Heavy fermion superconductivity: X-boson treatment

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We use the X-boson method to study the heavy fermion superconductivity phase employing an extension of the periodic Anderson model in the $U=\infty$ limit with a nearest neighbor attractive interaction between the localized $f$-electrons. We show that higher values of the hybridization parameter implies in lower values associated to the maximum of the superconducting critical temperature $T_c$, indicating that the real charge transfer between bands tends to destabilizes the Cooper pairing. Moreover, we show that the superconductivity is constrained to the vicinity of a range of densities where the $f$-band density of states at the Fermi level $\rho_f(\mu)$ have sufficiently high values and it was found both for configurations where the system presents intermediate valence and heavy fermion behavior, as experimentally observed. Finally, as the total occupation is raised and for larges hybridization parameter $V$ there is an insulator-superconductor transition, which is related to the existence of a hybridization gap that cannot be accessed by the slave boson method, because when the chemical potential lies in or above the gap the system suffers the second order phase transition characteristic of that method.

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I. INTRODUCTION

In the present paper we study the heavy fermion superconductivity employing an extension of the periodic Anderson model (PAM) in the $U=\infty$ limit taking into account the effect of a nearest neighbor attractive interaction between $f$ electrons. The model was primarily designed to study the heavy fermions systems, but it could fit in a description of the high temperature superconductors compounds (HTSC) as well, if regarded as a simplified extension of the Emery model.

Heavy fermion materials present a great variety of ground states: antiferromagnetic (AF) (UAgCu$_4$, UCu$_7$), superconductors (CeCu$_2$Si$_2$, UPt$_3$), Fermi liquids (FL) (CeCu$_6$, CeAl$_3$) and Kondo insulators (KI) (Ce$_3$B$_4$Pt$_3$, YbB$_12$). An uniform high temperature Curie-like magnetic susceptibility, a common feature to these compounds, is related to the fact that they are composed of elements with the incomplete $f$-shells like $Ce$ and $U$. As the temperature decreases up to a certain range, the system presents a temperature independent uniform susceptibility (Pauli susceptibility) signaling the annihilation or binding of the magnetic moments of the localized $f$-states, resembling the single-impurity Kondo problem. A consistent description of the overall properties of the heavy fermions is achieved by the competition between the Kondo effect, dealing with the annihilation or binding of the localized magnetic moments, and the Ruderman Kittel Kasuya Yosida (RKKY) interaction, which favors the appearance of a magnetic ground state; thus, the Hamiltonian that describes the basic physics of the system may be a regular lattice of $f$-moments which interact with an electron gas and with themselves through these electrons as proposed by the PAM. As concerns the heavy fermion superconductivity, it is an experimental fact that the large specific heat jump at $T_c$, of the order of the normal phase specific heat, indicates that pairing takes place among the $f$-electrons and the coherent-length must be much shorter than the typical values for conventional superconductors. Furthermore, the narrow bandwidth of the $f$-electrons suggests a strong on-site Coulomb repulsion which precludes on-site pairing and may lead to non-s-wave or unconventional pairing. New results have also revealed the possibility that magnetic (mainly AF) phase may coexists with the superconductivity and that some heavy fermion compounds display pseudogap behavior at the normal phase which is a common feature of the high critical temperature superconductors.

These rich phenomena motivate us to study the superconducting phase in context of the PAM with the recently developed X-boson technique, that was applied to the PAM in the limit $U\to\infty$ and produces satisfactory results, because they are very close to those obtained by the slave boson method, which is $\Phi$– derivable and is a very good approximation at high temperature $T$. The unphysical second order phase transitions that appear in the slave boson approach when $\mu >> E_{f,j}\sigma = E_f$ at low $T$, $\mu$ being the total chemical potential and $E_f$ the energy level of the $f$-electrons,

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and also for all parameters at intermediate temperatures $T$, are then eliminated by the X-boson treatment. Coleman [15] has observed that these phase transitions are artifacts of the theory, and the advantage of the present treatment is that those spurious phase transitions do not occur. Although in the X-boson there is no relevant spatial dependence in the self-energies of theCHA, they do retain some local time dependence. In the mean-field slave boson the corresponding self-energy vanishes, showing that all the local time dependence is completely lost in the self-energies of that method. The spurious phase transition observed by the slave-boson method are absent from the X-boson description, and this result indicates that the time dynamics retained in theCHA is able to suppress those transitions [16].

In the present paper we adopt the schematic classification proposed by Varma [23] and recently reintroduced by Steglich et al. [6, 24] to describe the exemplary Ce-based compounds. It is given in terms of the dimensionless coupling constant for the exchange between the local $f$ spin and the conduction-electron spins, $g = N_F |J|$, where $N_F$ is the conduction-band density of states at the Fermi energy and $J$ is connected to the parameters of the PAM via a Schrieffer-Wolff transformation [25]. $J = 2V^2 / E_f$ when $U \to \infty$. Therefore, within the X-boson technique,

$$g = \rho_c(\mu)2V^2/|E_f|,$$  

where $\rho_c(\mu)$ is the conduction density of states at the chemical potential $\mu$, $V$ is the hybridization parameter and $E_f$ is the renormalized $E_f$ introduced by the X-boson method, as shall be explained below, and the behavior of these compounds can be qualitatively driven through this parameter: when $g > 1$, the compound under consideration presents an intermediate valence (IV) behavior while for $g < 1$ it presents heavy fermion Kondo regime (HF). There exists a critical value $g_c$, at which the Kondo and the RKKY interactions have the same strength and non Fermi-liquid (NFL) effects have been postulated for systems with $g = g_c$. For $g_c < g < 1$, the magnetic local moments do not exist at very low temperatures and the system presents a Fermi liquid behavior while for $g < g_c$ we have the local magnetic moment regime. We observe that we use the parameter $g$ to classify the regimes of the PAM in a very qualitative way. Finally, as concerns to the X-boson chain approach, its present form only includes hybridization effects to second order in $V$, therefore the RKKY effects are not taken into account and we cannot discuss non Fermi liquid behavior at the present stage of the work.

