Short-range antiferromagnetic correlations in Kondo insulators

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Abstract

We study the influence of short range antiferromagnetic correlations between local f-electrons on the transport and thermodynamic properties of Kondo insulators. We use a Kondo lattice model with an additional Heisenberg interaction between nearest neighboring f-moments, as first proposed by Coqblin et al. [1] for metallic heavy fermions. The inter-site magnetic correlations produce an effective bandwidth for the f-electrons. They are treated on the same footing as the local Kondo correlations such that two energy scales appear in our approach. We discuss the competition between these two scales on the physical properties.

Key words: Kondo insulators. Strongly correlated systems. Hybridization

1 Introduction

Kondo insulators form a group of compounds that at high temperatures behave as dirty metals but at very low temperatures have their thermodynamic and transport properties determined by the existence of a small gap (10-100K) that arises from the hybridization of local electrons and the conduction band [2,3]. This family of compounds can be characterized as strongly correlated semiconductors due to the f or d character of the relevant electrons and includes FeSi [4], Ce3Bi4Pt3 [5–7], SmB6 [8], YbB12 [9] and CeFe4P12 [10].

Many theoretical models have been used to describe Kondo insulators. Some of them considered a two-band system, a large uncorrelated band of s electrons and another narrow correlated band which describes the f or d electrons [11–13]. Others considered an Anderson lattice, a conduction band and localized f states, with the correlation in these states generally treated within the slave-boson method [14,15].
Although Kondo insulators do not present long range magnetic order, the occurrence of short range antiferromagnetic correlations in these materials has been observed by inelastic neutron scattering [16], suggesting that a good model to describe Kondo insulators must include antiferromagnetic correlations between neighbors $f$-moments. We also point out that the magnetic susceptibility of Kondo insulators in the Curie-Weiss regime has a negative Curie temperature, as shown in Table 1 for some compounds. This is a clear indication of the presence of antiferromagnetic correlations in these materials.

In this letter we study some physical properties of the Kondo lattice taking into account short-range antiferromagnetic correlations between the localized $f$-electrons (only first neighbors) as first proposed by Coqblin et al.[1]. These authors have used this approach to describe metallic heavy-fermions while here we shall use it to investigate Kondo insulators. We calculate the density of states and study its behavior with increasing temperature and increasing magnetic correlations. We evaluate some physical properties such as optical conductivity, magnetic susceptibility and electrical resistivity. The format of the present letter is as follows. In section 2 we present the Hamiltonian and describe the approach used. In section 3 we calculate the density of states and some physical quantities in order to analyze the influence of magnetic correlations in the system.

## 2 Model Hamiltonian

We consider the following Hamiltonian to describe the system [1]:

$$
H = \sum_{k,\sigma} \varepsilon_k n^c_{k\sigma} + E_0 \sum_{i,\sigma} n^f_{i\sigma} - J_K \sum_i \vec{S}_i \cdot \vec{S}_i - J_H \sum_{i,\delta} \vec{S}_i \cdot \vec{S}_{i+\delta},
$$

where $n^c_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma}$, $n^f_{i\sigma} = f_{i\sigma}^\dagger f_{i\sigma}$. $\vec{S}_i$ are the spin operators associated to localized $f$-moments and $\vec{S}_i$ to conduction electrons at site $i$. The first term represents the conduction band. The operators $c_{k\sigma}$ and $c_{k\sigma}$, respectively, create and annihilate electrons in the conduction band state labeled by the wave vector $\vec{k}$ and spin $\sigma$. The second term, proportional to $E_0$, represents the binding

| Compound         | $\Theta$ |
|------------------|----------|
| $Ce_3Bi_4Pt_3$   | -125 K   |
| $YbBi_12$        | -79 K    |
| $FeSi$           | -1030 K  |

Table 1
Table of Curie Temperature for some compounds
energy of the \( f \)-electrons. The third term is the \( s-f \) exchange interaction \( J_K \) which gives rise to the Kondo coupling. In this model, following Coqblin et al. [1], we add a Heisenberg-like interaction \( J_H \) between nearest neighboring \( f \)-moments.

