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X-boson cumulant approach to the topological Kondo insulators

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Abstract.

In this work we present a generalization of our previous work of the $X-$boson approach to the periodic Anderson model (PAM), adequate to study a novel class of intermetallic $4f$ and $5f$ orbitals materials: the topological Kondo insulators, whose paradigmatic material is the compound SmB_6.

For simplicity, we consider a version of the PAM on a $2D$ square lattice, adequate to describe $Ce-$based compounds in two dimensions. The starting point of the model is the $4f-Ce$ ions orbitals, with $J=5/2$ multiplet, in the presence of spin-orbit coupling. Our technique works well for all of the parameters of the model and avoids the unwanted phase transitions of the slave boson mean field theory. We present a critical comparison of our results with those of the usual slave boson method, that has been intensively used to describe this class of materials. We also obtain a new valence first order transition which we attribute to the $\vec{k}$ dependence of the hybridization.

1. Introduction

In this work we study a novel class of intermetallic $4f$ and $5f$ orbitals materials: the topological Kondo insulators; in which strong interactions between itinerant and predominately localized degrees of freedom give rise to a bulk insulating state at low temperatures, while the surface remains metallic. This effect arises due to inversion of even parity conduction bands and odd parity very narrow f electron bands. For an odd number of band inversions, the metallic surface states are chiral and therefore remain robust against disorder and time reversal invariant perturbations.

The topological Kondo insulators have been studied employing the slave boson mean field theory (SBMFT) [1], both in the limit of the Coulomb repulsion $U\to\infty$ [2, 3], and for finite correlation U [4]. This approximation is attractive because with a small numerical effort, it is capable of qualitatively describe the Kondo regime, but as the temperature is increased or when $(\mu >> E_{f,\tau}=E_f)$ at low temperatures, and also for all parameters at intermediate temperatures, the SBMFT presents an unphysical second order phase transition with the conduction and the localized electrons decoupling from each other. In the impurity case this transition occurs when $T>T_K$, and defines the Kondo temperature.

To circumvent these problems, maintaining the simplicity of the calculation and the ideas involved, we have developed the X-boson method [6], inspired by the slave boson formalism. To solve the problem of non-conservation of probability (completeness) that appears when we use the X Hubbard operators, we use the chain cumulant Green's functions.

The SBMFT continues to be an attractive approach to treat the extreme Kondo limit of the Anderson model, where the localized occupation number is equal to $n_f = 1$ at very low temperatures, but it is less adequate to describe intermediate valence (IV) systems like the new topological Kondo insulator SmB_6, where the localized occupation number associated with the opening a gap at low temperatures, is $n_f \simeq 0.7 - 0.8$ [8] in this compound. On the other hand, the X-boson approach does not capture the Kondo peak physics in the limit of $n_f = 1$, as the SBMFT does, but it is more adequate to describe IV systems because this formalism does not present spurious phase transitions for any of the system parameters.

We generalize our previous work of the $X-$boson approach to the periodic Anderson model (PAM) for f electrons states with a total angular momentum J and z-axis component M, while the conduction electron states are described by a momentum $\mathbf{k}$ and spin σ; in our previous calculation we considered $J = 1/2$. The spin-orbit coupled Wannier states of the conduction electrons are then decomposed in terms of plane-wave states, and this gives rise to momentum-dependent form factors with symmetries that are uniquely determined by the local symmetry of the f states.

2. The $2D$ periodic Anderson model

The present paper deals with the periodic Anderson model (PAM) in the limit of infinite Coulomb repulsion ($U = \infty$), adequate to treat Ce-based compounds in two dimensions (2D) [5], and we employ the Hubbard X operators to write its Hamiltonian in the form

$$H = \sum_{\mathbf{k}\sigma} E_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{j\tau} E_{f,j\tau} X_{j,\tau} + \sum_{j\tau,\mathbf{k}\sigma} \left(V_{\sigma\tau}(\vec{k}) X^{\dagger}_{j,0\tau} c_{\mathbf{k},\sigma} + V^{*}_{\sigma\tau}(\vec{k}) c^{\dagger}_{\mathbf{k},\sigma} X_{j,0\tau} \right), \qquad (1)$$