The paper is organized as follow: In Section II we introduce the main ideas of heavy fermion superconductivity, in Section III we make a brief revision of the X-boson method developed earlier [15], in Section IV we present the model, in Section V we calculate in a mean field approximation the Gorkov’s anomalous function written in Zubarev’s notation and the gap equation, in Section VI we obtain numerically the superconducting phase diagram for several hybridization parameters and we discuss the model results; finally in the Section VII we present the conclusions and the future directions of the work.

II. THE X-BOSON METHOD

The periodic Anderson model (PAM) in the limit of infinite Coulomb repulsion $U \to \infty$ is given by

$$H = \sum_{k,\sigma} \epsilon_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{j,\sigma} E_{f,j,\sigma} X_{j,\sigma,\sigma}$$
$$+ \sum_{j,\sigma} \left( V_{j,\sigma} k X_{j,0,\sigma} c_{k,\sigma} + V_{j,\sigma,0} X_{j,0,\sigma} c_{k,\sigma}^\dagger X_{j,0,\sigma} \right),$$  

where the first term is the kinetic energy of the conduction electrons ($c$-electrons), the second term describes independent localized electrons ($f$-electrons) of energy $E_f$, and the last term is the hybridization Hamiltonian giving the interaction between the $c$-electrons and the $f$-electrons.

We employ the Hubbard operators [28] to project the double occupation state $|j, 2\rangle$ with two local electrons out of the space of local states at site $j$, as the X-Hubbard operators do not satisfy the usual commutation relations, the diagrammatic methods based on Wick’s theorem are not applicable, one has to use product rules instead:

$$X_{j,ab} X_{j,cd} = \delta_{bc} X_{j,ad}.$$  

The identity decomposition in the reduced space of local states at a site $j$ is then

$$X_{j,00} + X_{j,\sigma\sigma} + X_{j,\sigma\sigma} = I_j,$$  

where $I = \delta - \sigma$, and the three $X_{j,aa}$ are the projectors into $|j,a\rangle$. Because of the translational invariance, the occupation numbers $n_{j,aa} = \langle X_{j,aa}\rangle$ satisfy $n_{j,aa} = n_a$ (independent of $j$), and from Eq. (4) we obtain the “completeness” relation

$$n_0 + n_\sigma + n_{\sigma\sigma} = 1.$$  

In Coleman’s “slave boson” method [17–27], the Hubbard X operators are written as a product of ordinary bosons and fermions: $X_{j,00} \to b_j^\dagger b_j$, $X_{j,\sigma\sigma} \to b_j^\dagger f_j \sigma$, $X_{j,\sigma\sigma} \to f_j \sigma^\dagger b_j$, and a condition, that is equivalent to Eq. (4), is imposed to avoid states with two electrons at each site $j$. In the mean field approximation $b_j^\dagger \leftrightarrow b_j^\dagger = \sqrt{2}$ and the method of Lagrangian multipliers is employed to minimize the free energy subject to that condition. The problem is then reduced to an uncorrelated Anderson lattice with renormalized hybridization $V \to \sqrt{2}V$ and $f$ level $\epsilon_f \to \epsilon_f + \lambda$, and the conservation of probability in the space of local states is automatically satisfied because they are described by Fermi operators.

The approximate GF obtained by the cumulant expansion [28, 30] do not usually conserve probability (i.e. they
do not satisfy Eq. (5), and the procedure we adopt to recover this property in the X-boson method is to introduce

\[ R \equiv < X_{j,00} > = < b_j^\dagger b_j > , \]  

(6)
as variational parameter, and to modify the approximate GF so that it minimizes an adequate thermodynamic potential while being forced to satisfy Eq. (5). To this purpose we add to Eq. (2) the product of each Eq. (4) into a Lagrange multiplier \( \Lambda_j \), and employ this new Hamiltonian to generate the functional that shall be minimized by employing Lagrange’s method. To simplify the calculations we use a constant hybridization \( V \), as well as site independent local energies \( E_{f,j,\sigma} = E_{f,\sigma} \) and Lagrange parameters \( \Lambda_j = \Lambda \). We then obtain a new Hamiltonian with the same form of Eq. (2):

\[
H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \sum_{\mathbf{j},\sigma} \tilde{E}_{f,\sigma} X_{\mathbf{j},\sigma}\sigma \\
+ V \sum_{\mathbf{j},\mathbf{k},\sigma} \left( X_{\mathbf{j},0,\sigma} c_{\mathbf{k},\sigma} + c_{\mathbf{k},\sigma}^\dagger X_{\mathbf{j},\sigma}\sigma \right) \\
+ N_s \Lambda (R - 1),
\]

(7)
but with renormalized localized energies

\[
\tilde{E}_{f,\sigma} = \epsilon_{f,\sigma} + \Lambda. 
\]

(8)
The parameter

\[
R = 1 - \sum_{\sigma} < X_{\sigma}\sigma > 
\]

(9)
is now varied independently to minimize the thermodynamic potential, choosing \( \Lambda \) so that Eq. (5) be satisfied. While at this stage the electrons in the slave boson Hamiltonian have lost all the correlations, the Eq. (7) is still in the projected space and it is not necessary to force the correlations with an extra condition. On the other hand we do not have an exact solution for this new problem, and we then consider the most simple approximation obtained within the cumulant formalism, the Chain approximation (CHA) \[13, 21\]. The need of minimizing a thermodynamic potential arises because the completeness relation is not automatically satisfied for approximate cumulant solutions, and although the two procedures are formally very similar, they have a rather different meaning.