We examine the model above, specifically in the situation where the ground state of the system is an insulating state. First we construct an effective Hamiltonian, rewriting the original one, Eq.(1), in terms of new operators, as performed by Ruppenthal et al. [18]. Since we intend to describe the Kondo effect, we choose an operator \( \hat{\lambda}_{i,\sigma} \) that couples \( c \) and \( f \) electrons. In order to describe short-range magnetic correlations we introduce another operator \( \hat{\Gamma}_{i,\sigma} \) that couples \( f \) electrons in neighboring sites. These Hermitian operators are given by:

\[
\hat{\lambda}_{i\sigma} \equiv \frac{1}{\sqrt{2}}(c_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger c_{i\sigma}) \tag{2}
\]

and

\[
\hat{\Gamma}_{i+\delta,\sigma} \equiv \frac{1}{\sqrt{2}}(f_{i\sigma}^\dagger f_{i+\delta,\sigma} + f_{i+\delta,\sigma}^\dagger f_{i\sigma}). \tag{3}
\]

The spin components can be written in terms of the new operators. Using an additional constraint, that excludes the double \( f \)-occupancy, we get:

\[
s_i^x S_i^x + s_i^y S_i^y = -\frac{1}{2} \sum_\sigma \hat{\lambda}_{i\sigma} \hat{\lambda}_{i,-\sigma},
\]

\[
s_i^z S_i^z = \frac{1}{4}(n_i^c + n_i^f) - \frac{1}{4} n_i^c n_i^f - \frac{1}{2} \sum_\sigma \hat{\lambda}_{i,\sigma}^2,
\]

\[
S_i^x S_{i+\delta}^x + S_i^y S_{i+\delta}^y = -\frac{1}{2} \sum_\sigma \hat{\Gamma}_{i+\delta,\sigma} \hat{\Gamma}_{i,\sigma+\delta},
\]

\[
S_i^z S_{i+\delta}^z = \frac{1}{4}(n_i^f + n_{i+\delta}^f) - \frac{1}{4} n_i^f n_{i+\delta}^f - \frac{1}{2} \sum_\sigma \hat{\Gamma}_{i+\delta,\sigma}^2,
\]

where \( n_i^\alpha = n_i^{\alpha\uparrow} + n_i^{\alpha\downarrow} \). Since we are describing an insulating state at low temperatures, we use the constraints \( < n_i^c > = < n_i^f >= 1 \). Furthermore applying the decoupling,

\[
< n_{i\sigma}^\alpha n_{j\sigma}^\beta > \approx < n_{i\sigma}^\alpha > n_{j\sigma}^\beta + < n_{j\sigma}^\beta > n_{i\sigma}^\alpha,
\]

we find that the terms containing the number operators cancel out. Note that we are interested in non-magnetic solutions such that \( < n_{i\sigma}^\alpha > = < n_{i,-\sigma}^\alpha > \).
Finally we can write the Kondo and Heisenberg parts of the Hamiltonian as:

\[ H_K = \frac{1}{2} J_K \sum_{i\sigma} (\hat{\lambda}_{i\sigma} + \hat{\lambda}_{i,-\sigma}) \hat{\lambda}_{i\sigma}, \]  

(6)

\[ H_H = \frac{1}{2} J_H \sum_{i+\delta\sigma} (\hat{\Gamma}_{i+\delta\sigma} + \hat{\Gamma}_{i+\delta,-\sigma}) \hat{\Gamma}_{i+\delta\sigma}. \]  

(7)