where we follow the notation of the paper in the reference [3]. The first term is the Hamiltonian of the conduction electrons (c-electrons), with momentum $\vec{k}$ and spin σ, the second term describes independent localized electrons (f-electrons), with pseudospin τ belonging to one representation γ of some multiplet state at the site j. The last term is the hybridization Hamiltonian giving the interaction between the c-electrons and the f-electrons. As there is no local hybridization process between s and f electrons in rare earth ions, the hybridization process results from the nearest-neighbor hopping from the f electrons at a site j to the s electron at the vicinity of this site. To determine the structure of the $V_{\sigma\tau}(\vec{k})$ we must specify the representation γ of the localized electron and the corresponding conduction electrons. Considering the $j = 5/2$ multiplet structure the hopping hybridization matrix can be written as $V_{\sigma\tau}(\vec{k}) = V[\mathbf{\Phi}]_{\sigma\tau}(\vec{k})$, where $[\mathbf{\Phi}]_{\sigma\tau}(\vec{k})$ is the form factor, which is associated with the $\vec{k}$ dependence and the non trivial orbital structure of the hybridization. Following the derivation presented in reference [3], the form factor can be written as [5] $\mathbf{\Phi}(k) = \vec{d}(k) \circ \vec{\sigma}$, where for a $2D$ square lattice, $\vec{d}(k) = 2[sin(k_x), sin(k_y)]$ and $\vec{\sigma}$ are the Pauli spin matrices.

The X operators are very convenient to work with local states associated to the sites j of a lattice, and are defined in general by $X_{j,ab}{=}|j,a\rangle \langle j,b|$, where the set $\{|j,a\rangle\}$ is an orthonormal basis in the space of local states of interest. When $U \to \infty$ the identity I_j at site j should satisfy the completeness relation: $X_{j,00} + X_{j,\tau\tau} + X_{j,\overline{\tau}\overline{\tau}} = I_j$, where $\overline{\tau}$ is the pseudospin component opposite to τ, and the $X_{j,aa}$ are the projectors into $\mid j,a\rangle$.

3. The X-boson approach

The Hamiltonian can be treated by a generalization of the X-boson approach [6] for the lattice case, and the cumulant Green's function (GF) are then given by

$$G^{f}_{\mathbf{k}\sigma}(z)=\frac{-D_\tau\left(z-\varepsilon_{\mathbf{k}\sigma}\right)}{\mathcal{E}(z)},\quad G^{c}_{\mathbf{k}\sigma}(z)=\frac{-\left(z-\widetilde{E}_{f,\tau}\right)}{\mathcal{E}(z)}\quad,\quad G^{fc}_{\mathbf{k}\sigma}(z)=\frac{-|V|D_\tau\Delta(\vec{k})}{\mathcal{E}(z)},\tag{2}$$

with $\mathcal{E}(z)=\left(z-\widetilde{E}_{f,\tau}\right)\left(z-\varepsilon_{\mathbf{k}\sigma}\right)-|V|^2D_\tau\mathbf{\Delta}^2(\vec{k})$, where $z=\omega+i\eta$, with $\eta\to0^+$ and the roots of $\mathcal{E}(z)$ are given by

$$\omega_{\mathbf{k},\sigma}(\pm)=\frac{1}{2}\left(\varepsilon_{\mathbf{k},\sigma}+\widetilde{E}_f\right)\pm\frac{1}{2}\sqrt{\left(\varepsilon_{\mathbf{k},\sigma}-\widetilde{E}_f\right)^2+4|V|^2D_\tau\mathbf{\Delta}^2(\vec{k})},\tag{3}$$

