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ScienceDirect
Journal of Magnetism and Magnetic Materials 320 (2008) e490–e492
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Superconductivity and hybridization in a two-dimensional extended Hubbard model: Strong coupling regime

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Available online 2 March 2008

Abstract

In this work we study the effect of hybridization on the superconductivity within an attractive two-band Hubbard model. We describe the interband effects through an one body mixing term, differently from standard approaches. We consider a s-wave superconducting gap and a Hubbard-I approximation to describe the strongly correlated superconducting regime. We use Greens' function method to obtain the order parameter Δ_0 and the superconducting critical temperature T_c for various values of the hybridization strength V and the attractive potential U. The results show that for fixed values of U and V the gap raises for low temperatures and diminishes abruptly as the temperature increases. Also, T_c diminishes as V increases, and there exist a critical value V_c for which superconductivity is suppressed.

PACS: 75.30.−m; 75.30.Kz; 75.50.Ee; 77.80.−e; 77.84.Bw

Keywords: Hybridization; Superconductivity; Two-band

1. Introduction

The influence of hybridization on superconductivity has been extensively discussed in the literature [1–6]. A two-band mechanism for superconductivity was proposed by Suhl et al. [1], and Kondo [2], and later investigated by several others [3–7]. In particular, in Ref. [5] it was studied that the influence of an one body hybridization on superconductivity in two-band systems through a sp–d model of overlapping bands close to the Fermi level. The physical meaning of the hybridization is to create, in the normal state, new bands with mixed features. In Ref. [5], U was treated within the BCS theory, i.e., a weak correlation regime.

On the other hand, with the discovery of the high temperature superconductors (HTSC) a lot of new systems have been considered. In particular, the cuprates have been extensively studied, but a great number of questions related to them remain to be answered. It is recognized that the electrons which move in the CuO_2 planes are the most relevant to describe their superconducting properties [8]. In particular, there is no doubt that the d–d electrons plays a fundamental role in the superconductivity. Therefore, we adopt an extended two-band Hubbard model, with a Hubbard-I treatment [9] for the d–d attractive correlation.

In this work we calculate the superconducting gap Δ_0 and the superconducting critical temperature T_c, with both: a k-dependent hybridization $V_{\mathbf{k}}$, and a constant one, focusing in a s-wave gap symmetry. We verify that T_c is renormalized by a parameter α, which gives the ratio of the effective band masses. Moreover, there is also a critical value V_c for which T_c vanishes. Some considerations involving HTSC materials, as well as transitions metals superconductors, are also made.

2. The model

In order to study the dynamics of the carriers with correlations and the basic attractive interaction we consider

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0304-8853/$ - see front matter
doi:10.1016/j.jmmm.2008.02.165

a Hubbard Hamiltonian

$$H = \sum_{\langle\langle ij\rangle\rangle\sigma} t_{ij}^{\rm d} d_{i\sigma}^{\dagger} d_{j\sigma} + \sum_{\langle\langle ij\rangle\rangle\sigma} t_{ij}^{\rm s} c_{i\sigma}^{\dagger} c_{j\sigma} - U \sum_{\langle ij\rangle\sigma} n_{i,\sigma}^{\rm d} n_{j,-\sigma}^{\rm d} + \sum_{\langle ij\rangle\sigma} V_{ij}(c_{i\sigma}^{\dagger} d_{j\sigma} + d_{i\sigma}^{\dagger} c_{j\sigma}), \quad (1)$$