Consistently with the decoupling used above, Eq.(5), we deal with the product of operators in equations (6) and (7) introducing the mean fields \( \lambda_i = \langle \hat{\lambda}_{i\sigma} \rangle \) and \( \Gamma_i = \langle \hat{\Gamma}_{i\delta\sigma} \rangle \). Furthermore due to translational invariance, \( \lambda_i = \lambda \) and \( \Gamma_i = \Gamma \). Performing a Fourier transform, using \( \varepsilon_k = -\frac{W}{z} \sum_R \cos(kR) \) where \( z \) is the number of neighbors and \( 2W \) is the band width, we obtain the effective Hamiltonian:

\[ H' = \sum_{k,\sigma} \varepsilon_{k\sigma} n_{k\sigma}^{\varepsilon\sigma} + J_K \lambda \sum_{k\sigma} (c_{k\sigma}^f f_{k\sigma} + f_{k\sigma}^f c_{k\sigma}) + \sum_{k,\sigma} \left( E_0 - b\varepsilon_k \right) n_{k\sigma}^f \]

\[ - 2J_K \lambda^2 - 2J_H \Gamma^2, \]  

(8)

where

\[ b = \frac{J_H W}{\Gamma}. \]  

(9)

We have then arrived at a new picture where the magnetic correlations \( J_H \) give rise to a narrow band of \( f \)-electrons of effective width \( 2bW \) (\( b \) is temperature dependent). The interaction \( J_K \) (using \( J_K < 0 \), since we are describing the Kondo effect) introduces an effective hybridization between the conduction and the renormalized \( f \) bands.

The new quasi-particles associated with the Hamiltonian (9) can now be obtained. This is done by calculating the one-electron Green’s functions which are found from their equations of motion. These Green’s functions are given by,

\[ G_{k,\sigma}^{ff}(\omega) = \frac{A^f(\varepsilon_k, \omega)}{\omega - \omega_1(\varepsilon_k)} - \frac{A^f(\varepsilon_k, \omega)}{\omega - \omega_2(\varepsilon_k)}, \]  

(10)

\[ G_{k,\sigma}^{cf}(\omega) = \frac{J_K \lambda}{(\omega_1(\varepsilon_k) - \omega_2(\varepsilon_k)) \left( \frac{1}{\omega - \omega_1(\varepsilon_k)} - \frac{1}{\omega - \omega_2(\varepsilon_k)} \right)}, \]  

(11)

\[ G_{k,\sigma}^{cc}(\omega) = \frac{A^c(\varepsilon_k, \omega)}{\omega - \omega_1(\varepsilon_k)} - \frac{A^c(\varepsilon_k, \omega)}{\omega - \omega_2(\varepsilon_k)}. \]  

(12)
where $G_{\alpha\beta}^{\kappa,\kappa'} = \langle \alpha_{\kappa \sigma} \rangle \langle \beta_{\kappa' \sigma'} \rangle$ for $\alpha, \beta = c, f$ and

$$
A^c(\varepsilon_k, \omega) = \frac{\omega - (b\varepsilon_k + E_0)}{\omega_1(\varepsilon_k) - \omega_2(\varepsilon_k)},
$$

(13)

$$
A^f(\varepsilon_k, \omega) = \frac{\omega - \varepsilon_k}{\omega_1(\varepsilon_k) - \omega_2(\varepsilon_k)}.
$$

(14)

We have expressed the Green’s functions in terms of simple poles corresponding to two hybridized quasi-particle bands with dispersion relations given by

$$
\omega_{1,2}(\varepsilon_k) = \frac{1}{2}[(1 + b)\varepsilon_k + E_0] \pm \frac{1}{2}\sqrt{[(1 - b)\varepsilon_k - E_0]^2 + 4J^2 K^2 \lambda^2}.
$$

(15)

---

**Fig. 1.** The energy dispersion relations $\omega_{1,2}(k)$ for the hybridized bands found in the mean-field approximation using $\varepsilon_k = -W \cos(ka/\pi)$, where $G/2 = \pi/2a$ is half a reciprocal lattice vector. Solid line is used for $J_H = 0$ and dashed line for $J_H < 0$.