III. THE SUPERCONDUCTIVITY MODEL

In order to have a superconducting state, we add to the usual PAM given by Eq. (2) an effective interaction \( H_W \) among the heavy \( f \)-electrons,

\[
H_W = \frac{1}{2} \sum_{\langle i,j\rangle,\sigma,\sigma'} W_{i,j} X_{i,\sigma}\sigma X_{j,\sigma'\sigma'},
\]

(10)
where

\[
X_{i,\sigma}\sigma = X^\dagger_{i,0}\sigma X_{i,\sigma}\sigma.
\]

(11)
The term \( H_W \) describes an effective attraction between two neighboring \( f \) sites \( (W_{i,j} < 0) \), which is responsible for the heavy fermion superconductivity in the model. We only consider the superconductivity arising from \( f \)-electron pairing. As the conduction electrons exist at the Fermi surface the possibility of formation of \( c-c \) Cooper pairs cannot be excluded \[1\], but we do not consider these pairs here. Indeed, there are experimental evidence that pairing occurs between the heavy \( f \)-electrons. In this framework the correlated \( f \)-electrons hybridize with the conduction band, and interact via a non-retarded nearest neighbor attraction. The interaction is proposed on a phenomenological basis and its microscopic origin is not investigated. The same approach was also used by Romano et. al. \[2\], Zielinski and Matlak \[3\], and Araújo et. al. \[4\]. Moreover, Tachiki and Maekawa \[22\] studied the superconductivity in the Periodic Anderson Model with a small dispersion of the \( f \)-band in the heavy fermion state and they have concluded that pairing between \( f \)-electrons are responsible for superconductivity, rather than between the conduction electrons.

It is more interesting to work with the Fourier transform of the Hubbard operators

\[
X_{i,0}\sigma = \frac{1}{\sqrt{N}} \sum_l e^{i \mathbf{k}_l \cdot \mathbf{R}_l} X_{\mathbf{k},0}\sigma,
\]

(12)
\[
X^\dagger_{i,0}\sigma = \frac{1}{\sqrt{N}} \sum_l e^{-i \mathbf{k}_l \cdot \mathbf{R}_l} X^\dagger_{\mathbf{k},0}\sigma,
\]

(13)
where \( N \) is the number of the lattice sites. Considering Cooper pairing only in the singlet channel, the model defined by Eqs. (7) and (10) in the momentum space can be written as

\[
H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} \tilde{E}_{f}\mathbf{k}\sigma X_{\mathbf{k},\sigma}\sigma \\
+ \sum_{\mathbf{k},\sigma} V(X^\dagger_{\mathbf{k},0}\sigma c_{\mathbf{k},\sigma} + c_{\mathbf{k},\sigma}^\dagger X_{\mathbf{k},0}\sigma) \\
+ \sum_{\mathbf{k},\mathbf{k}'} W_{\mathbf{k},\mathbf{k}'} b^\dagger_{\mathbf{k}} b_{\mathbf{k}'} \\
+ N_s \Lambda (R - 1),
\]

(14)
where

\[
b^\dagger_{\mathbf{k}} = X^\dagger_{\mathbf{k},0}\sigma X^\dagger_{-\mathbf{k},0}\sigma
\]

(15)
and

\[
W_{\mathbf{k},\mathbf{k}'} = W \sum_\delta e^{i \mathbf{k} \cdot \mathbf{k}' \cdot \delta},
\]

(16)
where the summation over \( \delta \) runs over the nearest neighbors and we consider the hybridization constant \( V = V_{\mathbf{j},\sigma,\mathbf{k}} \).
The superconducting term in the right hand side of the Eq. (14) is responsible for the Cooper pair formation. The parameter $W$ is negative, where $W_{k\k'} = W_{\eta_k \eta_{k'}}$ and $\eta_k$ is assigned according to the symmetry of the superconducting order parameter. 

For most of the superconducting materials the charge carriers can couple in the $s$, $p$, $d$, etc. channels. For heavy fermions, although both the crystalline anisotropy and spin-orbit interaction are important [31], and the order parameter should be written in terms of a complete set of basis-function multiplets for the appropriate symmetries. However, as a first study of the effect of the hybridization over the superconducting phase diagram and how the hybridization affects $T_c$, we only consider the case of an isotropic $s$-wave superconducting gap in our numerical calculations.

IV. THE GREEN’S FUNCTIONS

Since our model Hamiltonian, Eq. (14), does not depend explicitly on the time, the corresponding Green’s functions GF are only functions of the difference $t - t' = \tau$. In the aforementioned Zubarev’s notation [32] the GF can be written as $G_{\sigma}^{\tau}(k, \tau) = \theta(\tau)(c_{k,\sigma}(\tau)c_{k,\sigma}(0)) - \theta(-\tau)(c_{k,\sigma}^\dagger(0)c_{k,\sigma}(\tau))$ for this fermionic system, where the operator $c_{k,\sigma}(t)$ is in the Heisenberg representation. Formally, besides the $(r, t)$ representation of the GF, the model admits the $(r, \omega)$ representation defined by the Fourier transform $\tilde{G}_{\omega}(r, \omega)$. Hence the $(k, \omega)$ representation is defined by the discrete Fourier transform

$$G_{\omega}(k, \omega) = \frac{1}{N} \sum_k G_{\omega}(k, \omega)e^{ikr},$$

which could be simply denoted by

$$G_{\sigma}(k, \omega) \equiv \langle c_{k,\sigma}, c_{k,\sigma}^\dagger \rangle \omega.$$

Analogously, the Gorkov’s anomalous function is defined by

$$\mathcal{F}_{\sigma}(k, \omega) \equiv \langle X_{k,0\sigma}, X_{-k,0\sigma}^\dagger \rangle \omega.$$