where $c_{i\sigma}^{\dagger}(c_{i\sigma})$ and $d_{i\sigma}^{\dagger}(d_{i\sigma})$ are the fermionic creation (annihilation) operator at site $\mathbf{r}_i$ for the s and d bands, respectively. The lattice parameter for the square lattice is $a = 1$, and spin $\sigma = \{\uparrow\downarrow\}$. $n_{i\sigma}^{\rm d} = d_{i\sigma}^{\dagger} d_{i\sigma}$ is the density operator, $t_{ij}^{\rm d}$ and $t_{ij}^{\rm s}$ are the hopping integrals between sites i and j nearest-neigbours and next-nearest-neigbours for the s and d electrons. U is the nearest-neigbour attractive potential between the d electrons, which can result from the elimination of the electron–phonon coupling through a canonical transformation or, as suggested by Hirsch and Scalapino [10], it may be provided by the competition between on-site and nearest-neigbours site Coulomb interaction for some range of parameters. V_{ij} is the nearest-neigbours hybridization of the two bands, which may be k-dependent, arising from a non-local character of the mixing, or a constant one, representing an average hybridization over the Brillouin zone.

Since the d-band density of states is much higher than the s one at the Fermi level, we assume throughout this work, that the superconducting pairs originate at the d-band. To obtain the superconductor order parameter, we calculate the equations of motion in the Wannier representation of the propagators $\langle\langle d_{i\sigma}; d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$, $\langle\langle d_{i,-\sigma}^{\dagger}; d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$, $\langle\langle c_{i\sigma}; d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$ and $\langle\langle c_{i,-\sigma}^{\dagger}; d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$ [5]. We calculate also the equations of motion for the newly generated Greens' functions $\langle\langle n_{j,-\sigma}^{\rm d} d_{i\sigma}; d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$ and $\langle\langle n_{j\sigma}^{\rm d} d_{i,-\sigma}^{\dagger}; d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$, considering the classical Hubbard-I approach and a mean-field treatment: $2U\sum_{jp}\langle\langle n_{p,-\sigma}^{\rm d} n_{j,-\sigma}^{\rm d} d_{i\sigma}; d_{l\sigma}^{\dagger}\rangle\rangle_{\omega} \approx \tilde{U}\sum_{p}\langle\langle n_{p,-\sigma}^{\rm d} d_{i\sigma}; d_{l\sigma}\rangle\rangle_{\omega} + 2\langle n^{\rm d}\rangle\sum_{p}\Delta_{pi}\langle\langle d_{p,-\sigma}^{\dagger}; d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$, where $\tilde{U} = 2U\langle n^{\rm d}\rangle$, and $\Delta_{ij} = U\langle d_i^{\dagger} d_{j,-\sigma}^{\dagger}\rangle$ is the superconducting order parameter. From the above relations one obtains the gap self-consistent gap equation for a s-wave symmetry

$$\Delta = \frac{1}{N_{\rm s}}\sum_{k} 2\Delta U\left[\frac{F_{1\mathbf{k}} + G_{1\mathbf{k}}\tanh(\beta E_{1\mathbf{k}}/2)}{2E_{1\mathbf{k}}(E_{1\mathbf{k}}^2 - E_{2\mathbf{k}}^2)(E_{1\mathbf{k}}^2 - E_{3\mathbf{k}}^2)}\right] + \frac{1}{N_{\rm s}}\sum_{k} 2\Delta U\left[\frac{F_{2\mathbf{k}} + G_{2\mathbf{k}}\tanh(\beta E_{2\mathbf{k}}/2)}{2E_{2\mathbf{k}}(E_{2\mathbf{k}}^2 - E_{1\mathbf{k}}^2)(E_{2\mathbf{k}}^2 - E_{3\mathbf{k}}^2)}\right] + \frac{1}{N_{\rm s}}\sum_{k} 2\Delta U\left[\frac{F_{3\mathbf{k}} + G_{3\mathbf{k}}\tanh(\beta E_{3\mathbf{k}}/2)}{2E_{3\mathbf{k}}(E_{3\mathbf{k}}^2 - E_{1\mathbf{k}}^2)(E_{3\mathbf{k}}^2 - E_{2\mathbf{k}}^2)}\right], \quad (2)$$