As shown in figure 1 the two bands are separated by an indirect gap between the lower band at $k = G/2$ and the upper band at $k = 0$. For increasing values of the magnetic correlation $|J_H|$, the indirect gap gets larger while the direct gap remains constant. The direct gap $\Delta_{dir}$ is governed only by $J_K$. It is easy to see that $\Delta_{dir} = 2J_K \lambda$ and it occurs at $E_0 = (1 - b)\varepsilon_k$.

An insulating ground state, as observed in $Ce_3Bi_4Pt_3[5]$ or $YbB_{12}[9]$, is obtained when the lower band is completely filled. This corresponds to the half-filled band case where the occupation numbers assume the values $< n^f_i > = < n^c_i > = 1$. Furthermore, we take $E_0 = \mu = 0$ and symmetric bands with respect to the chemical potential $\mu$. Since the $f$-moments are correlated antiferromagnetically, which corresponds to $J_H < 0$, for $J_K \neq 0$ we always have an insulating ground state with the chemical potential fixed in the middle of the gap of the density of states.

The parameters $\lambda$ and $\Gamma$ are obtained from the two coupled equations that have to be solved self-consistently for each temperature:
\[ 1 = J_K \sum_k \frac{1}{(\omega_1 - \omega_2)} \left( \frac{f(\omega_1) - f(\omega_2)}{\omega - \omega_1} - \frac{f(\omega_1) - f(\omega_2)}{\omega - \omega_2} \right) \] (16)

\[ \Gamma = -\sum_k \frac{1}{(\omega_1 - \omega_2)} \left( \frac{(\omega_1 - \varepsilon_k)f(\omega_1)}{\omega - \omega_1} - \frac{(\omega_2 - \varepsilon_k)f(\omega_2)}{\omega - \omega_2} \right) \] (17)

where \( f(\omega) = \frac{1}{\exp(\beta(\omega - \mu)) + 1} \) is the Fermi distribution and \( \omega_{1,2} = \omega_{1,2}(\varepsilon_k) \) is given by Eq.(15).

The present method has many similarities with the slave-boson mean field approach and like it, presents a critical temperature \( T_c \) where the conduction and the \( f \) electrons become decoupled [14,15]. In our model, this arises for \( \lambda(T_c) = \Gamma(T_c) = 0 \) which implies the vanishing of the effective hybridization term \( \lambda \). So, these mean-field methods are useful to study the properties of Kondo insulators only in the low temperature regime, below the critical temperature \( T_c \) of the spurious phase transition. We shall present results here for \( T \ll T_c \) such that the present approach is valid.

3 Theoretical Results and Comparison with Experiments

As discussed previously, the magnetic correlations modify the band structure of the system, increasing the indirect gap. In this section we analyze the influence of these correlations in some physical properties, calculating \( \lambda \) and \( \Gamma \) self-consistently for each value of temperature. For simplicity we consider a uniform density of states of width \( 2W \) for the conduction electrons.

3.1 Density of states

Using that \( \langle n_{k,\sigma}^{\alpha,\beta} \rangle = \frac{1}{\pi} \text{Im}[G_{k,\sigma}^{\alpha,\beta}(\omega)] \) we obtain the \( c \) and \( f \) contributions to the density of states. In figures 2 and 3, we show the density of states which consists of two hybridized bands separated by a gap. The density of states is very sharp near the band edges independently of the form of the unperturbed bands.

Temperature renormalizes the density of states decreasing the gap (figure 2). With increasing temperatures the density of states become more peaked near the band edges. The density of states also depends on the magnetic correlations represented here by the parameter \( b \). The last term in Eq.(9) produces an effective \( f \)-band and its weight renormalizes with \( b \). In a system where the Fermi level is inside the gap, the main effects of short range antiferromagnetic correlations are to increase the gap and enhance the density of states near the band edges, as we can see in figure 3.
Fig. 2. $f$ contribution to the density of states for different temperatures. $J_K/W = -0.4$, $J_H/W = -0.1$.

Fig. 3. $f$ contribution to the density of states for two different values of $J_H$ and $k_B T/W = 0$.