In a similar way one defines

$$G^{\sigma}(k, \omega) \equiv \langle X_{-k,0\sigma}, X_{k,0\sigma}^\dagger \rangle \omega,$$

$$G^{\sigma}(k, \omega) \equiv \langle X_{k,0\sigma}, X_{-k,0\sigma}^\dagger \rangle \omega,$$

$$\mathcal{F}_{\sigma}(k, \omega) \equiv \langle X_{k,0\sigma}, X_{-k,0\sigma}^\dagger \rangle \omega.$$

From the above definitions, one can show that $\mathcal{F}_{\sigma}(k, \omega)$ satisfies the equation of motion

$$i\omega \mathcal{F}_{\sigma}(k, \omega) = \langle Z_{k,\sigma}, X_{-k,0\sigma}^\dagger \rangle \omega,$$

where $Z_{k,\sigma} = [X_{k,\sigma}^\dagger, H]$. We employ the equation of motion method and we obtain a chain of equations that shall be broken by a mean-field approximation and further calculations furnish the quasi-particles spectrum. Therefore, the final system of equations to be solved is

$$(i\omega_n - \epsilon_k)g^{\sigma}(k, \omega_n) = Vg^{\sigma}(k, \omega_n),$$

$$(i\omega_n + \epsilon_k)g^{\sigma}(k, \omega_n) = -Vg^{\sigma}(k, \omega_n),$$

$$(i\omega_n + \tilde{E}_f)g^{\sigma}(k, \omega_n) = -V\sigma g^{\sigma}(k, \omega_n) + \Delta_1^{\sigma}\sigma \tilde{g}^{\sigma}(k, \omega_n),$$

$$(i\omega_n - \tilde{E}_f)g^{\sigma}(k, \omega_n) = V\sigma g^{\sigma}(k, \omega_n) + \Delta_2^{\sigma}g^{\sigma}(k, \omega_n) + D_{\sigma},$$

where $\Delta_k$ is the superconducting gap defined by

$$\Delta_k = \sum_{k\k'} W_{k\k'} \langle b^\dagger_{k\k'} \rangle$$

and the quantity $D_{\sigma}$ is given by

$$D_{\sigma} = \langle X_{00} + X_{\sigma\sigma} \rangle.$$

In the X-boson method employed here all the correlations are included in the quantity $D_{\sigma}$ and, indeed, making $D_{\sigma} = 1$ the above system of equations with the mapping $V \leftrightarrow \sqrt{V}$ and $W \leftrightarrow s^2W$ is identical to the slave boson’s result given in Appendix A similar to those obtained by Araújo et al. [3]. Further, in the absence of the hybridization term the $f$-band and the conduction band decouples and solving the remaining system of equations for the $f$-band one formally recover the BCS result though with a distinct physical meaning, here the energy $E^f_\sigma$ assumes a constant value and the strong correlations presented are taken into consideration via the parameter $D_{\sigma}$.

Considering the paramagnetic case ($D_{\sigma} = D_{\sigma\sigma}$) and solving Eqs. (24) – (27) for the anomalous GF one find

$$\mathcal{F}_{f\sigma}(k, \omega) = -\sum_{j=1}^{4} \frac{B_{ij}}{\omega_n - \omega_j},$$

where

$$B_{2} = \Delta_1^{\sigma} D_{\sigma}^2 (\omega^2 - \epsilon_k^2),$$

$$B_{4} = \Delta_2^{\sigma} D_{\sigma}^2 (\omega^2 - \epsilon_k^2),$$

with $B_1 = -B_2$ and $B_3 = -B_4$. The four poles representing the above quasi-particle (QP) excitations given by

$$\omega_2 = \sqrt{\frac{\alpha - \frac{1}{2} \sqrt{\alpha^2 - 4\beta}}{2}},$$

$$\omega_4 = \sqrt{\frac{\alpha + \frac{1}{2} \sqrt{\alpha^2 - 4\beta}}{2}},$$

and
\[ \omega_1 = -\omega_2 \text{ and } \omega_3 = \omega_4, \text{ where} \]
\[ \alpha = \Delta_k^2 + 2V^2D_\sigma + \epsilon_k^2 + \tilde{E}_F^2, \]  \tag{35}
and
\[ \beta = V^4D_\sigma^2 - 2V^2D_\sigma \epsilon_k \tilde{E}_F + \Delta_k^2 \epsilon_k^2 + \epsilon_k^2 \tilde{E}_F^2. \]  \tag{36}