with

$$F_{i\mathbf{k}} = E_{i\mathbf{k}}^2[E'_{1\mathbf{k}} + E'_{2\mathbf{k}} - \varepsilon_{s\mathbf{k}}] - \varepsilon_{s\mathbf{k}} E'_{1\mathbf{k}} E'_{2\mathbf{k}}, \quad (3)$$

$$G_{i\mathbf{k}} = E_{i\mathbf{k}}[E_{i\mathbf{k}}^2 - \varepsilon_{s\mathbf{k}}[E'_{1\mathbf{k}} + E'_{2\mathbf{k}}] + E'_{1\mathbf{k}} E'_{2\mathbf{k}}], \quad (4)$$

$$E_{1\mathbf{k}} = \sqrt{-\frac{A_{\mathbf{k}}}{3} + 2\sqrt{\frac{|p_{\mathbf{k}}|}{3}}\cos\frac{\phi_{\mathbf{k}}}{3}}, \quad (5)$$

$$E_{2,3\mathbf{k}} = \sqrt{-\frac{A_{\mathbf{k}}}{3} - 2\sqrt{\frac{|p_{\mathbf{k}}|}{3}}\cos\frac{\phi_{\mathbf{k}} \pm \pi}{3}}, \quad (6)$$

$$E'_{1,2\mathbf{k}} = -\frac{\tilde{\varepsilon}_{\mathbf{k}} + \tilde{U}}{2} \pm \frac{\sqrt{(\tilde{\varepsilon}_{\mathbf{k}} + \tilde{U})^2 + 4(2\tilde{U}\varepsilon_{s\mathbf{k}} - \varepsilon_{d\mathbf{k}}\varepsilon_{s\mathbf{k}})}}{2}, \quad (7)$$

$$\cos\phi_{\mathbf{k}} = -\frac{q_{\mathbf{k}}}{2\sqrt{(|p_{\mathbf{k}}|/3)^3}}, \quad (8)$$

where $N_{\rm s}$ is the number of sites in the lattice, $p_{\mathbf{k}} = (3B_{\mathbf{k}}\text{-}A_{\mathbf{k}}^2)/3$, $q_{\mathbf{k}} = C_{\mathbf{k}} + 2A_{\mathbf{k}}^3/27 - A_{\mathbf{k}}B_{\mathbf{k}}/3$, $A_{\mathbf{k}} = 2\tilde{V}_{\mathbf{k}}\text{-}\tilde{\varepsilon}_{\mathbf{k}}^2$, $B_{\mathbf{k}} = \tilde{V}_{\mathbf{k}}^2 + 4\Delta_{\mathbf{k}}^2\tilde{U}^2$, $C_{\mathbf{k}} = 4\Delta_{\mathbf{k}}^2[2\tilde{U}\varepsilon_{s\mathbf{k}}V_{\mathbf{k}}^2 - (\tilde{U}^2\varepsilon_{s\mathbf{k}}^2 + V_{\mathbf{k}}^4)]$, $\tilde{V}_{\mathbf{k}} = \varepsilon_{s\mathbf{k}}\varepsilon_{d\mathbf{k}}\text{-}V_{\mathbf{k}}^2\text{-}\tilde{U}\varepsilon_{s\mathbf{k}}$, $\tilde{\varepsilon}_{\mathbf{k}} = \tilde{U} - (\varepsilon_{s\mathbf{k}} + \varepsilon_{d\mathbf{k}})$, and $\beta = 1/k_{\rm B}T$.

3. Numerical results and conclusions

To obtain Δ_0 and $T_{\rm c}$ for a specific value of V and U, Eq. (2) is solved self-consistently in the first Brillouin zone of the momentum space of a square lattice, together with the dispersion relation:

$$\varepsilon_{s\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] + 4t_2\cos(k_x)\cos(k_y) + \varepsilon_0. \quad (9)$$

