtained using the hybrid band density of states. The conductivity may be also found starting from the density of states and the Kubo-Greenwood formula.[11]

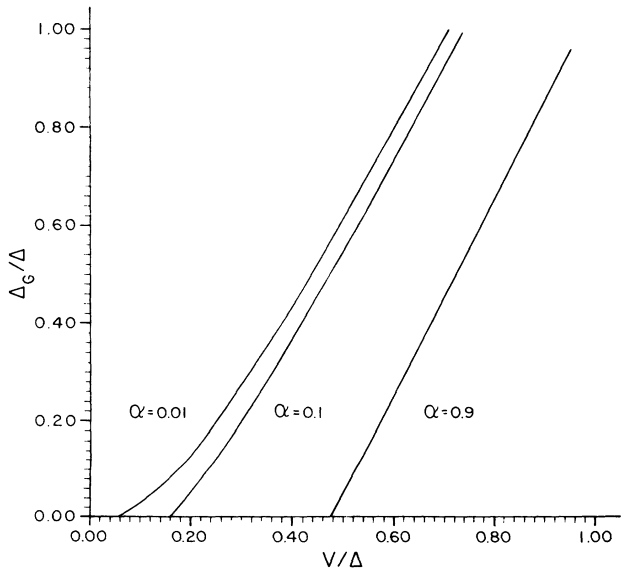

FIG. 1. The hybridization gap Δ_G as a function of hybridization V for different values of the ratio α between the effective masses (Δ is the bandwidth of the large s-like band).

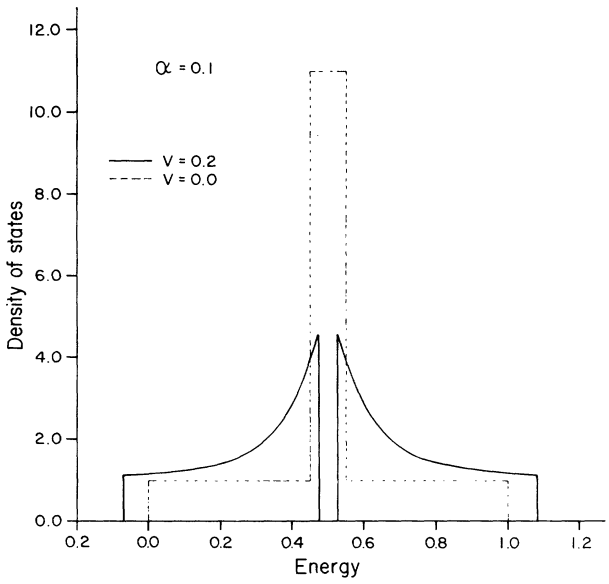

FIG. 2. The density of states of the two-band system before and after the hybridization is turned on. The lower hybrid band accommodates two electrons. The Fermi level is in the middle of the gap and is temperature independent due to the symmetry of the bands.

Notice that we can expand Eq. (21) close to V_c to obtain

$$\Delta_G \approx |V - V_c| \ .$$

Consequently, the gap exponent $s = \nu z$ defined by $\Delta_G \approx |V - V_c|^{\nu z}$ where ν and z are the correlation length and the dynamic exponents, respectively,[12] assumes the value $s = \nu z = 1$ within our approach. In fact, the exponents characterizing the zero-temperature metal-insulator transition at V_c may depend on the nature of the decouplings used to treat the many-body interactions.[13] However, the general features of our calculations as the existence of a $V_c \neq 0$ for the two-band problem, the typical behavior of the susceptibility shown in Fig. 3, which is due to the large density of states close to the edges of the gap, should be independent of any particular approximation.