Now we shall treat the hybridization and the superconducting terms \((H_V \text{ and } H_W \text{ respectively}) \) in the model Hamiltonian given by Eq. (14) as external perturbations and calculate the thermodynamic potential \(\Omega\) through the \(\lambda\) parameter integration \[32\]. One should minimize the free energy in order to find the Lagrange multiplier in the former Hamiltonian. But first we will focus on the contribution of \(H_W\) only, which is the only term responsible for the Cooper pair formation. Our discussion is analogous to imposing \(V = 0\) in our model. Under this constraint the difference of thermodynamic potential in the superconductor and normal states \(\Omega_s - \Omega_n\) is
\[ \Omega_s - \Omega_n = \int_0^1 d\lambda \langle H_W' \rangle, \]  \tag{37}
where
\[ H_W' = \sum_{k,k'} W_{kk'}b_k^\dagger b_{k'}. \]  \tag{38}
By a variable transformation the above difference defined by Eq. \[28\] is rewritten as \[\int_0^W \frac{dW'}{W'} \langle H_{W'} \rangle\]. In a Hartree-Fock approximation the average \(\langle H_{W}' \rangle\) can be “factorized” and \[\sum_k \eta_{kk'} \epsilon_{k'} = \Delta_k/W\] according to Eq. \[28\]. Hence Eq. \[27\] becomes
\[ \Omega_s - \Omega_n = \sum_k \int_0^W \frac{dW'}{W} \Delta_k b_k^\dagger b_k^\dagger. \]  \tag{39}
For an isotropic \(s\)-wave superconducting gap in the absence of an external magnetic field \(\Delta_k = \Delta = \Delta^*\) and \(\eta_k = 1\). Also notice that \(W^{-2} = -dW^{-1}/dW\) and after another variable transformation we get that
\[ \Omega_s - \Omega_n = -\int_0^\Delta d\Delta' \Delta' d\frac{d}{d\Delta'} \left( \frac{1}{W} \right), \]  \tag{40}
which is the same functional result given by Fetter and Walecka \[31\]. Notice that at temperatures higher than or equal to the superconducting critical temperature \(T \geq T_c\) the superconducting order parameter is assumed, as in the BCS theory, to be zero. Therefore \(\Omega_s - \Omega_n = 0\) at \(T = T_c\) and henceforth we shall disregard the contribution of \(H_W\) in order to calculate the Lagrange multiplier for the superconducting phase diagram and only consider the hybridization term contribution of the model Hamiltonian as an external perturbation. Further, for \(T \geq T_c\) the system is in the normal state and the GFs yields to the previous result obtained in the CHA of the PAM, obtained by taking the infinite sum of all diagrams that contains only second order cumulants terms. The GFs of the CHA have functional form which are close to the uncorrelated ones \((U = 0)\), but they cannot be reduced to them by any change of scale, except for \(D_\sigma = 1\), when we recover the slave-boson GFs if we put \(V \rightarrow \sqrt{2}V\). Nevertheless, notice that although the condition that forces completeness in the CHA is identical to that employed in the slave-boson method to force \(n_\uparrow \leq 1\), it has a rather different origin, being only a consequence of using a reduced set of diagrams in the perturbative expansion, and the departures from completeness are usually very moderate. In the formalism described here, it is this essential difference between the two methods that eliminates the spurious phase transition appearing in the slave-boson method. Imposing \(\Delta = 0\) at the system of equations given by Eqs. \[24\]-\[27\] one find that
\[ G^{\text{ff}}_\sigma(-k,\omega_n)|_{T=T_c} = \frac{A}{i\omega_n - \omega_+} + \frac{B}{i\omega_n - \omega_-}, \]  \tag{41}
where the poles \(\omega_+, \omega_-\) are
\[ \omega_{\pm} = \left( \epsilon_k + \tilde{E}_f \right) \pm \sqrt{\left( \epsilon_k - \tilde{E}_f \right)^2 + 4V^2D_\sigma}, \]  \tag{42}
and the above coefficients are
\[ A = D_\sigma \frac{\epsilon_k - \omega_+}{\omega_+ - \omega_-}, \]  \tag{43}
\[ B = D_\sigma \frac{\omega_- - \epsilon_k}{\omega_+ - \omega_-}. \]  \tag{44}
Also notice that
\[ (i\omega_n - \epsilon_k)V^{-1}G^{\text{ff}}_\sigma(-k,\omega_n) = G^{\text{ff}}_\sigma(-k,\omega_n) \]  \tag{45}
and one get that
\[ G^{\text{ff}}_\sigma(-k,\omega_n) = \frac{V D_\sigma}{\omega_+ - \omega_-} \times \left[ \frac{1}{i\omega_n - \omega_+} - \frac{1}{i\omega_n - \omega_-} \right]. \]  \tag{46}
Moreover,
\[ G^{\text{sc}}_\sigma(k,\omega_n) = \frac{1}{(i\omega_n - \tilde{E}_f)(i\omega_n - \epsilon_k) - V^2D_\sigma}. \]  \tag{47}
Since the thermodynamic potential was already calculated in detail by one of us and collaborators elsewhere \[15\] treating the hybridization Hamiltonian \(H_V\) as an external perturbation, we shall just briefly outline its solution below. According to the \(\lambda\) parameter integration
\[ \Omega = \Omega_0 + N_s \Lambda (R - 1) + \int_0^1 d\lambda \langle H_V(\lambda) \rangle, \]  \tag{48}
where, regarding Eq. \[15\], the average \(\langle H_V(\lambda) \rangle\) is
\[ \langle H_V(\lambda) \rangle = 4\lambda V^2D_\sigma \frac{n_F(\omega_+) - n_F(\omega_-)}{\omega_+ - \omega_-}. \]  \tag{49}
and \( n_F \) is the Fermi function. At the above Eq. (17), the quantity \( \Omega_0 \) is the thermodynamic potential associated to the unperturbed part of the Hamiltonian at \( T = T_c \) and \( N_s \Lambda (R - 1) \) was already introduced to impose the completeness relation (4). Minimizing \( \Omega \) with respect to \( R \), we get

\[
\Lambda = \frac{1}{N_s} \sum \n\sum V^2 - \frac{n_F(\omega_n) - n_F(\omega_{n+1})}{\sqrt{(\epsilon_k - E_f)^2 + 4V^2D_s}}. \tag{49}
\]

Finally, the average \( \langle b_k^\dagger \rangle \) can be found from Eq. (30) and the self-consistent gap equation is obtained according to the definition in Eq. (4). Notice that Eq. (50) is identical to Eq. (49), (56) and (57) and provide the superconducting phase diagram.

In the next section we calculate the superconducting phase diagram for \( T_c \) as a function of the total electron number \( N_t = N_f + N_c \), where these occupation numbers are calculated for the Green’s functions given by Eqs. (31), (36) and (40) considering a constant conduction density of states as defined in Eq. (55).

