Metal-insulator transition in Kondo insulators: A functional-integral approach

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We present a theory to describe the metal-insulator transition as a function of pressure and temperature in Kondo insulators. A two-band model is introduced and we treat the electronic correlations using a functional-integral approach in the static approximation. The effects of pressure and temperature on the electronic structure of the system and the phase diagram are discussed. In particular we find the critical line separating the (paramagnetic) insulating from the metallic phase and the exponents characterizing the vanishing of the gap close to this line. We compare our results with experiments and previous theoretical approaches. [S0163-1829(98)01112-6]

I. INTRODUCTION

The metal-nonmetal transition in rare-earth compounds with applied pressure and temperature has been extensively studied.[1–5] This transition is observed in homogeneously mixed-valence materials, Sm compounds, especially SmB_6 and SmS under pressure.[5] Measurements of the electrical resistivity,[1] the dynamical conductivity,[2] the specific heat,[2] and the Hall coefficient[3] show that these materials are paramagnetic semiconductors with an energy gap at low temperatures which is also confirmed by direct tunneling experiments.[4] At high temperatures they behave as metals with no evident energy gap. More recently it became clear that these materials belong to a more general class of compounds known as *Kondo insulators*.[6] These systems at first look appear to behave as semiconductors with a small gap. However detailed studies[7] reveal a more complex behavior where correlations as expected from the narrow f orbitals involved play a fundamental role.

Recently some of us[8] studied the metal-insulator transition in Kondo insulators. A two-band model was introduced and the hybridization between them, when larger than a critical value V_c, produces a gap in the density of states giving rise to an insulating state for the considered electron counting. Electronic correlations within the narrow band were treated in the Hubbard I approximation. The value of V_c turned out to be inversely proportional to the mass of the quasiparticles in this narrow band. Also, since the gap is small in Kondo insulators, this indicates that these systems are close to a metal-insulator transition and universality concepts become relevant to describe their physical behavior. The critical exponents for this transition, at zero temperature, were obtained and it was argued that such a transition is in fact in the universality class of the *density-driven* metal-insulator (MI) transition[9] for which the exponents are known.[10] In this work the effect of temperature in the gap was not considered although the susceptibility obtained with a temperature independent gap shows a good qualitative agreement with experimental data. In a related work the same authors took into account excitonic correlations in these Kondo insulators.[11] The main effect was to renormalize the hybridization but the universality class of the zero temperature MI transition was not changed. Another approach to the Kondo insulator problem was taken by Fu and Doniach.[12] In order to deal with correlations these authors worked in infinite dimensions. The gap they find is fully renormalized by correlations even at zero temperature.

In the present paper we consider the effect of temperature in the gap and address the question of how this gap behaves with increasing temperature. For this purpose we use a functional integral approach to deal with the electronic correlations. This turns out to include temperature effects in a natural way. The correlated two-band model is transformed into an alloy problem which is treated within a coherent potential approximation (CPA). Such an approach was used previously to study a periodic Anderson model (PAM).[13] However, contrary to the present two-band theory[14] the PAM does not require a finite critical value of the hybridization to produce a gap ($V_c=0$). As a consequence the phase diagrams are different in the two approaches.

We finally propose and study an excitonic mechanism which, as with our CPA treatment, also gives rise to a *temperature-driven* metal-insulator transition, in this case due to the temperature dependence of excitonic correlations. The critical exponents characterizing the vanishing of the gap at the critical temperature are obtained and turn out to be the same in both cases.