where $\mathbf{\Delta}^2(\vec{k})=\frac{1}{2}Tr[\mathbf{\Phi}(\vec{k}).\mathbf{\Phi}^*(\vec{k})]$. The correlations appear in the X-boson approach through the quantity $D_\tau=R+n_{f,\tau}$, with $R=\langle X_{0,0}\rangle$ and $n_{f,\tau}=\langle X_{\tau,\tau}\rangle$. In the X-boson approach the quantity D_τ must be calculated self-consistently through the minimization of the corresponding thermodynamic potential with respect to the parameter R, at the same time $\widetilde{E}_{f,\tau}=E_{f,\tau}+\Lambda$, where Λ is a Lagrange multiplier. We shall consider a spin independent tight-binding conduction band on a $2D$ square lattice

$$\varepsilon_{\mathbf{k}}=-2t[cos(k_x)+cos(k_y)],\tag{4}$$

where we employ the hopping between neighboring sites of the $2D$ square lattice, $t=1$ as the energy unit. In the X-boson method [6], after the minimization of the thermodynamic potential $\Omega=-k_BT\ln(\mathcal{Q})$, (where $\mathcal{Q}$ is the grand partition function) with respect to the R parameter we obtain the X-boson parameter Λ

$$\Lambda=\frac{-V^2}{\pi^2}\int_{-\pi}^{\pi}dk_x\int_{-\pi}^{\pi}dk_y\mathbf{\Delta}^2(\vec{k})\frac{n_F\left(\omega_{\mathbf{k}}(+)\right)-n_F\left(\omega_{\mathbf{k}}(-)\right)}{\sqrt{\left(\varepsilon_{\mathbf{k}}-\widetilde{E}_f\right)^2+4V^2D_\tau\mathbf{\Delta}^2(\vec{k})}},\tag{5}$$

where $n_F\left(x\right)$ is the Fermi-Dirac distribution $n_F(z)=\left[1+\exp\left(\beta\ z\right)\right]^{-1}$, N_s is the number of sites and $\mathbf{\Delta}^2(\vec{k})=4[sin^2(k_x)+sin^2(k_y)]$. After the numerical calculation of the parameter Λ, we calculate the occupation numbers employing the Green's functions and we use the completeness relation $\langle X_{j,00}\rangle+\langle X_{j,\tau\tau}\rangle+\langle X_{j,\overline{\tau\tau}}\rangle=I_j$, to calculate the parameter $R=D_\tau-n_{f,\tau}$. All the calculations are repeated again until the convergence of the X-boson parameters Λ and R is attained.

The density of states is obtained numerically through the relation

$$\rho(\omega)=\frac{-1}{\pi}Im\int_{-\pi}^{\pi}dk_x\int_{-\pi}^{\pi}dk_y\frac{1}{\omega-\omega_{\mathbf{k}}(\pm)+i\eta},\tag{6}$$

where $\omega_{\mathbf{k}}$ is given by the Eq. 3.

In a similar way as it is done with the slave boson Hamiltonian [1], we have shown [6] that the X-boson Hamiltonian Eq. 1 can be written in an uncorrelated form H^u as

$$H^u=\sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}\ c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}+\sum_{k,\tau}\widetilde{\varepsilon}_f\ f^\dagger_{\mathbf{k},\tau}f_{\mathbf{k},\tau}+N_s\Lambda(R-1)+\sum_{\mathbf{k},\sigma\tau}\left(\overline{V}_{\sigma,\tau}(\mathbf{k})f^\dagger_{\mathbf{k},\tau}\ c_{\mathbf{k},\sigma}+\overline{V}_{\sigma,\tau}(\mathbf{k})^*c^\dagger_{\mathbf{k},\sigma}\ f_{\mathbf{k},\tau}\right),\tag{7}$$

with $\overline{V}_{\sigma\tau}(\mathbf{k})=\sqrt{D_\tau}V_{\sigma\tau}(\mathbf{k})$. This Hamiltonian can be easily diagonalized, and following Tran's work [3], we can write

$$\mathcal{H}^u=\sum_{\mathbf{k}}\Psi^\dagger(\mathbf{k})H^u(\mathbf{k})\Psi(\mathbf{k})+N_s\Lambda(R-1),\tag{8}$$

