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Effect of hybridization in a two-band Hubbard superconductor: Strong coupling limit with extended s-wave gap

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Abstract

The critical temperatures T_c, for different hybridization strengths V, are obtained, within a Hubbard-I approximation, using an extended two-band Hubbard model. Here we considered an extended s-wave gap symmetry and a two-dimensional square lattice. The results show that for a fixed value of the attractive potential U and fixed hybridization V the gap raises for low temperatures, and diminishes as the temperature increases. Moreover, the gap behavior with hybridization is such that when V increases the gap diminishes.

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1. Introduction

The electronic hybridization has been extensively used to study the superconductivity in the framework of a BCS theory [1–4]. Since some high-T_c materials, as well as superconducting heavy fermions, show strong electronic correlations [5,6], we apply here a Hubbard-I approximation [6] to obtain the zero temperature superconducting gap Δ_0 and the critical temperature T_c in a two-band Hubbard model, in the presence of a one-body hybridization. We consider an extended s-wave gap symmetry [7] and a constant and a k-dependent hybridization.

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

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

where $c^{\dagger}_{i\sigma}(c_{i\sigma})$ and $d^{\dagger}_{i\sigma}(d_{i\sigma})$ 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 $\sigma = \{\uparrow\downarrow\}$. $n^{d}_{i\sigma} = d^{\dagger}_{i\sigma} d_{i\sigma}$ is the density operator; t^{d}_{ij} and t^{s}_{ij} are the hopping integrals between sites i and j nearest-neigbors and next-nearest-neigbors for the s and d electrons. U is the attractive potential between the d electrons, which can be provided by the competition between on-site and nearest-neigbors site Coulomb interaction for some range of parameters [8]. V_{ij} is the 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 $\langle\langle d_{i\sigma}; d^{\dagger}_{l\sigma}\rangle\rangle_{\omega}$, $\langle\langle d^{\dagger}_{i,-\sigma}; d^{\dagger}_{l\sigma}\rangle\rangle_{\omega}$, $\langle\langle c_{i\sigma}; d^{\dagger}_{l\sigma}\rangle\rangle_{\omega}$and $\langle\langle c^{\dagger}_{i,-\sigma}; d^{\dagger}_{l\sigma}\rangle\rangle_{\omega}$ [6]. We calculate the equations of motion for the new generated Greens's functions $\langle\langle n^{d}_{j,-\sigma} d_{i\sigma}; d^{\dagger}_{l\sigma}\rangle\rangle_{\omega}$ and $\langle\langle n^{d}_{j\sigma} d^{\dagger}_{i,-\sigma}; d^{\dagger}_{l\sigma}\rangle\rangle_{\omega}$, following the Hubbard-I approach and a mean-field treatment: $(2U\sum_{jp}\langle\langle n^{d}_{p,-\sigma} n^{d}_{j,-\sigma} d_{i\sigma}; d^{\dagger}_{l\sigma}\rangle\rangle_{\omega} \approx \tilde{U}\sum_{p}\langle\langle n^{d}_{p,-\sigma} d_{i\sigma};$

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$d_{l\sigma}\rangle\rangle_\omega + 2\langle n^{\rm d}\rangle \sum_p \Delta_{pi}\langle\langle d^\dagger_{p,-\sigma}; d^\dagger_{l\sigma}\rangle\rangle_\omega$),where $\tilde{U} = 2U\langle n^{\rm d}\rangle$, and $\Delta_{ij} = U\langle d^\dagger_i d^\dagger_{j,-\sigma}\rangle$ is the superconducting order parameter. In the momentum space, and considering an extended s-wave gap symmetry, the order parameter is given by [7]: $\Delta_{\mathbf{k}} = 2\varDelta^{\max}|\cos(k_x) + \cos(k_y)|$, where $\varDelta^{\max} = \varDelta$ is the maximum gap amplitude and it is independent of momentum. From the above relations one obtains the gap self-consistent gap equation for an extended s-wave symmetry