3.2 Optical conductivity

The optical conductivity can be written as [19]:

$$\sigma(\nu) = \frac{\pi}{2W} \sum_\sigma \int d\varepsilon \int d\omega \rho^c_\sigma(\varepsilon, \omega) \rho^c_\sigma(\varepsilon, \omega + \nu) \left[ f(\omega) - f(\omega + \nu) \right] \frac{f(\omega) - f(\omega + \nu)}{\nu}$$

where $\rho^c_\sigma(\varepsilon, \omega)$ is the one particle spectral density of the conduction electrons.

In the optical conductivity, shown in figure 4, the behavior of the gap in-
Fig. 4. Optical conductivity for $J_K/W = -1.0$, $J_H/W = -0.1$ varying the temperature. The frequency $h\nu$ is in units of the bandwidth $W$.

Involves two characteristic temperature scales as observed experimentally for $Ce_3Bi_4Pi_3$ [20] and $FeSi$ [4]. Firstly the high temperature regime, compared to the width of the conductivity gap $\Delta_c$, where the gap $\Delta_c$ itself is strongly renormalized with $T$, as we can see in figure 4. The optical conductivity also presents a Drude-like feature at low frequencies, as observed recently by Gorshunov et al [21] in dynamical conductivity measurements in $SmB_6$. This peak indicates that the low-energy transport is determined by free charge carriers. Then the second temperature scale is set by the width of this Drude peak. Only at small temperatures the gap is completely opened. At these low temperatures the variation in the intensity of this peak, whose weight is transferred to the high frequency region of the spectrum, is the main effect of temperature. The gap itself remaining unchanged as the low-energy behavior changes from being dominated by free carriers to more localized carriers. We point out that the interaction $J_H$ has no effect in the gap size of the optical conductivity.

3.3 Magnetic susceptibility and electrical resistivity

In this subsection we calculate the electrical resistivity and the magnetic susceptibility for different values of $J_H$ to analyze the influence of antiferromagnetic correlations in these properties. The electric conductivity is obtained from the limit $\nu \to 0$ of the optical conductivity.

$$\sigma(0) = \frac{\pi \beta}{2W} \int d\varepsilon \int d\omega [\rho_\sigma^c(\varepsilon, \omega)]^2 f(\omega)[1 - f(\omega)], \quad (19)$$
where \( \beta \equiv 1/T \). The resistivity is given by \( \rho = 1/\sigma(0) \). Notice that this expression must be used with care. In the problem considered here, there is translational invariance and consequently \( \mathbf{k} \) is a good quantum number. However in real systems impurity scattering is always present and this limits the electron mean free path. In the calculations presented below, this is taken into account by including a finite lifetime for the conduction electrons. Formally this is done by replacing, \( \omega \rightarrow \omega + i\Gamma \), in the Green’s functions, where \( \Gamma \) is temperature independent. We point out that here we are interested in the temperature dependence of the conductivity which is not affected by the magnitude of \( \Gamma \).

If an external magnetic field \( h \) with its direction along the z-axis is applied, the quasi-particle energies become

\[
\omega_{i,\sigma}(\varepsilon_k) = \omega_i(\varepsilon_k) - \sigma h.
\] (20)

The free energy in the presence of the field, using the new quasi-particles energies (20), is written as

\[
F(\lambda, \Gamma, T) = -\frac{1}{\beta} \sum_{i=1,2} \sum_{k,\sigma} \ln \left( 1 + \exp \left( -\beta \omega_{i,\sigma}(\varepsilon_k) \right) \right) + 2J_H \lambda^2 + 2J_H \Gamma^2
\] (21)