II. FORMULATION OF THE PROBLEM

The Hamiltonian which describes our system is

$$H = H_0 + H_1, \tag{1}$$

where

$$H_0 = \sum_{lj\sigma} T^c_{lj} c^\dagger_{l\sigma} c_{j\sigma} + \sum_{lj\sigma} T^f_{lj} f^\dagger_{l\sigma} f_{j\sigma} + \sum_{lj\sigma} V_{lj} (f^\dagger_{l\sigma} c_{j\sigma} + c^\dagger_{j\sigma} f_{l\sigma}) \tag{2}$$

and

$$H_1 = (U/2) \sum_{l\sigma} n^f_{l\sigma} n^f_{l-\sigma}. \tag{3}$$

T^λ_{lj} represents the hopping integrals between l and j sites with $\lambda = c$ (or f) referring to a wide, uncorrelated band of width $2W$ and a narrow band, respectively. V_{lj} is the hybridization between c and f bands and U is the repulsive Coulomb interaction in the narrow band. The operators $c^\dagger_l$, c_l create and destroy electrons in the wide band and $f^\dagger_l$, f_l are creation and annihilation operators of electrons in the narrow band at site l. $n^f_{l\sigma} = f^\dagger_{l\sigma} f_{l\sigma}$ is the occupation number operator for f electrons at site l with spin σ. If it was not for the repulsive term, the Hamiltonian above could be exactly diagonalized giving rise to two hybrid bands.[8] However, the many body term due to the effective repulsive interaction U makes this a difficult problem for which an approximation must be introduced. In order to treat the electronic correlations we employ the functional integral method,[15] so that the partition function associated to the Hamiltonian above is

$$Z = \mathrm{Tr} e^{-\beta H_0} T_s e^{-\int_0^\beta U \Sigma_{l\sigma} n^f_{ls\sigma} n^f_{ls-\sigma} ds}, \tag{4}$$

where $\beta = 1/kT$ and T_s is the *time ordering* operator. Using the Hubbard-Stratonovich relation[15] and choosing to represent the Coulomb interaction term in the Ising-like representation, namely,

$$\sum_l n^f_{ls\uparrow} n^f_{ls\downarrow} = \frac{1}{4} \sum_{ls} [(n^f_{ls\uparrow} + n^f_{ls\downarrow})^2 - (n^f_{ls\uparrow} - n^f_{ls\downarrow})^2], \tag{5}$$

we can rewrite the partition function as

$$Z = \int \Pi_{ls} d\xi_{ls} d\nu_{ls} e^{-\int_0^\beta (U/4) \Sigma_l (\xi^2_{ls} + \nu^2_{ls}) ds} \times \mathrm{Tr} e^{-\beta H_0} T_s e^{\int_0^\beta (U/2) \Sigma_{l\sigma} (i\nu_{ls} + \sigma \xi_{ls}) n^f_{ls\sigma} ds}, \tag{6}$$

where we have introduced auxiliary charge (ν_{ls}) and spin fields (ξ_{ls}). It is not trivial to calculate this partition function related to the *time s*. We can neglect the dynamic effects of the fluctuating fields through the elimination of the time dependence of these operators which corresponds to adopting the static approximation.[15] Then we have

$$Z = \int \Pi_l d\xi_l d\nu_l \exp\left\{ -\beta \sum_l \left[(U/4)(\xi^2_l + \nu^2_l) - \frac{1}{\beta} \ln \mathrm{Tr} \exp(-\beta \widetilde{H}) \right] \right\}, \tag{7}$$

where the new effective Hamiltonian $\widetilde{H}$ is given by

$$\widetilde{H} = \sum_{l\sigma} \epsilon^c_0 n^c_{l\sigma} + \sum_{lj\sigma} T^c_{lj} c^\dagger_{l\sigma} c_{j\sigma} + \sum_{l\sigma} \epsilon^f_{l\sigma} n^f_{l\sigma} + \sum_{lj\sigma} T^f_{lj} f^\dagger_{l\sigma} f_{j\sigma} + \sum_{lj\sigma} V_{lj} (f^\dagger_{l\sigma} c_{j\sigma} + c^\dagger_{j\sigma} f_{l\sigma}) \tag{8}$$

and the effective energy $\epsilon^f_{l\sigma}$ by

$$\epsilon^f_{l\sigma} = \epsilon^f_0 - (U/2) \eta_l, \tag{9}$$

where $\eta_l = i\nu_l + \sigma \xi_l$. Through the Hubbard-Stratonovich relation, the initial system with the Coulomb interaction between the f electrons becomes an effective one-electron problem under the influence of magnetic (ξ) and electric (ν) fluctuating fields. Then the partition function of the original system reduces to the calculation of a Gaussian average over these fluctuating fields.