with

$$H^u(\mathbf{k}) = \begin{pmatrix} \varepsilon_{\mathbf{k}} & V\Phi_{\mathbf{k}} & 0 & 0 \\ V\Phi^*_{\mathbf{k}} & \widetilde{\varepsilon}_f & 0 & 0 \\ 0 & 0 & \varepsilon_{\mathbf{k}} & -V\Phi_{\mathbf{k}} \\ 0 & 0 & -V\Phi^*_{\mathbf{k}} & \widetilde{\varepsilon}_f \end{pmatrix}, \tag{9}$$

where $\Psi^\dagger(\mathbf{k}) = (c^\dagger_{\mathbf{k},\uparrow} f^\dagger_{\mathbf{k},(-)} c^\dagger_{\mathbf{k},\downarrow} f^\dagger_{\mathbf{k},(+)})$ is a four component Dirac spinor, with $\varepsilon_{\mathbf{k}} = E_{\mathbf{k}} - \mu$, $\widetilde{\varepsilon}_f = \widetilde{E}_f + \Lambda - \mu$ and $\Phi_{\mathbf{k}} = 2[sin(\mathbf{k_x}) - isin(\mathbf{k_y})]$. Expanding $\Phi_{\mathbf{k}}$ for small values of $\mathbf{k_x}$ and $\mathbf{k_y}$, we obtain an effective Dirac theory given by the Hamiltonian

$$H^u(\mathbf{k}) = \begin{pmatrix} \varepsilon_{\mathbf{k}} & 2V(\mathbf{k_x} - i\mathbf{k_y}) & 0 & 0 \\ 2V(\mathbf{k_x} + i\mathbf{k_y}) & \widetilde{\varepsilon}_f & 0 & 0 \\ 0 & 0 & \varepsilon_{\mathbf{k}} & -2V(\mathbf{k_x} + i\mathbf{k_y}) \\ 0 & 0 & -2V(\mathbf{k_x} - i\mathbf{k_y}) & \widetilde{\varepsilon}_f \end{pmatrix}, \tag{10}$$

whose spectrum can be written in a Dirac form $E_\pm(p) = \varepsilon \pm \sqrt{A^2(p_x^2 + p_y^2) + M^2}$, with $\varepsilon = (\varepsilon_{\mathbf{k}} + \widetilde{\varepsilon}_f)/2$, $M = (\varepsilon_{\mathbf{k}} - \widetilde{\varepsilon}_f)/2$ and $A = 4V$. This discussion shows that the X-boson captures the behavior of the Dirac cones in the spectral density at around $\mathbf{k} \approx \mathbf{0}$, as indicated in Fig. 3.

4. Results and discussion

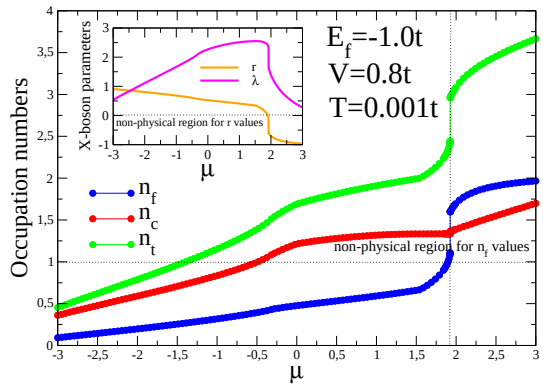

Figure 1. Slave boson occupation numbers.

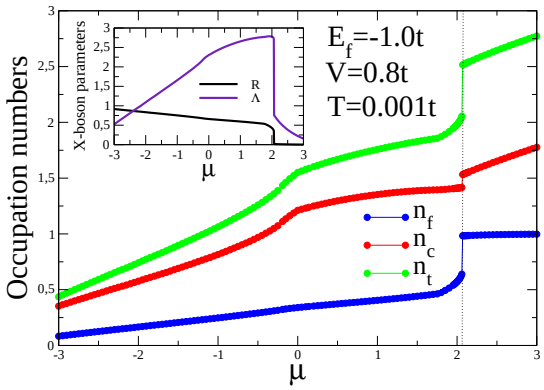

Figure 2. X-boson occupation numbers.

