Heavy fermion $d$ wave superconductivity: a X-boson approach

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Abstract

From 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, we compare the obtained superconducting phase diagram of a two dimensional $d$-wave superconductor with the results obtained for an isotropic $s$-wave superconductor employing the X-boson method.

Key words: X-boson method, superconductivity phase diagram, pairing symmetries

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1. Introduction

Recently, we have used the X-boson method \cite{1} to study the superconducting phase diagram of the PAM in the $U \to \infty$, where $U$ is the on-site Coulomb repulsion, in the presence of an attractive interaction between the localized $f$-electrons,

\begin{equation}
H = \sum_{k,\sigma} \epsilon_{k,\sigma} c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} E_f X_{k,\sigma}\sigma
+ \sum_{k,\sigma} V(X^\dagger_{k,0\sigma} c_{k,\sigma} + c^\dagger_{k,\sigma} X_{k,0\sigma})
+ \sum_{k,k'} W_{k,k'} b^\dagger_k b_{k'} ,
\end{equation}

where we only considered site independent local energies $E_{f,j,\sigma} = E_{f,\sigma}$ and a constant hybridization $V = V_{j,\sigma,k}$. The operator $b^\dagger_k = X^\dagger_{k,0\sigma} X^\dagger_{-k,0\sigma}$ creates Cooper pairs, where $X_{k,\sigma\sigma'}$ is the Hubbard operator. We have shown \cite{2} that the existence of superconductivity is constrained to a region where the $f$-band densities of states $\rho_f(\omega)$ at $\omega = \mu$ is sufficiently high. A high $\rho_f(\mu)$ usually implicates higher values of $T_c$, what suggests that the Kondo behavior of the system favors superconductivity in the X-boson approach. Nevertheless, as charge carriers are added to the system the superconductivity was found both for configurations where the system presented intermediate valence (IV) and heavy fermion (HF) behavior and we have recovered the three characteristic regimes of the PAM: Kondo, IV and magnetic. This behavior which cannot be found for the same model by the slave-boson treatment \cite{3}, since it breaks down when the $f$-occupation number $N_f \to 1$.

Despite the fact that the model was primarily designed to the study of the heavy fermion compounds, theoretical descriptions of the superconducting phases based on two-band models have application for a large variety of systems and the model could fit into the description of the high temperature superconductors compounds (HTSC) \cite{4} or into the new two-band superconductor MgB$_2$. Meanwhile, unconventional superconductors may exhibit different pair symmetries. For instance, HTSC cuprates appears to present $d_{x^2-y^2}$ superconductivity for some compounds and $s$-wave for others while for the HF compounds the crystallographic anisotropies and strong spin-orbit coupling make the task of determining the pair...
symmetry very difficult, although $d$-wave model is still one of the leading candidates to describe superconductivity in UPt$_3$ [5].

In this paper we employ the X-boson approach to compare the results for the superconducting phase diagram of an isotropic $s$-wave superconductor with the results provided by a $d_{x^2-y^2}$ superconductor.

2. The Method

The X-boson approach consists of introducing the variational parameter $R = 1 - \sum \sigma < X_{\sigma\sigma} >$, which modifies the Green’s functions (GF) so that it minimizes an adequate thermodynamic potential while being forced to satisfy the “completeness” relation $n_0 + n_\sigma + n_{\bar{\sigma}} = 1$, where $n_{j,\sigma} = < X_{j,\sigma\sigma} >$. To this purpose we added to the model the product of each “completeness” relation into a Lagrange multiplier $\Lambda_j$, and use this new Hamiltonian to generate the functional that shall be minimized by employing the Lagrange’s method.

At the critical temperature the Green’s functions yields to the previous result found in the chain approximation of the PAM, [6] but now with the localized energy levels $E_f$ and $D_\sigma = R + n_\sigma$ renormalized, and we solve the mean-field superconducting gap equation [2] at $T = T_c$ constrained to the “completeness” relation above. For the two dimensional $d_{x^2-y^2}$ superconductor we use the tight-binding band dispersion $\epsilon(k) = -2t \sum_{x,y} \cos(k_x) + \cos(k_y)$ and an attractive interaction with a $\cos(k_x) - \cos(k_y)$ dependence in $k$-space leads to the same superconducting gap symmetry. On the other hand, the superconducting phase diagram for the $s$-wave isotropic gap is obtained using a constant conduction density of states, $\rho(\epsilon_c) = 1/2D$, only defined for the interval $-D \leq \epsilon_c - \mu \leq D$. We make $E_f = -0.15$, $V = 0.3$ and the superconducting interaction $W = -0.20$ in units of the half-bandwidth $D$ or the hopping parameter $t$. Finally, the total electron number $N_t = N_f + N_c$, is kept constant and the chemical potential is calculated self-consistently while the electrons are allowed to transfer between bands.

3. Results

In Fig. 1 the superconducting phase diagrams for a 2-$d$ $d_{x^2-y^2}$ superconductor and an isotropic $s$-wave superconductor are shown. As previously obtained [2] the superconductivity is constrained to a region where $\rho_f(\mu)$ is high and our results show that $d$-wave pairing exhibits the highest $T_c$ up to occupations of about $N_t \approx 1.4$, which is in the vicinity of the Kondo regime. For higher occupations, both systems present a superconductor-insulator transition when the chemical potential $\mu$ crosses the hybridization gap, what means that $\mu$ lies in the region between the peaks of the density of states and the system presents a IV behavior. Notice that for even more higher occupations, $\mu$ reaches the upper band, what cannot be obtained by the slave-boson method, since it breaks down when $N_f \rightarrow 1$. For $N_t \gtrsim 1.4$ a crossover occurs into a regime where the isotropic $s$-wave pairing becomes the most stable for the parameters considered.

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