Since the effective Hamiltonian describes a disordered system we use a CPA, in which the random energy levels $\epsilon^f_{l\sigma}$ are substituted by the self-energy $\Sigma^f_\sigma(\omega)$, which is determined self-consistently by

$$\Sigma^f_\sigma(\omega) = \langle \eta_\sigma \rangle + \{ \langle \eta^2_\sigma \rangle - [\Sigma^f_\sigma(\omega)]^2 \} G^{ff}_\sigma(\omega). \tag{10}$$

The average over the fluctuating fields is calculated by

$$\langle \eta^n_\sigma \rangle = \frac{\int d\xi d\nu \eta^n e^{-\beta[U/4(\xi^2+\nu^2) + g(\xi,\nu)]}}{\int d\xi d\nu e^{-\beta[U/4(\xi^2+\nu^2) + g(\xi,\nu)]}} \tag{11}$$

with

$$g(\xi,\nu) = \frac{1}{\pi} \sum_\sigma \int d\omega f(\omega) \mathrm{Im} \ln[1 - (\epsilon^f_\sigma - \Sigma^f_\sigma) G^{ff}_\sigma(\omega)]. \tag{12}$$

The one-particle Green's function for f electrons is given by

$$G^{ff}_\sigma(\omega) = \sum_k \frac{\omega - \epsilon^c_k}{(\omega - \epsilon^c_k)[\omega - \epsilon^f_{k\sigma} - \Sigma^f_\sigma(\omega)] - |V_k|^2}. \tag{13}$$

For c electrons we have

$$G^{cc}_\sigma(\omega) = \sum_k \frac{\omega - \epsilon^f_{k\sigma} - \Sigma^f_\sigma(\omega)}{(\omega - \epsilon^c_k)[\omega - \epsilon^f_{k\sigma} - \Sigma^f_\sigma(\omega)] - |V_k|^2}. \tag{14}$$

In order to obtain explicit results for the electronic densities of states for c and f electrons we adopt the homothetic band model[8] for the bare dispersion relations

$$\begin{cases} \epsilon^c_k = \epsilon_k, \\ \epsilon^f_{k\sigma} = \alpha \epsilon_{k\sigma} + \gamma. \end{cases}$$

The quantity α ($\alpha < 1$) may be interpreted as taking into account the different effective masses of the electrons in the narrow f band and the broad c band, i.e., $(m_c/m_f) = \alpha$. The quantity γ gives the shift of the narrow band with respect to the wide band. Within this model a single density of states, that of the wide band, is sufficient to specify the problem.

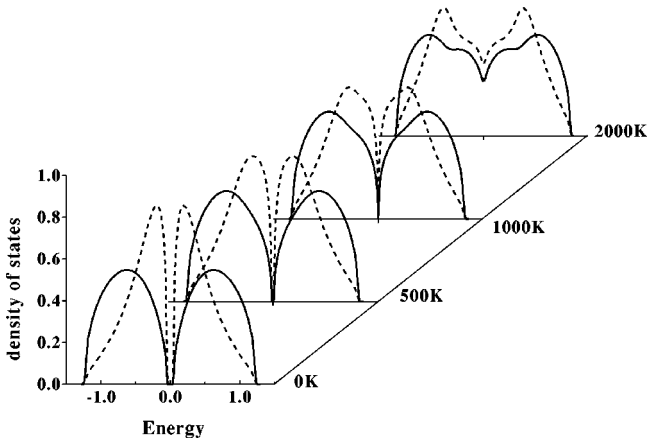

FIG. 1. Density of states for different values of temperature showing the *temperature-driven* metal-insulator transition. In this case $\alpha = m_c/m_f = 0.2$, $U/W = 1.3$, and $V/W = 0.5 < (V/W)_c$ with $W = 1$ eV such that at $T = 0$ the system is a paramagnetic insulator. The MI transition occurs for $T_c \approx 1400$ K.