In Figs. 1 and 2 we compare the occupations numbers calculated employing both the SBMFT [1] and the X-boson approach [6]. We choose the following set of parameter: $E_f = -1.0t$, $V = 0.8t$ and $T = 0.001t$. The new interesting result, is that both methods show a first order transition in the occupation numbers in the local magnetic moment regime (LMM)[7]. In the SBMFT the transition is not physical, because it occurs in the region where $n_f > 1$, but in the X-boson case the corresponding transition, presented in Fig. 2, is physical because it occurs in a region where $n_f < 1$. It is possible to observe in Fig. 1 that the proximity of the spurious transition of the SBMFT distorts all the occupation numbers in the intermediate valence (IV) region, indicating that the SBMFT is not completely adequate do describe the topological Kondo insulators. This X-boson first order transition is not observed when we consider a constant hybridization V (cf. Fig. 12 of our paper [6]), and in this case we obtain a

crossover from the IV to the Kondo region. We can associate this first order transition to the $j = 5/2$ multiplet structure of the hopping hybridization matrix employed to describe the Ce ions, which introduces a $\vec{k}$ dependence and a non trivial orbital structure in the hybridization.

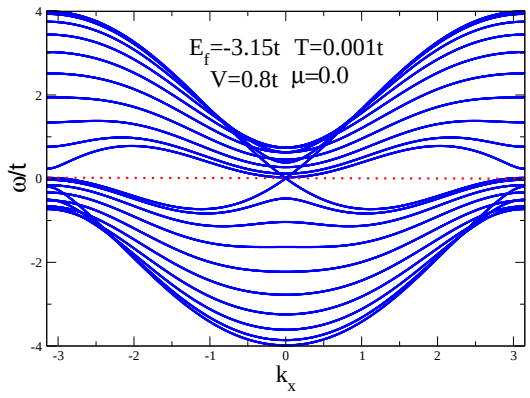

Figure 3. Single-particle band spectrum for the X-boson.

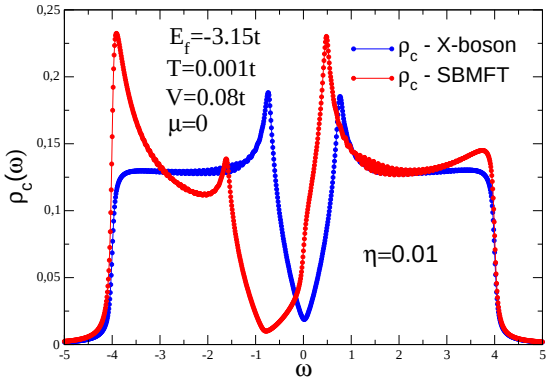

Figure 4. Density of states of the conduction electrons for the X-boson and slave boson.

In Figs. 3 we represent the X-boson single-particle band spectrum for $E_f = -3.15t$, $V = 0.8t$, $T = 0.001t$, along the x axis, $k = k_x$, and several k_y values for $\mu = 0.0$ in the IV regime, corresponding to an insulator situation. The Fig. 3 represents a strong topological Kondo insulator, because the spectral function presents a small gap at the border of the zone boundary and the Dirac cones crosses the chemical potential at $\mu = 0.0$ [2]. In Fig. 4 we plot the density of states of the conduction electrons for the X-boson and the slave boson methods, calculated with the same parameters of Fig. 3. The X-boson presents a typical insulator situation, with the localized occupation number being $n_f = 0.66$ whereas the slave boson breaks down in this region producing an unphysical density of states of $n_f = 1.37$. Due to numerical instabilities [9] associated with the analytic continuation of the Green's functions to the real axis, we represent the density of states for $\eta = 0.01$, but it is clear from the figure that it represents an insulator.

Acknowledgments
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