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

where $F_{i\mathbf{k}} = E^2_{i\mathbf{k}}[E'_{1\mathbf{k}} + E'_{2\mathbf{k}} - \varepsilon_{s\mathbf{k}}] - \varepsilon_{s\mathbf{k}}E'_{1\mathbf{k}}E'_{2\mathbf{k}}$, $G_{i\mathbf{k}} = E_{i\mathbf{k}}[E^2_{i\mathbf{k}} - \varepsilon_{s\mathbf{k}}[E'_{1\mathbf{k}} + E'_{2\mathbf{k}}] + E'_{1\mathbf{k}}E'_{2\mathbf{k}}]$ and $E_{1\mathbf{k}} = [-A_{\mathbf{k}}/3 + 2(|p_{\mathbf{k}}|/3)^{1/2}\cos\phi_{\mathbf{k}}/3]^{1/2}$, $E_{2,3\mathbf{k}} = [-A_{\mathbf{k}}/3 - 2(|p_{\mathbf{k}}|/3)^{1/2}\cos(\phi_{\mathbf{k}} \pm \pi)/3]^{1/2}$, $E'_{1,2\mathbf{k}} = -(\tilde{\varepsilon}_{\mathbf{k}} + \tilde{U})/2 \pm [(\tilde{\varepsilon}_{\mathbf{k}} + \tilde{U})^2 + 4\zeta_{\mathbf{k}}]^{1/2}/2$, $\cos\phi_{\mathbf{k}} = -q_{\mathbf{k}}/[2(|p_{\mathbf{k}}|/3)^{3/2}]$, and $N_{\rm s}$ is the number of sites in the lattice, $\gamma_{\mathbf{k}} = |\cos(k_x) + \cos(k_y)|$,$p_{\mathbf{k}} = (3B_{\mathbf{k}} - A^2_{\mathbf{k}})/3$, $q_{\mathbf{k}} = C_{\mathbf{k}} + 2A^3_{\mathbf{k}}/27 - A_{\mathbf{k}}B_{\mathbf{k}}/3$, $\zeta_{\mathbf{k}} = 2\tilde{U}\varepsilon_{s\mathbf{k}} - \varepsilon_{d\mathbf{k}}\varepsilon_{s\mathbf{k}}$, $A_{\mathbf{k}} = 2\tilde{V}_{\mathbf{k}}$-$\tilde{\varepsilon}^2_{\mathbf{k}}$, $B_{\mathbf{k}} = \tilde{V}^2_{\mathbf{k}} + 4\varDelta^2_{\mathbf{k}}\tilde{U}^2$, $C_{\mathbf{k}} = 4\varDelta^2_{\mathbf{k}}[2\tilde{U}\varepsilon_{s\mathbf{k}}V^2_{\mathbf{k}} - (\tilde{U}^2\varepsilon^2_{s\mathbf{k}} + V^4_{\mathbf{k}})]$, $\tilde{V}_{\mathbf{k}} = \varepsilon_{s\mathbf{k}}\varepsilon_{d\mathbf{k}}$- $V^2_{\mathbf{k}} - \tilde{U}\varepsilon_{s\mathbf{k}}$, $\tilde{\varepsilon}_{\mathbf{k}} = \tilde{U} - (\varepsilon_{s\mathbf{k}} + \varepsilon_{d\mathbf{k}})$, and $\beta = 1/k_{\rm B}T$.

To obtain $\varDelta_0$ 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, for $\langle n^{\rm d}\rangle = \langle n^{\rm s}\rangle = 1.0$, together with the dispersion relation: $\varepsilon_{s\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] + 4t_2\cos(k_x)\cos(k_y) + \varepsilon_0$. We start with initial values of $\varDelta$ and T, then Eq. (2) is iterated, until the limit $T \to T_{\rm c}$ is obtained. Here t is the hopping integral for the nearest-neigbors and t_2 the hopping integral for the next-nearest-neigbors. ε_0 is an adjustable parameter. Also, we introduce now the homothetic relation concerning the dispersion relation for s and d electrons [6]: $\varepsilon_{d\mathbf{k}} = \alpha\varepsilon_{s\mathbf{k}}$, where α is a phenomenological parameter which 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.