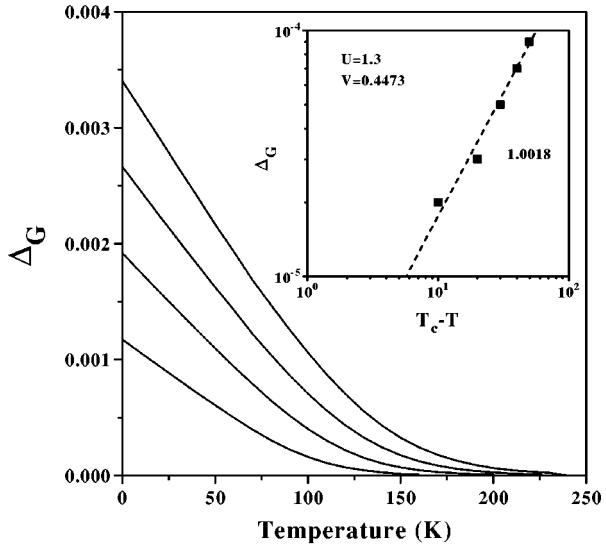

FIG. 2. The gap $\Delta_G(T)$ as function of temperature for $U/W = 1.3$, $W = 1$ eV, $\alpha = m_c/m_f = 0.2$, and different ratios V/W. From bottom to top $(V/W, T_c)$ = (0.4480, 160 K), (0.4485, 200 K), (0.4490, 225 K), and (0.4495, 240 K). The inset shows the behavior of the gap close to the *temperature-driven* metal-insulator transition. It vanishes linearly close to T_c, i.e., $\Delta_G(T) \propto |T - T_c|^{\mu}$ with $\mu = 1$.

At this point our problem has been reduced to a self-consistent solution of Eqs. (10)–(12) within the homothetic band model. The sums over **k**, to obtain the local Green's function, Eqs. (13) and (14), are transformed into integrals by introducing the bare density of states of the wide band. Before dealing with the self-consistent equations, we introduce a further simplification which consists in making the integral over the charge fields ν within the saddle point approximation. This amounts to substitute the charge field ν by its average value $\langle \nu \rangle = n^f$, where n^f is the total number of f electrons. We will be interested here in the symmetric case, where both, the narrow and wide bands are symmetrically located around the Fermi level. This corresponds to take $n^c = n^f = 1$ and these values remain constant as parameters such as temperature or hybridization change.[8,9,11] This condition also fixes the parameter γ in the homothetic band relation.

The self-energy we obtain has both a real and an imaginary part. The effects of temperature are contained in the averages of the random fields $\langle \eta_\sigma \rangle$ and $\langle \eta_\sigma^2 \rangle$, defined in Eq. (11). Due to the saddle point approximation in the charge fields these averages are essentially related to those over the random magnetic fields ξ. Since we are interested here in nonmagnetic solutions $\langle \xi \rangle = 0$ and we drop all spin indexes. Furthermore to an excellent approximation $\langle \xi^2 \rangle \approx k_B T U/2$ for sufficiently low temperatures.[13] At $T = 0$ our self-energy is frequency independent, purely real, and reduces to the usual random phase approximation (RPA) result $\Sigma_\sigma^f(\omega, T = 0) = U \langle n^f_{-\sigma} \rangle = (U/2) n^f$.