The results are

\[
G^{ff}(\omega) = -\frac{D_s}{\omega - E_f} - \left( \frac{D_sV}{\omega - E_f} \right)^2 \times \log \left[ \frac{(\omega - \omega_1) (\omega - \omega'_1)}{(\omega - \omega_2) (\omega - \omega'_2)} \right], \tag{58}
\]

\[
G^{cc}(\omega) = -\frac{1}{2}\beta - \frac{V D_s}{\omega - E_f} \log \left[ \frac{(\omega - \omega_1) (\omega - \omega'_1)}{(\omega - \omega_2) (\omega - \omega'_2)} \right], \tag{59}
\]

\[
G^{fc}(\omega) = -\frac{V D_s}{\omega - E_f} \log \left[ \frac{(\omega - \omega_1) (\omega - \omega'_1)}{(\omega - \omega_2) (\omega - \omega'_2)} \right], \tag{60}
\]

where

\[
w_1^2 = \frac{1}{2} \left[ (E_f - D_+) + \sqrt{(E_f - D_+)^2 + 4D_sV^2} \right], \tag{61}
\]

\[
w_2^2 = \frac{1}{2} \left[ (E_f - D_-) + \sqrt{(E_f - D_-)^2 + 4D_sV^2} \right], \tag{62}
\]

with \( D_\pm = D \pm \mu \).

Also,

\[
N_f = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \, n_F(\omega) \Im \left[ G^{ff}(\omega) \right], \tag{64}
\]

\[
N_c = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \, n_F(\omega) \Im \left[ G^{cc}(\omega) \right], \tag{65}
\]

where \( n_F \) is the Fermi function.

V. RESULTS AND DISCUSSION

In this section we solve the self-consistent system of equations Eqs. (19), (20) and (27) for \( T_c \). All the
energies are expressed in units of $D$, numerical calculation are performed making $E_f = -0.15$ and the superconducting interaction parameter is $W = -0.10$.

In Fig. 1 we present the superconducting phase diagram for $T_c$ as a function of $N_t$, where each $N_t$ corresponds to a distinct sample with a certain stoichiometric composition and the chemical potential is found self-consistently constrained to the furnished $N_t$. The superconducting interaction $W$ is kept constant for every set of parameters, since its main effect is simply to raise the $T_c$ value.

Our results for the superconducting phase diagram show that the existence of the superconductivity is constrained to the vicinity of a range of occupations where the values of the $f$-band densities of states $\rho_f(\mu)$ at $\omega = \mu$ are sufficiently high. Moreover, high values of $\rho_f(\mu)$ usually implicate higher values of $T_c$, what suggests that the Kondo behavior of the system favors superconductivity in the X-boson approach. Nevertheless, the reduction of the hybridization parameter $V$ causes a general increasing on the maximum of the superconducting critical temperature $T_c$, this is due to the diminution of the charge fluctuations between the conduction and the $f$ electron states. Indeed, Fig. 2 shows the behavior of $T_c$ as a function of the hybridization $V$ in the low and high occupation regimes. As $V$ increases, the critical temperatures diminishes and at very small values of the hybridization, the critical temperatures tend to a finite value; this behavior is similar to that obtained by Araújo et. al. using the slave boson method. Note that for $N_t = 1.8$ the superconductivity phase is suppressed for the interval $V \sim [0.03, 0.06]$, which is related to the appearance of a hybridization gap in the $\rho_f(\omega)$.

Regarding the superconducting phase diagram, at low

FIG. 1: The superconducting critical temperature $T_c$ as a function of the total electron number $N_t$ for (a) $V = 0.1$, (b) $V = 0.3$, (c) $V = 0.5$ grouped in the three different regimes.

FIG. 2: The occupation numbers $N_c$ and $N_f$ as a function of $N_t$. Other parameters are the same as in Fig. 1.

FIG. 3: The critical temperature $T_c$ as a function of the hybridization $V$ for $N_t = 1.4$ and $N_t = 1.8$. Other parameters are the same as in Fig. 1.
the hybridization parameter, perconducting phase diagram systematically by varying the temperature \( T \) or the chemical potential \( \mu \) the value \( V = \sqrt{2}V = 0 \) is presently reached, leading to \( N_f \rightarrow 1 \) and the decouple of the two types of electrons, what can be interpreted as a change of phase related to a symmetry breaking of the mean-field Hamiltonian. These unphysical second-order phase transitions that appear in the slave-boson approach are artifacts of the theory, as already observed by Coleman [30], while the present X-boson treatment prevents those spurious phase transitions. Therefore, we were motivated to study the superconducting phase diagram systematically by varying the hybridization parameter \( V \) and our results provide three distinct regimes for the superconducting phase diagram as can be seen in Fig. 4. (a) for small values of \( V \) the superconductivity shows up in a broad interval of occupations and the function \( T_c(N_f) \) have a single maximum for our numerical data; (b) as \( V \) is increased, \( V \sim 0.2 - 0.4 \), the range of occupations where there is superconductivity is narrowed and shifted to higher values. The function \( T_c(N_f) \) presents two local maxima and between them the superconductivity is suppressed, which is related to the appearance of a hybridization gap in the \( \rho_f(\omega) \) and the system becomes an insulator in this region; (c) as \( V \) increases even more, \( V \sim 0.4 - 0.5 \), the superconductivity shows up in a smaller range of occupation and the superconducting region related to the first local maximum is suppressed. As the total occupation is raised, the system crosses an insulating region until it becomes superconducting. For larger values of the hybridization parameter \( V > 0.5 \) the superconductivity is completely suppressed.