Here, $t = 1.0$ is the hopping integral for the nearest-neigbours and it is the energy unit, $t_2 = 0.55t$ is the value of the hopping integral for the next-nearest-neighbours, and it is known to describe well the HTSC phase diagram [11]. ε_0 is an adjustable parameter. Also, we introduce now the homothetic relation concerning the dispersion relation for s and d electrons [5]: $\varepsilon_{d\mathbf{k}} = \alpha\varepsilon_{s\mathbf{k}}$, where α is a phenomenological parameter and plays the role of the effective band masses, and gives a fair approximation for the description of the two-band system. For the symmetric case, $\varepsilon_{s\mathbf{k}}$ and $\varepsilon_{d\mathbf{k}}$ are centered at the Fermi level. To solve Eq. (2) we start with an initial guess for Δ and $k_{\rm B}T$. Then, these values are changed and Eq. (2) is iterated until the limit $T \to T_{\rm c}$ is achieved. In Fig. 1 we exhibit the behavior of the gap curves as a function of $V_{\mathbf{k}}$ for a constant hybridization, for half filled bands ($\langle n^{\rm d}\rangle = \langle n^{\rm s}\rangle = 1$), and strong coupling limit $U = 8t$. One sees that as the magnitude of V increases, Δ_0 and $k_{\rm B}T_{\rm c}$ diminish. For low temperatures the gaps increase and, as the temperatures increase, the gaps diminish abruptly. Also, we can see that the critical hybridization is $V_{\rm c} = 7t$. We want to point out that in general the hybridization increases with applied pressure. So, our results imply that the superconducting gap decreases with increasing hybridization V. This behavior is observed for HTSC as well as in some transitive metals, such as Niobium [5]. It is important to remember that, in our calculations we have considered a Hubbard-I approach, which is beyond the usual BCS.

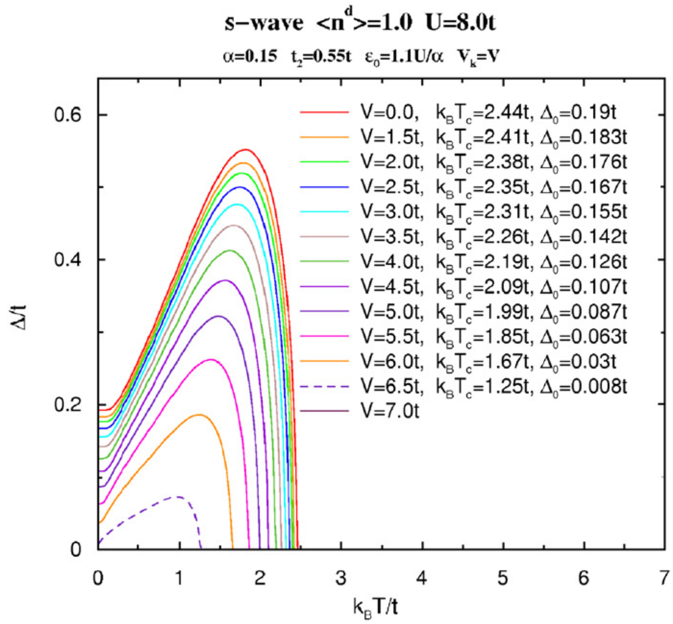

Fig. 1. The figure shows the behavior of the gap curves when V changes. As one can see, as V increases, k_BT_c and Δ_0 diminish. The results are for a constant hybridization. We have obtained the same results for a k-dependent hybridization. Notice that, for low temperatures the curves increase and, as the temperature increases, the curves abruptly decrease. For $V>7.0t$ there is no superconductivity. Therefore, $V_c=7.0t$ for these parameters.