and the magnetic susceptibility is given by

\[
\chi(T) = \frac{\partial^2 F}{\partial h^2} \Big|_{h=0} = \frac{1}{4} \beta \sum_{i=1,2} \sum_{k,\sigma} \text{sech}^2 \left( \frac{1}{2} \beta \omega_{i,\sigma}(\varepsilon_k) \right).
\] (22)
temperature resistivity and susceptibility curves were fitted using the activated forms \( \chi(T) = (C/T) \exp(-\Delta_\chi/kT) \) and \( \rho(T) = \rho_0 \exp(-\Delta_\rho/kT) \), which describe the experimental data in Kondo insulators. As we can see in figure 5, these analytical expressions give also a good description of the theoretical results, indicating that our model describes very well the low temperature properties of these systems. The fittings of the theoretical results yield values for the transport \( \Delta_\rho \) and magnetic \( \Delta_\chi \) gaps [4]. In figure 6 we show these gaps for different values of \( J_H \). \( \Delta_\chi \) and \( \Delta_\rho \) increase for increasing values of \( |J_H/W| \) but their ratio remains the same \( \Delta_\chi/\Delta_\rho \approx 2.2 \) suggesting that magnetic correlations do not influence the relation between them.

![Fig. 6. Magnetic (full squares) and transport (full circles) gaps versus \( J_H \) for \( J_K/W = -0.4 \).](image)

**3.4 Analysis**

Experimental results yield different values for the gaps of Kondo insulators. The gap measured in optical conductivity \( \Delta_c \) has larger values than the gaps measured in neutron scattering and susceptibility measurements, \( \Delta_\chi \) or in transport measurements, \( \Delta_\rho \) [20]. On the other hand, comparing the spin and transport gaps, experimental results show that \( \Delta_\chi \geq \Delta_\rho \) [4,7]. The present theory accounts for these observations and introduces a new discussion about the role of short-range magnetic correlations in the properties of these gaps.

We have discussed in section 2 the influence of antiferromagnetic correlations in the indirect and direct gaps in the density of states. Although in the calculations of section 3 we used a square band, without a defined dispersion relation, we point out that, since our results show that the frequency gap \( \Delta_c \)
in the optical conductivity does not renormalize as \( J_H \) varies, we may conclude that this quantity is determined by the direct gap. This is expected, since due to the negligible momentum of the photon, optical excitations involve essentially an energy transfer. On the other hand the results in figure (6) show that the transport and susceptibility gaps are strongly renormalized by magnetic correlations indicating the indirect nature of the gap that determines these physical properties.

4 Conclusions

In this work we have discussed a model for Kondo insulators which takes into account the influence of short-range magnetic correlations in these systems. We used a Kondo lattice with an additional Heisenberg term and we treated the problem within a mean-field approach in order to obtain an effective Hamiltonian where the additional term gives rise to an effective bandwidth for the \( f \) electrons. Although the Kondo interaction leads to an indirect coupling between the local electrons, we have added explicitly to the Hamiltonian an interaction between them. In this way we can make a straightforward analysis of the influence of these magnetic correlations on the properties of the system.

We have obtained the density of states of the new quasi-particles and observed that their energy bands are renormalized by temperature and antiferromagnetic correlations. We have calculated the magnetic susceptibility and electric resistivity to get the magnetic and transport gaps which turn out to be strongly renormalized by magnetic correlations. Calculating the optical conductivity we find a Drude-like peak at very low frequencies, as observed recently in dynamical conductivity measurements of \( SmB_6 \)[21]. However, the gap in the optical conductivity remains the same for different values of the strength of magnetic correlations. This gap is determined by the direct gap in the band structure, while the magnetic and transport gaps arise mostly from the indirect gap. The antiferromagnetic correlations change substantially the physical properties related to the indirect gap but do not change the quantities related to the direct one. These observations can produce an insight for future experimental analysis.

This letter discusses explicitly the short-range magnetic correlations which have not been explored previously in the theoretical study of Kondo insulators. The model is able to reproduce their physical properties, including their temperature dependence, and is in good qualitative agreement with experimental results.
Acknowledgments

The authors like to thank M. A. Gusmão for useful discussions and sending a pre-print of his work. This work was supported by The Brazilian agencies Conselho Nacional de Desenvolvimento Científico (CNPq) and CAPES.

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