The self-consistent solution of the self-energy allows us to obtain the density of states, $n_\alpha(\omega) = -1/\pi \mathrm{Im} G^{\alpha\alpha}(\omega)$, $\alpha = c, f$. Figure 1 shows the total density of states for a specified set of parameters and different temperatures. As can be seen from the figure the zero temperature gap closes as temperature increases indicating a temperature-driven metal-insulator transition. We have investigated the behavior of the gap Δ_G close to the critical temperature T_c. Figure 2 shows that this gap vanishes linearly close to T_c, i.e., $\Delta_G \propto |T_c - T|$. At zero temperature we have obtained previously that the gap vanishes close to the $T = 0$ critical point as $\Delta_G(T = 0) \propto |(W/V)_c - (W/V)|^{\nu z}$ with $\nu z = 1$, where W/V is the ratio of the half-bandwidth of the wide band and the hybridization. At zero temperature this value of νz is exact and valid for any dimension.[9] The present approach extends this result to finite temperatures. However, it is not clear if the exponent we obtain for the temperature-driven transition is also exact or a consequence of the approximations we used.

The phase diagram (T/V) versus (W/V) close to the quantum critical point (QCP) at $(W/V)_c$ is shown in Fig. 3. The critical line separating the paramagnetic insulator from the paramagnetic metal close to the QCP is given by $T_c \propto |(W/V)_c - (W/V)|^{\psi}$ which defines the *shift exponent* ψ. We find that $\psi = 1/2$ describes very well our results. This value for the shift exponent is typical of mean-field theories. As the ratio of the effective masses $\alpha = m_c/m_f$ decreases, i.e., the

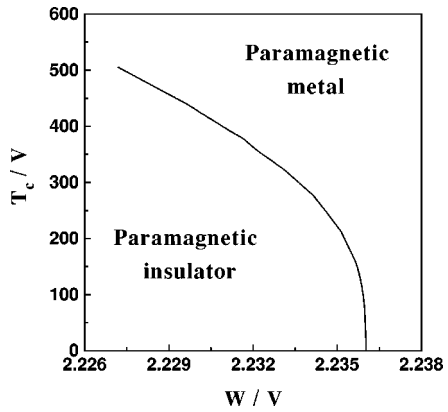

FIG. 3. Phase diagram of a Kondo Insulator as function of temperature close to the zero temperature critical point $(W/V)_c$ for $\alpha = m_c/m_f = 0.2$, $U/W = 1.3$, $W = 1$ eV. Note that $\alpha = 0$ corresponds to the PAM and in this case $V_c = 0$. The critical line vanishes close to the quantum critical point as $T_c \propto |\delta|^{\psi}$ with the exponent $\psi = 1/2$.

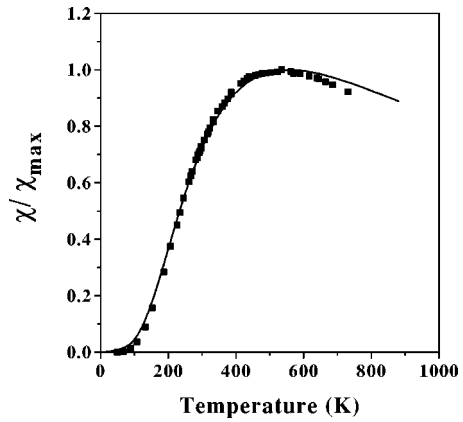

FIG. 4. The temperature dependent susceptibility obtained from Eq. (16) compared with experimental data for FeSi (Ref. 22). The parameters are $U/W=1.3$, $\alpha=0.2$, $V/W=0.65$, with $W=0.25$ eV. The MI transition occurs for these parameters at $T_c\approx 500$ K.

quasiparticles in the narrow band become heavier, the critical ratio $(W/V)_c$ increases. In the case $\alpha=0$, which corresponds to the PAM, any value of the hybridization opens a gap and drives the system to an insulating state $(V_c=0)$.