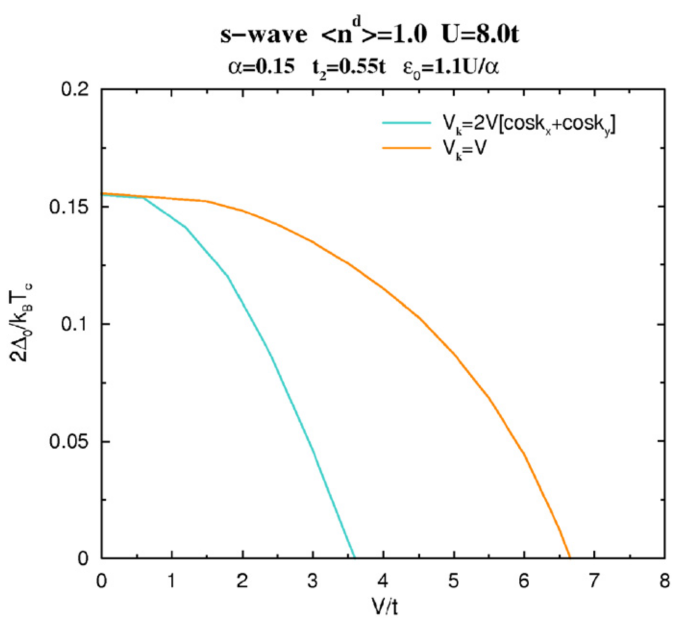

Fig. 2. Here we have the dependence of $2\Delta_0/k_BT_c$ when V changes for a constant and a k-dependent hybridization. For $V_{\mathbf{k}}=0$, $\Delta_0\approx 0.16t$ for both hybridizations. Notice that when V increases, $2\Delta_0/k_BT_c$ becomes null for both: the k-dependent and the constant hybridizations.

Fig. 2 shows the behavior $\zeta=2\Delta_0/k_BT_c$ for a k-dependent and a constant $V_{\mathbf{k}}$. One sees that there is an abrupt change in ζ when one goes from small V regime to large one, clearly showing the presence of a non-BCS regime (small V) to a BCS one (large V).

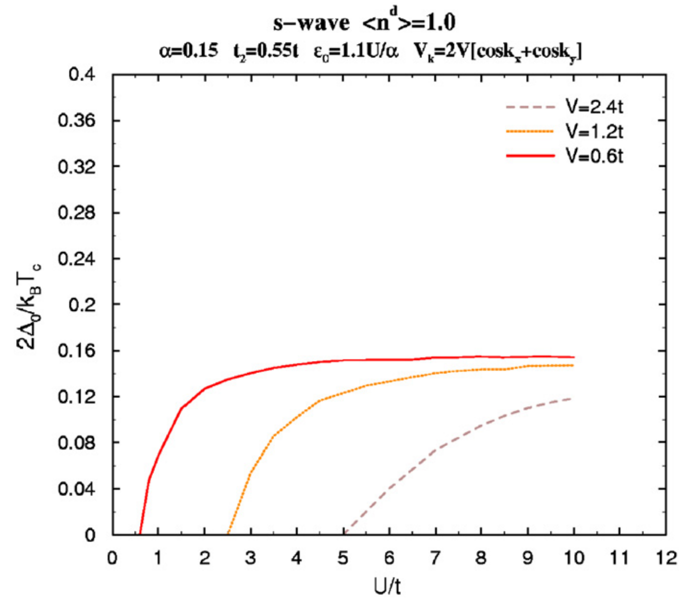

Fig. 3. Here we have the dependence of $2\Delta_0/k_BT_c$ on U, for a k-dependent hybridization, for three different hybridization strengths.

Fig. 3 shows the behavior of ζ when U changes, for a k-dependent hybridization. For low values of U, ζ decreases and becomes null. As U increases, going into the strong coupling limit region ($U/t\gg 1$), ζ seems to stabilize in a specific value. This feature appears also in s-wave superconductors in the inhomogeneous two-dimensional attractive Hubbard model [12]. In fact, in some materials ζ seems to have a constant value. The results for a constant $V_{\mathbf{k}}$ are quite similar. A more complete work on the thermodynamics arising from the model presented here will be published elsewhere [13].

Acknowledgments

We acknowledge partial financial support from CNPq and FAPERJ, Brazilian agencies. This work was also financed by PRONEX No. E-26/171.168/2003 from CNPq/FAPERJ.

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