According to our data for the superconducting phase diagram in the first regime, the function \( T_c(N_f) \) has a single maximum, as can be seen in Fig. 4a. For this low \( V \) regime the \( f \)-band density of states is located in a narrow region of the bandwidth, since the electrons are more localized, the two peaks of the density of states are sharp and the distance between them is small, about 0.02\( D \), as can be seen in Figs. 4a-4c. Notice that in this small interval defined by the distance between peaks, the densities of states for both bands are zero and when the chemical potential lies in this hybridization gap the system presents an insulating behavior unless the conducting electrons have enough kinetic energy to tunnel through the gap. In this low hybridization regime the superconducting critical temperature is larger than the

![Figure 4](image_url)
distance between the chemical potential $\mu$ and the border band peaks, and since the average kinetic energy of the conducting electrons should be proportional to $T_c$ for a given occupation in the phase diagram, the conducting electrons have enough energy to tunnel through the hybridization gap and the system does not present an insulating behavior. Notice that $T_c$ is larger for $V = 0.1$ because the existence of the superconductivity phase is related to a high value for the $f$-band density of states at the chemical potential.

The phase diagram for the second regime is presented in Fig. 4b. The critical temperature $T_c$ is non-null only when the $f$-band density of states at the chemical potential is sufficiently high, what also indicates the range of occupations where there is superconductivity. Notice the two local maxima for $T_c$ and the suppression of superconductivity between them when $\mu$ crosses the hybridization gap. In this region the Matsubara’s summation defined by Eq. 59 is close to zero and, hence, there is no non-null solution for $T_c$. Indeed, in Figs. 4d - 4f we present the results for the chemical potential localization, the $f$-band density of states, and the conducting electrons density of states $\rho_c(\omega)$ corresponding to different values of $N_f$. Moreover, Fig. 5 presents the behavior of the chemical potential as a function of $N_f$ for the three regimes found. Notice that there is an abrupt variation of $\mu$ when it crosses the hybridization gap, the slope is larger as the distance between peaks of the DOS is larger. Indeed, Fig. 5 shows the appearance of a hybridization gap when the chemical potential lies in a region between bands where superconductivity is suppressed because the system becomes an insulator. An analogous transition was found by Romano studying the same model taking into account $s$, $p$, $d$ anisotropic pairing and for $U = 1$, in units of $D$ for the value of $N_f$ close to the half filling. Indeed, notice that when the values of the hybridization parameter are raised the two peaks of the density of states are lowered and the distance between peaks is broadened, evidencing two main factors responsible for the appearance of an insulator region under the constraints of the furnished parameters in the X-boson approach: on one hand, when $V$ increases, the $f$-band density takes up smaller values, what causes the overall superconducting critical temperature to diminish, since $T_c$ is non-null only when the value of $\rho_f(\mu)$ is sufficiently large, indicating that the average kinetic energy of the fermions in the system is decreased; on the other hand, since the distance between peaks are broadened, the demand of kinetic energy required by the conducting electrons to tunnel through the hybridization gap becomes larger. Therefore, as the total occupation is increased the chemical potential roughly also increases, as seen in Fig. 4 and when it crosses the hybridization gap, the conducting electrons do not have the required energy to tunnel through the gap and the system becomes an insulator. Again, this result would not be obtained by the mean-field slave boson method, since the approach breaks down in the Kondo region when $N_f \to 1$ and the upper band cannot be reached.

For the third regime, superconductivity is constrained to a small range of occupation, as can be seen in Fig. 4c. This regime is characterized by high values of the hybridization parameter and the superconducting region, related to the first local maximum of $T_c$, is suppressed. Therefore, as the total occupation is raised, or charge carriers are added to the $f$-band, the system suffers a insulator-superconductor transition. Again, our results for the superconducting phase diagram can be inferred from the behavior of the chemical potential compared to several plots of the the $f$-band density of states. Indeed, as can be seen in Figs. 4g-4i, the $f$-band DOS is asymmetric and the first peak, which is related to the first local maximum of $T_c$, is smaller; hence, for this range of occupations the values of $\rho_f(\mu)$ are not sufficiently large and the superconductivity is suppressed.

It is interesting to compare the results obtained by the X-boson approach with those obtained by the slave boson approach (see Appendix A): first note that while the effective superconducting interaction $W$ is mapped according to $W \to D_x^2 W$ for the X-boson method, the effective $W$ for the slave boson method is $W \to z^2 W$, see Appendix A. Note that $D_x$ is a bounded quantity varying from 1 to 0.5 as the $f$-band occupation raises, while $z \to 0$ as $N_f \to 1$ and the main effect of the $z^2 W$ interaction is to cause a general reduction of $T_c$ for the occupations where the superconductivity exists. Hence, only for a large value of the $W$ parameter we could find a value for $T_c$ in the slave boson method which is comparable to those obtained by the X-boson approach, what means...
that the slave boson method requires greater values of $W$ to produce the same critical temperatures reached by the X-boson method, see Fig. 6. Furthermore, Fig. 6a presents the superconducting phase diagram for $T_c$ as a function of $N_l$ for $V = 0.2$ and $W = -0.5$. Note that as $N_l$ increases, the chemical potential also increases, but $z$, which is essentially the expectation value of the $f$-holes, tends to zero (Fig. 6b) causing $T_c$ to be null before $\mu > \tilde{E}_f$ (Fig. 6c).