Figures 4 and 5 show the temperature dependent susceptibility $\chi(T)$ and the optical conductivity $\sigma(\omega,T)$ as calculated in our model. They are obtained from the following expressions[12]

$$\sigma(\omega,T)=\int_{-\infty}^{\epsilon_F} dE n(E)n(E+\omega)[1-f(E+\omega,T)], \tag{15}$$

where $f(E)$ is the Fermi function and the susceptibility is given by

$$\chi(T)\propto \lim_{\omega\to 0}\sigma(\omega,T)/T. \tag{16}$$

These quantities, as can be seen from Figs. 4 and 5, show an overall agreement with the experimental data.[6,7]

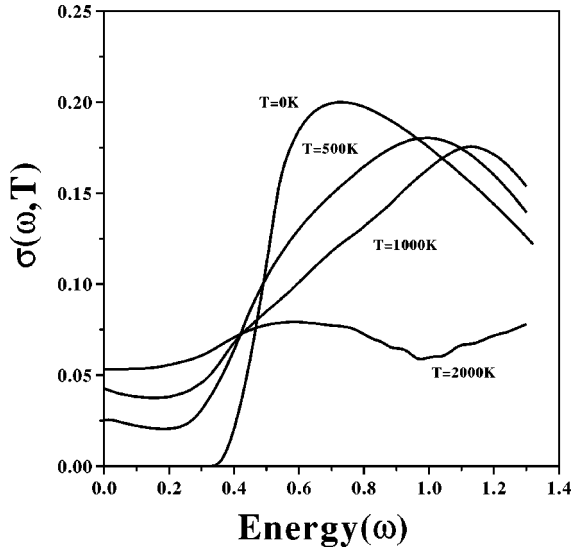

FIG. 5. The frequency dependent optical conductivity, Eq. (15), for different temperatures, obtained using the same parameters of Fig. 4.

We should point out that our two-band model requires a finite critical value V_c of the hybridization to open a gap. This occurs because we consider f-f overlap in the narrow band. Notice that in the PAM model, differently from our approach, there is no metal-insulator transition since any V is sufficient to open a gap. The existence of a finite critical hybridization modifies the scaling laws as compared with those of the PAM model and is responsible for the power-law behavior of the physical quantities, close to the MI transition, that we obtain here. For simplicity, in our numerical calculations we have not considered the k dependence of hybridization and consistently any details of the f-band structure. The reason is that we are interested on general aspects of the physics of Kondo insulators related to the proximity of these materials to the MI transition.

III. EXCITONIC EFFECTS IN KONDO INSULATORS

The effect of excitonic correlations in the zero temperature metal-insulator transition has been investigated.[11,16] It was shown that such correlations although renormalizing the hybridization do not change the universality class of this transition which is that of *density-driven* MI transitions.[11] We now investigate how temperature affects these results. The relevant Hamiltonian is given by

$$H=\sum_k \epsilon_k^c c_k^\dagger c_k+\sum_k \epsilon_h^f f_k^\dagger f_k+\sum_k V_k(c_k^\dagger f_k+f_k^\dagger c_k)$$
$$-\sum_{k,k',q} G(q)c_{k+q}^\dagger c_k f_{k'-q}^\dagger f_{k'} \tag{17}$$

which describes two hybridized c and f bands and an attractive interaction $G(q)$ between electron and holes. Within the random-phase approximation the temperature dependent correlation function Δ_{eh} can be obtained:

$$\Delta_{eh}(T)=\sum_k \langle f_k^\dagger c_k\rangle=\int d\omega f(\omega)\mathrm{Im}G^{cf}(\omega) \tag{18}$$

with

$$G^{cf}(\omega)=\sum_k \frac{\tilde{V}(T)}{(\omega-\epsilon_k^c)(\omega-\epsilon_k^f)-\tilde{V}^2(T)},$$