In Fig. 1 we exhibit the behavior of the gap as a function of the hybridization for half-filled bands, and strong coupling $U = 8t$. Here we plot the case of a k-dependent hybridization, the results for a constant V being quite similar. We observe that, for small T, the gap increases slightly, whereas when T increases the gap decreases abruptly. Fig. 2a shows the behavior of $\xi = 2\varDelta_0/k_{\rm B}T_{\rm c}$ for the same set of parameters of Fig. 1, for a k-dependent hybridization. One sees that when U increases, ξ seems to stabilize in the region of validity of the approximation for U. Fig. 2b shows the behavior of ξ for different V, for both: a k-dependent and a constant hybridization, for $U = 8.0t$. We want to point out that in general the hybridization increases with applied pressure. So, some of our results imply that $\varDelta_0$ decreases with increasing V. Therefore, our theoretical calculations can be used to understand the behavior of $T_{\rm c}$ under pressure of some two-band systems, e.g., heavy fermion intermetallic compounds.

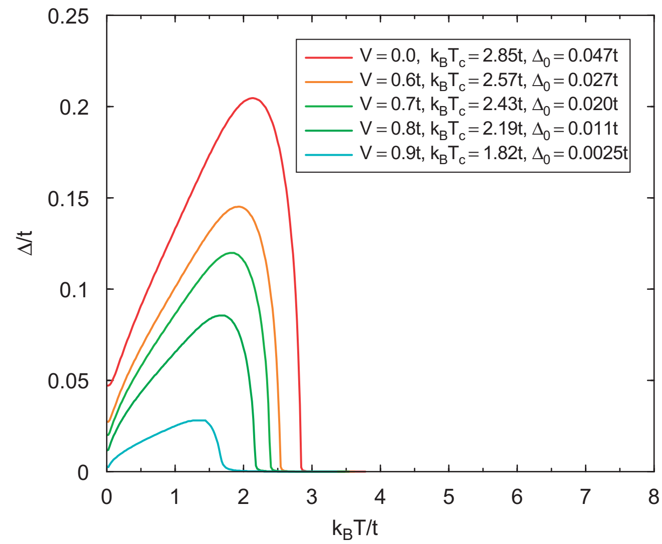

Fig. 1. Gap curves for different V. For a critical value $V_{\rm c}(\approx 1.0t)$, the gap disappears.

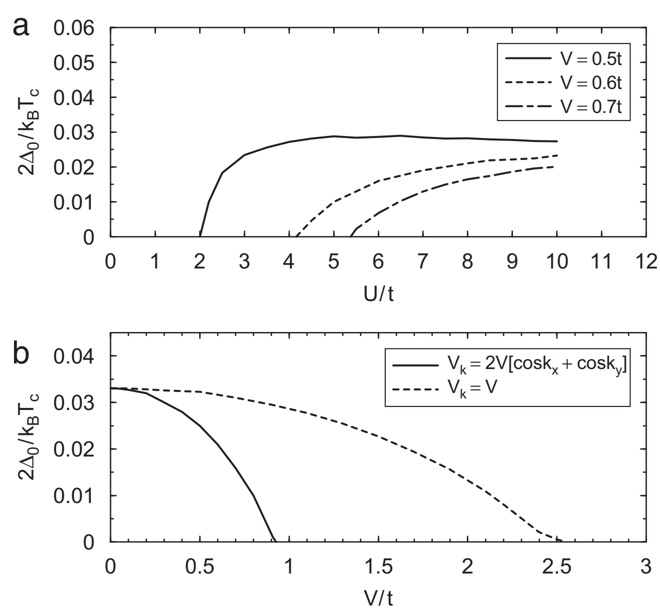

Fig. 2. In (a) we show the behavior of $2\varDelta_0/k_{\rm B}T_{\rm c}$ when U changes. In (b) we show the results of $2\varDelta_0/k_{\rm B}T_{\rm c}$ for two cases: a k-dependent and a constant $V_{\mathbf{k}}$.

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