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On intraband and interband BCS pairings in presence of hybridization in two band superconductors

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Abstract

We discuss the stability of the intraband (r = dd) and interband (r = sd) couplings in the presence of a constant hybridization on a two-band system. We calculate the critical temperature $T_{c,r}$ associated to both type of couplings and then we obtain the values of $\epsilon r = 2|U_r|\Delta_r(0)/k_B T_{c,r}$ and the isotope coefficients γ_r . One shows that under some circumstances, one can obtain values for ϵ_r and γ_r which differ considerably from standard BCS couplings for both Cooper pairings.

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1. Introduction

The effect of the electronic hybridization on narrow band superconductivity has been extensively investigated in the literature [1]. In previous works [2,3], we investigated the effect of one-body hybridization on the superconductivity of a two-band model differently from the standard approaches [1] for the uncoupled system (we can only form Cooper pairing of one kind d-d or s-d). Within the one-body formulation only single electrons are transferred between different bands, so that, for a local character hybridization, $V = V_0$, we verified that there is a critical value of the hybridization V_c depending on α (which gives the ratio of the effective band masses) and θ_D (Debye frequency) for which the most of superconductor parameters vanishes. We obtain the critical temperature $T_{c,r}$ and the order parameter $\Delta^* r(0) = |U_r|\Delta_r(0)$ for the uncoupled system to calculate the value of $\epsilon_r^* = \Delta^* r(0)/k_B T_{c,r}$ as a functions of V_0 . We also obtain an exact expression for the isotope coefficient $\overline{\gamma}_r$ directly from the BCS gap equation. In the absence of hybridization our results reproduce the standard BCS results [4].

2. The Hamiltonian

The Hamiltonian describing our system is

$$H = H_0 + H_a + H_h,\tag{1}$$

where

$$H_0 = \sum_{i,j,\sigma} T^{(s)}_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i,j,\sigma} T^{(d)}_{ij} d^{\dagger}_{i\sigma} d_{j\sigma}, \qquad (2)$$

$$H_{\rm a} = U_{\rm dd} \sum_{i,\sigma} n^{\rm d}_{i\sigma} n^{\rm d}_{i,-\sigma} + U_{\rm sd} \sum_{i,\sigma} n^{\rm s}_{i\sigma} n^{\rm d}_{i,-\sigma}, \tag{3}$$

$$H_{\rm h} = \sum_{i,\sigma} V_{ii} (c^{\dagger}_{i\sigma} d_{i\sigma} + d^{\dagger}_{i\sigma} c_{i\sigma}). \tag{4}$$

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 H_0 represents the (s) and (d) bands without interaction. H_a represents a net attractive interaction between electrons of opposite spin at the same site ($U_r < 0$, r = dd or r = sd) [5]. H_h is the mixing term which represents a oneparticle hybridization Hamiltonian in presence of the periodic lattice. We take $V_{ii} = V_0 = \text{constant}$. The Hamiltonian (4) is used to take into account the formation of both d–d and s–d pairings. We derive an exact expression for the isotope coefficient directly from the gap equation at $T = T_c$, using the relation $T_c \sim M^{-1/2}$ within the BCS framework for any form of *DOS*. The gap equation as a function of the absolute temperature $\beta = 1/k_BT_c$ is given by

$$\Delta_{\rm r}^* = \frac{U_{\rm r}}{8\pi} \int_{-\hbar\omega_{\rm D}}^{\hbar\omega_{\rm D}} \rho_{\rm s}(z) d\sum_{n=1}^2 L_{n\rm r}(z) \frac{1}{\omega_n(z)} \\ \times \tanh\left(\frac{\beta}{2}\omega_n(z)\right)$$
(5)

with

$$L_{nr}(z) = \left[1 - (-1)^n \frac{m_r(z)}{F(z)}\right] \Delta_r^* - (-1)^n C_r V$$
$$\times \omega_n(z) \Delta_{r'}^*, \tag{6}$$

and

$$\omega_n(z) = \left\{ \frac{1}{2} [A(z) - (-1)^n F(z)] \right\}^{1/2},\tag{7}$$

$$A(z) = (\alpha^2 + 1)z^2 + 2(V_0^2 + \Delta_{\rm sd}^{*2})\Delta_{\rm dd}^{*2}, \tag{8}$$