where $\tilde{V}(T)=V+G\Delta_{eh}(T)$ and the k dependence of V and G has been dropped. Again we have a self-consistency problem to be solved. We consider the same bare bands used previously. The excitonic correlation function as a function of temperature for the specified set of parameters is shown in Fig. 6. $\Delta_{eh}(T)$ decreases with temperature but never vanishes since there is no real excitonic transition in our model due to the presence of hybridization as we pointed out before.[14] The reason is that hybridization acts as a conjugate field to the excitonic order parameter. There is, however, a metal-insulator transition for $n^c=n^f=1$, associated with the vanishing of the gap at a critical temperature, as shown in Fig. 7. We find again that the gap vanishes linearly close to the critical temperature, i.e., $\Delta_G\propto|T-T_c|^\mu$ with $\mu=1$. The physical reason for this transition is thermal agitation which destroys the electron-hole pairs decreasing the effective hy-

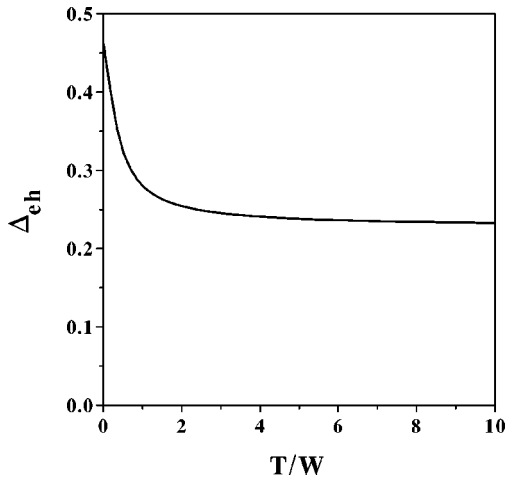

FIG. 6. The excitonic correlation function Δ_{eh} as function of temperature for $(U/W)=0$, $V/W=0.4$, and $G/W=0.11$. Δ_{eh} never vanishes due to the presence of hybridization which acts as a conjugate field.

bridization $\tilde{V}$. We emphasize that this metal-insulator transition is not an excitonic transition since $\Delta_{eh}(T)$ is always nonzero in our approach. We have then obtained an additional mechanism for a temperature-driven metal-insulator transition due to excitonic correlations. This mechanism for the MI transition is totally different from the previous one, although in both cases, the gap vanishes linearly close to the critical temperature. The present mechanism arises from the electron-hole attraction while before the driving force was the Coulomb repulsion between electrons in the same narrow band. In the excitonic case the renormalization occurs in the off-diagonal part of the Hamiltonian while in the CPA it is the energy of the heavy quasiparticles that are renormalized. Since the effects of both processes add up it is difficult to separate them. Although the overall temperature dependence of the gap is quite distinct in both cases (compare Figs. 2 and 7), what is more relevant is that they yield the same critical

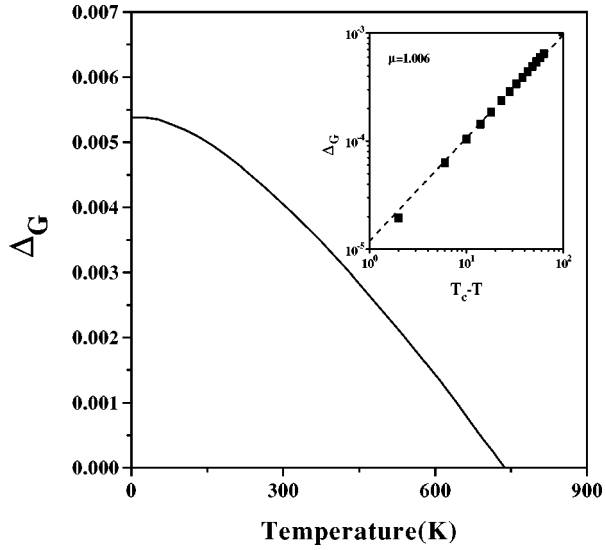

FIG. 7. The gap as function of temperature, showing the MI transition due to the excitonic mechanism. The inset shows that close to the critical temperature $\Delta_G(T)\propto|T-T_c|^{\mu}$ with $\mu=1$.