IV. THE EFFECT OF IMPURITIES

The hybridization gap which was found previously is due to the translation invariance of the system and also a many-body effect. Interactions, as we have shown, act to decrease the gap renormalizing the bare hybridization parameter but are not expected to destroy coherence. What happens when translation invariance is lost due to the ad-

dition of impurities or in the presence of phonon scattering? A simple although phenomenological way of taking into account the effect of disorder and also of inelastic scattering is to introduce a lifetime in the quasiparticles of the bare bands. This approach was used by Doniach[14] and Weger[15] to describe the sharp rise in the resistivity of some intermetallic compounds with increasing temperature and gives rise to a *dehybridization transition.* This occurs whenever $\hbar(\tau_{ff}^{-1}-\tau_{ss}^{-1})\geq 2\tilde{V}$, where τ_{ff}^{-1} and τ_{ss}^{-1} are the scattering rates of the f and s electrons, respectively. Essentially the bare quasiparticles due to their finite lifetime have their energies spread in a significant interval compared to the hybridization gap blurring it. This effect may be particularly important in the systems considered here where the gap is small. Since the scattering rates are, in general, temperature dependent, as in the case of phonon scattering, *dehybridization* may occur as a function of temperature. This effect is formally similar to that which arises in the slave-boson approach although the underlying physics is quite distinct being in that case due to the many-body interactions. In the *metallic* regime the lifetime of the electrons[15] in the large conduction band is given by $\tau_{sf}^{-1}=\tilde{V}^2\tau_{ff}/\hbar^2$. Then the temperature dependence of the resistivity in the *metallic* regime may give information on the scattering mechanisms of the highly correlated electrons. The formulation of dehybridization as discussed above suffers the same deficiency of the mean-field, slave-boson method in the sense that it gives rise to a phase transition, associated with the vanishing of the gap, at a given temperature.[6] This spurious transition here is due to the way of treating disorder by simply introducing a finite lifetime for the bare quasiparticles. In spite of this formal difficulty, which should be circumvented in a more elaborate approach, this mechanism must be considered when discussing the effect of doping and disorder on hybridization gap materials. Also it affects the temperature dependence of the thermodynamic and transport properties since it gives rise to a temperature-dependent gap.

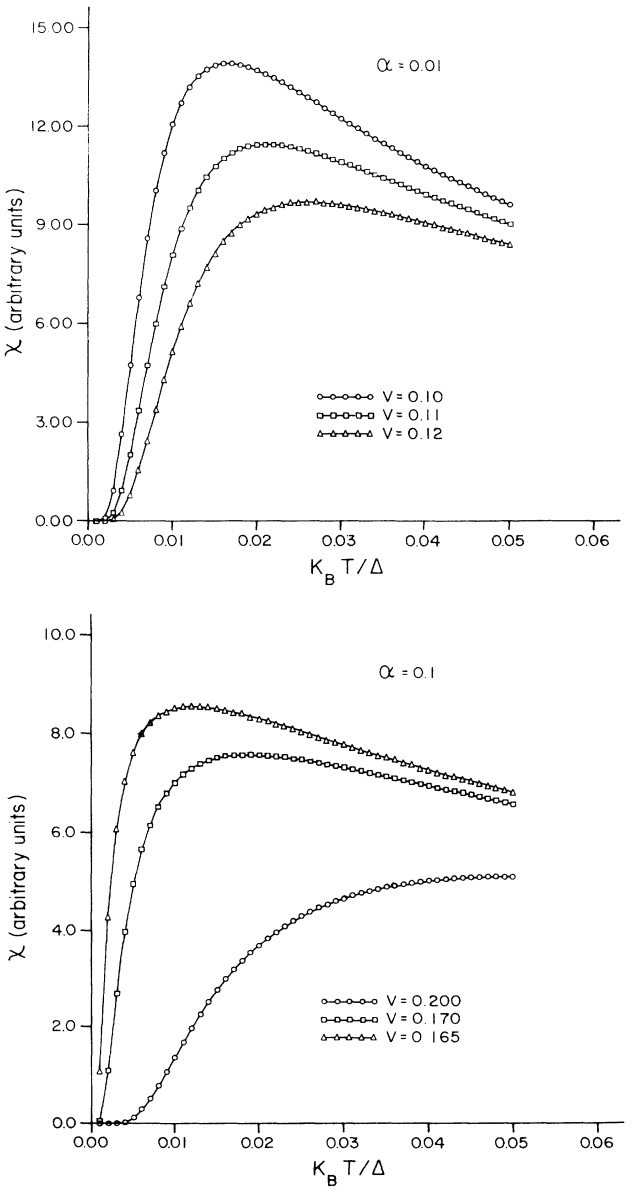

FIG. 3. The magnetic susceptibility, in arbitrary units, as a function of temperature for different parameters. Δ is the bandwidth of the large band.