Finally, in Fig. 7 we show the parameter $g$ defined by the Eq. 1 as a function of $N_l$ for the three regimes. As can be seen in Fig. 7 according to the criteria established in [6, 24], as $N_l$ increases we recover the three characteristic regimes of the PAM: Kondo, IV and magnetic; the same cannot be found for the slave-boson treatment, since it breaks down when $N_l \to 1$. Also notice that the criteria is consistent to the picture that as $\mu$ approaches $E_f$ within an interval of width $\Delta_A \propto V^2$, there exists the possibility of charge fluctuations between the bands. For $V = 0.5$, the superconductivity only exists for a range of $N_l$ where the system presents a IV behavior ($g > 1$). As the value of the hybridization is lowered, we prevent the possibility of charge fluctuation between bands for broader ranges of $N_l$ and the superconductivity arises even in the regions where the system presents Kondo or magnetic behaviors. Since high values of $\rho_f(\mu)$ usually imply in higher values of $T_c$, the X-boson approach favors the superconductivity around the Kondo resonance. Nevertheless, as $\mu$ crosses the hybridization gap, when the chemical potential lies in the region between the peaks of the density of states, the quantity $\rho_c(\mu) \to 0$, and one gets that $g = 0$, since it is proportional to the $c$-band density of states at the chemical potential and nothing can be inferred about the magnetic order within the system. Moreover, as $N_l \to 1$, the parameter $g$ decreases. Indeed, since $T_{RKKY} \sim g^2$ and $T_K \propto e^{-1/g}$ [6, 24], when $g \ll 1$ one should expect that the RKKY interaction, which scales to $k_BT_{RKKY}$, to be much larger than $k_BT_K$, suggesting that the magnetic ordering at $T_{RKKY}$ pre-empts Kondo singlet formation, and the system might go from a FL paramagnetic state to an RKKY magnetic phase with well-localized moments according to the established criteria.

VI. CONCLUSIONS

In conclusion, in this paper we studied within the X-boson approach the paramagnetic case of the PAM with a phenomenological superconducting term and we obtained the phase diagram of the model. Although high values of $\rho_f(\mu)$ usually imply higher values of $T_c$, what indicates that the X-boson approach favors superconductivity around the Kondo resonance, superconductivity was found both for configurations where the system presented IV and HF behavior. This behavior is in agreement to experimental results, since superconductivity was found both in heavy fermion materials as well as in intermediate valence compounds [57, 58]. Moreover, we show that higher values of the hybridization parameter implies in lower values associated to the maximum of the superconducting critical temperature, indicating that the real charge exchange between bands tends to destabilizes the Cooper pairing, in agreement to the previous results obtained by the slave-boson approach [3] and by
perturbative approach \[2\]. Furthermore, as the total occupation is raised and for larger \(V\), the system presents a superconductor-insulator transition, which is related to the appearance of a hybridization gap that cannot be obtained by the slave-boson method, which breaks down in this region. These results could be experimentally tested since the hybridization coupling \(V\) can be increased by an applied external pressure.

Also, the detailed discussion of the magnetic solutions of the model within the X-boson approach, the possibility of coexistence between superconductivity and magnetic order and even how the different symmetries of the superconducting order parameter can alter the results obtained in the present paper will be subject of investigation in future works.

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**APPENDIX A: SLAVE BOSON APPROACH**

We apply the Coleman’s “slave boson” method \[17\] described in Section 2 to the Hubbard operators in the original Hamiltonian given in Eq. 2 plus the term \(\sum_{k,k'} W_{k,k'} b_k^\dagger b_{k'}\), which is responsible for the Cooper pair formation in the singlet state. Here we only assume a constant hybridization \(V\), as well as site independent local energies \(E_{f,j,\sigma} = E_{f,\sigma}\). Also, we are constrained to the subspace where the identity \(I = b^\dagger b + \sum_{\sigma} f_{\sigma}^\dagger f_{\sigma}\) is preserved. Therefore, the operator \(Q \equiv \Lambda \left( z + \sum_{k,\sigma} f_{k,\sigma}^\dagger f_{k,\sigma} - 1 \right)\) is added to the mean-field Hamiltonian rewritten in the slave-boson’s representation and the parameters \(z\) and \(\Lambda\) are determined by minimization of the free energy. In terms of this new representation the model Hamiltonian becomes

\[
H = \sum_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma} \tilde{E}_f f_{k,\sigma}^\dagger f_{k,\sigma} + \sum_{k,\sigma} \sqrt{z} V (c_{k,\sigma}, f_{k,\sigma} + c_{k,\sigma}^\dagger f_{k,\sigma}^\dagger) + \sum_{k, k'} z^2 W_{k,k'} b_k^\dagger b_{k'} + \Lambda (z - 1),
\]

where the localized \(f\)-energy is renormalized by \(\tilde{E}_f = E_f + \Lambda\), and the operator \(b_k^\dagger\) is given by \(b_k^\dagger = f_{k,\uparrow}^\dagger f_{-k,\downarrow}^\dagger\).

Finally, in a mean-field approximation we find

\[
\begin{align*}
(i\omega_n - \epsilon_k) G_{\sigma}^{\omega f} (-k, \omega_n) &= V \sqrt{z} G_{\sigma}^{\omega f} (-k, \omega_n), \\
(i\omega_n + \epsilon_k) F_{\sigma, f,j} (k, \omega_n) &= -V \sqrt{z} F_{\sigma, f,j} (k, \omega_n), \\
(i\omega_n + \tilde{E}_f) F_{\sigma, f,j} (k, \omega_n) &= -V \sqrt{z} F_{\sigma, f,j} (k, \omega_n) + z^2 \Delta k^\ast (k) G_{\sigma}^{\omega f} (-k, \omega_n), \\
(i\omega_n - \tilde{E}_f) G_{\sigma}^{\omega f} (-k, \omega_n) &= V \sqrt{z} G_{\sigma}^{\omega f} (-k, \omega_n) + z^2 \Delta k F_{\sigma, f,j} (k, \omega_n) + 1,
\end{align*}
\]

where the superconducting gap was already defined in Eq. 28. Also note that the above system of equations with the mapping \(D_{\sigma} = 1\), \(V \leftrightarrow \sqrt{z} V\) and \(W \leftrightarrow z^2 W\) is identical to the X-boson’s result.

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