$$F(z) = \{ [(\alpha^2 - 1)z^2 + \Delta_{dd}^{*2}]^2 + 4V_0^2 [(\alpha + 1)^2 z^2 + \Delta_{dd}^{*2}] \\ + 4\Delta_{sd}^{*2} [(\alpha - 1)^2 z^2 + \Delta_{dd}^{*2}] \}^{1/2},$$
(9)

where

$$vm_r(z) = \begin{cases} r = \mathrm{sd}, \ r' = \mathrm{dd}, \ C_{\mathrm{sd}} = 2, \\ m_{\mathrm{sd}} = (\alpha - 1)^2 z^2 + 4V_0^2 + \Delta_{\mathrm{dd}}^{*2}, \\ r = \mathrm{dd}, \ r' = \mathrm{sd}, \ C_{\mathrm{dd}} = 4, \\ m_{\mathrm{dd}} = (\alpha^2 - 1)z^2 + 2V_0^2 + \Delta^{*2}, \end{cases}$$
(10)

being $z = E + i\delta$ and $\Delta^{*2} = 2\Delta_{sd}^{*2} + \Delta_{dd}^{*2}$.

3. The isotope coefficient

For a local character hybridization $V_{ii} = V_0$, we derive an exact expressions for the isotope coefficient $\gamma_i 3 = -d \ln T_{c,r}/d \ln M(r = dd, sd)$ using the gap equation (5) [2,4]. At the critical temperature $(U_r \Delta_r(T_{c,r}) = \Delta_r^*(T_{c,r}) = 0)$ is given by $1 - |U_r|\Gamma_r = 0$, using the relation $\omega_D \sim M^{-1/2}$, so that



Fig. 1. $\epsilon_r^* = 2\Delta_r^*(0)/k_B T_{c,r}$ and isotope effect as functions of the hybridization $V_0/|U_r|$ for several values of θ_D and the rate of α .

$$\gamma \mathbf{r}(\alpha^2, V_0^2, \theta_{\mathrm{D}}) = \frac{\rho_{\mathrm{s}}(\hbar\omega_{\mathrm{D}}) \sum_{n=1}^{2} \frac{L_{nr}(z)}{\omega_{0,n}(z)} \tanh\left(\frac{\beta_n^c(z)}{2}\right)|_{z=\hbar\omega_{\mathrm{D}}}}{\beta_{\mathrm{c}} \int_{-\hbar\omega_{\mathrm{D}}}^{\hbar\omega_{\mathrm{D}}} \rho_{\mathrm{s}}(z) \,\mathrm{d}z \sum_{n=1}^{2} L_{nr}(z) \frac{1}{\cosh^2\left(\frac{\beta_n^c(z)}{2}\right)}},\tag{11}$$

where $\beta_n^{c}(z) = \beta^{c} \omega_{0n}(z)$.

In Fig. 1, one gets for an arbitrary DOS, the following results: the value of $\epsilon_r^* = 2\Delta_r^*(0)/k_BT_{c,r}$ differs considerably from standard BCS result, in almost the whole range of validity of the hybridization. We define V_{\min} the value of a hybridization V_0 where the superconducting parameters attain their minimum values. Close to V_{\min} , ϵ_{dd}^* increases as compared to the BCS result whereas $T_{c,dd}$ tends towards zero. One sees that d-d pairing favors an enhancement of $\epsilon_{\rm dd}^*$, with increasing hybridization, contrary to the case of s-d pairing, where ϵ_{sd}^* diminishes when V_0 tends to a V_{min} like $T_{c,sd}$ does. For both pairings the isotope coefficient $\overline{\gamma}_r$ exhibits the following features: close to V_{min} , it reduces enormously as compared with BCS result; whereas for very small V_0 this coefficient is the same as obtained in [4], and it takes a maximum value for any value of $V_0/|U_r|$ depending on α and $\theta_{\rm D}$ ($\theta_{\rm D}$ = Debye frequency).

As a final comment: hybridization has a strong connection with applied external pressure *P* in transition metal like systems as well as in high T_c materials [6,7]. Under compression they can exhibit positive or negative dT_c/dP [8]. The analysis of this rather complicate dependence is beyond the scope of this article and will be discussed in a forthcoming work.

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