exponent $\mu=1$ for the gap $\Delta_G(T)$. The value of this exponent is an important result of our theory since it has experimental relevance. In fact the experiments show that there are no evident anomalies in the thermodynamic or transport properties which could signal the temperature-driven MI transition. However, if these quantities have, as expected, a thermally activated contribution, i.e., proportional to $\exp[-\Delta_G(T)/T]$, it is clear that their behavior and of their respective derivatives at T_c depend crucially on the exponent μ determining the critical behavior of Δ_G. It is interesting to compare the problem above with the case of spin-density wave materials, such as cromium, where a gap also opens below a critical temperature.[18] In this case the gap is a true order parameter and vanishes at T_c with an exponent which in mean field takes the value $\mu=1/2$. Values of $\mu<1$ imply strong anomalies in the derivatives of physical quantities with thermally activated contributions at T_c (Ref. 17) and these anomalies are in fact observed, for example, in the transport properties.[18]

IV. CONCLUSIONS

We have introduced a two-band model to investigate the physics of Kondo insulators at finite temperatures. For this purpose we have used a functional integral approach which naturally extends our previous zero temperature results.[8,9,11] We have found a *temperature-driven* metal-insulator transition associated with the vanishing of the gap at a critical temperature T_c. The gap turns out to vanish linearly close to T_c. This is similar to the $T=0$ result where the gap also vanishes linearly with the distance to the critical point. We have obtained a finite temperature phase diagram and found that the critical line close to the quantum critical point is governed by the mean-field shift exponent $\psi=1/2$. We found the heavier the quasiparticles in the narrow band the smaller is the hybridization required to open a gap in the $T=0$ density of states and to produce an insulating state. In our approach this together with a special electron counting condition are the main reasons for finding Kondo insulating behavior mostly in f compounds. Since the $T=0$ gap measures essentially the distance to the QCP, $\Delta_G(T=0)\propto|\delta|$, where $\delta=(W/V)_c-(W/V)$ and this gap is small in Kondo insulators, we have argued that these systems are close to the metal-insulator transition and universality concepts are useful to understand their physical properties. Although Coulomb correlations are essential to determine the finite temperature behavior of the system they do not affect the exponents of the zero temperature MI transition. This transition belongs to the universality class of the *density-driven* MI transitions for which all exponents are known.[9]

We point out that pressure is a fundamental tool to investigate the physical behavior of Kondo insulators. The reason is that the ratio W/V is sensitive to pressure and in this way it is possible to explore the zero temperature axis of the phase diagram of Fig. 3 as discussed in detail in Ref. 14. As concerns the behavior of the gap we obtain even at $T\neq0$ that it vanishes linearly with the distance to the critical point as at zero temperature. It is interesting that doping FeSi with Al drives this system to a metallic state and the MI transition is similar to that observed in an uncorrelated semiconductor such as SiP.[19] This irrelevance of correlations with respect to

the critical behavior is exactly what we obtain here. Note that this is valid as long as the MI transition is not accompanied by the appearance of long range magnetic order. Unfortunately doping FeSi also introduces strong disorder and it is this which ultimately is going to determine the critical behavior. Since we do not consider disorder, our $T=0$ approach is appropriate to describe the quantum MI transition in Kondo insulators which can be driven by pressure or magnetic field.[20] In this case our results suggest that this transition is similar, i.e., in the same universality class, to that observed for example in the metal ytterbium as a function of pressure.[21] Finally we point out that the reason the large Coulomb interactions become relevant at the small temperature scales typical of Kondo insulator behavior, as given, for example, by the temperature of smearing of the gap in the optical conductivity is a consequence of the proximity of these materials to the QCP.

ACKNOWLEDGMENTS

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