The metal *ytterbium* has physical properties which are useful to compare with those of the materials studied here. For moderate applied pressured Yb has a metal-insulator transition due to the opening of a hybridization gap.[16] This material can then be considered as a typical case for which the condition $V>V_c$ is not fulfilled but can be reached by applying pressure. On the other hand, the essential difference between Yb and the Kondo insulators is the strength of the many-body interactions which should be negligible in the former system. It is interesting that a large T^2 term occurs in the resistivity of metallic Yb which is enhanced as the metal-insulator transition is approached even though the f electrons are always sufficiently below the Fermi level and do not play any role in this transition.[17]

V. CONCLUSIONS

We have introduced a two-band model to describe the properties of the family of heavy-fermion materials known as Kondo insulators. This model is also appropriate to describe transition-metal compounds, such as FeSi which exhibit similar properties. We have shown, within an extended Hubbard-I approximation, that many-body effects renormalize the mixing parameter reducing it from its bare value. We also found, differently from the Anderson lattice approach, that there is a critical value of the hybridization parameter for a gap to appear. This value is significantly large and may be one of the reasons hybridization gap materials are rather unusual, in particular, when based in transition metals. Within our approach the spin gap in the Kondo insulators coincides with the charge gap in agreement with experimental results on transport and thermodynamic properties[1,3] of these systems.

We have calculated the magnetic susceptibility of the two-band model showing that it has the qualitative

features observed in the actual systems. We have argued that the main effect of impurities and phonon scattering is to destroy coherence and give rise to *dehybridization.* Our two-band model provides the appropriate framework to consider these mechanisms. Other competing effects as the formation of impurity bands or filling of the upper hybrid band[18] cannot however be ruled out.

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[1]G. Aeppli and Z. Fisk, Comments Condens. Mater Phys. **16**, 155 (1992).
[2]M. F. Hundley *et al.*, Phys. Rev. B **42**, 6842 (1990).
[3]J. D. Thompson *et al.*, in *Transport and Thermal Properties of f Electron Systems,* edited by H. Fujii, T. Fujita, and G. Oomi (Plenum, New York, in press).
[4]H. Tsunetsugu *et al.*, Phys. Rev. B **46**, 3175 (1992).
[5]P. Riseborough, Phys. Rev. B **45**, 13 984 (1992).
[6]C. Sanchez-Castro, K. Bedell, and B. R. Cooper, Phys. Rev. B **47**, 6879 (1993).
[7]J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963).
[8]See A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1975).
[9]T. M. Rice and K. Ueda, Phys. Rev. Lett. **55**, 995 (1985).
[10]R. Kishore and S. K. Joshi, Phys. Rev. B **2**, 1411 (1970).
[11]N. F. Mott and E. A. Davies, *Electronic Processes in Non-Crystalline Materials* (Clarendon, Oxford, 1971).
[12]M. A. Continentino, Phys. Rep. (to be published).
[13]M. A. Continentino, G. Japiassu, and A. Troper, J. Appl. Phys. (to be published).
[14]A. B. Kaiser and D. Doniach, Int. J. Magn. **1**, 11 (1970).
[15]M. Weger, Philos. Mag. B **52**, 701 (1985).
[16]D. B. McWhan, T. M. Rice, and P. H. Schimdt, Phys. Rev. **177**, B1063 (1969).
[17]R. Jullien and D. Jerome, J. Phys. Chem. Solids **32**, 257 (1971).
[18]P. Schlottmann, Phys. Rev. B **46**, 998 (1992).