On the Superconductivity in the Induced Pairing Model

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Abstract

The two component model of coexisting local electron pairs and itinerant fermions coupled via charge exchange mechanism, which mutually induces superconductivity in both subsystems, is discussed. The cases of isotropic $s$-wave and anisotropic pairing of extended $s$ and $d_{x^2-y^2}$-wave symmetries are analyzed for a 2D square lattice within the BCS-mean field approximation and the Kosterlitz-Thouless theory. We determined the phase diagrams and superconducting characteristics as a function of the position of the local pair (LP) level and the total electron concentration. The model exhibits several types of interesting crossovers from BCS like behavior to that of LP’s. Some of our results are discussed in connection with a two-component scenario of preformed pairs and unpaired electrons for exotic superconductors.

Key words:
Boson-Fermion model, Phase fluctuations

A system of interacting charged bosons (bound electron pairs) and electrons can show features which are intermediate between those of local pair superconductors and those of classical BCS systems. Such a two component (boson-fermion) model is of relevance for high temperature superconductors (HTS) and other exotic superconductors [1,2,3,4,5,6,7,8,9,10]. Recently, we have studied a generalization of this model to the case of anisotropic pairing [9,10]. Here, we shortly outline the study and present further results concerning the phase diagrams and superconducting properties of such a system in the case of isotropic $s$-wave pairing as well as for anisotropic pairings of $d$- and extended $s$-wave symmetries, for a 2D square lattice.

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1 The Model

We consider the model of coexisting electron pairs (formed by "d" electrons) and itinerant "c" electrons defined by the following effective Hamiltonian

\[
H = \sum_{k\sigma}(\epsilon_k - \mu)c_{k\sigma}^\dagger c_{k\sigma} + 2 \sum_i(\Delta_0 - \mu)b_i^\dagger b_i - \sum_{ij}J_{ij}b_i^\dagger b_j + \sum_{k,q}\left[V_q(k)c_{k+q/2,\uparrow}^\dagger c_{-k+q/2,\downarrow}^\dagger b_q + H.c.\right],
\]

(1)

where \( \epsilon_k \) refers to the band energy of the c-electrons, \( \Delta_0 \) measures the relative position of the LP level with respect to the bottom of the c-electron band, \( \mu \) is the chemical potential which ensures that the total number of particles in the system is constant, i.e. \( n = \frac{1}{N}(\sum_{k\sigma} < c_{k\sigma}^\dagger c_{k\sigma} > + 2 \sum_i < b_i^\dagger b_i >) = n_c + 2n_B \). \( n_c \) is the concentration of c-electrons, \( n_B \) is the number of d-pairs (hard-core bosons) per site. \( J_{ij} \) is the pair hopping integral The operators for local pairs \( b_i^\dagger, b_i \) obey the Pauli spin 1/2 commutation rules. \( V_q(k) \) describes the coupling between the two subsystems. Furthermore, we set \( J_{ij} = 0 \). We will analyze the case \( V_q(k) = V_0(k) = I\phi_k/\sqrt{N} \), and neglect its \( q \) dependence at small \( q \). The interaction term takes the form of coupling, via the center of mass momenta \( q \), of the singlet pair of c-electrons \( B_q^\dagger \) and the hard-core boson \( b_q \):

\[
H_1 = \frac{1}{\sqrt{N}} \sum_q I(B_q^\dagger b_q + b_q^\dagger B_q).
\]

(2)

\( B_q^\dagger = \sum_k \phi_k c_{k+q/2,\uparrow}^\dagger c_{-k+q/2,\downarrow}^\dagger \) denotes the singlet pair creation operator of c-electrons and \( I \) is the coupling constant. The pairing symmetry, on a 2D square lattice, is determined by the form of \( \phi_k \), which is 1 for on-site pairing \( (s) \), \( \phi_k = \gamma_k = \cos(k_x a) + \cos(k_y a) \) for extended s-wave \( (s^*) \) and \( \phi_k = \eta_k = \cos(k_x a) - \cos(k_y a) \) for d_{x^2-y^2}-wave pairing \( (d) \). In general, one can consider a decomposition \( I\phi_k = g_0 + g_s\gamma_k + g_d\eta_k \), with appropriate coupling parameters for different symmetry channels.

The numerical results presented below are based on the BCS-Mean-Field Approximation (MFA) and the Kosterlitz-Thouless (KT) theory for 2D superfluid. In the BCS-MFA the free energy of the system is calculated to be:

\[
F/N = -\frac{2}{\beta N} \sum_k \ln[2\cosh(\beta E_k/2)] - \frac{1}{\beta} \ln[2\cosh(\beta \Delta)] + C,
\]

(3)

\[
C = -\epsilon_b + \Delta_0 + \mu(n_c + 2n_B) - 2\mu - 2I|x_0|\rho_0^2,
\]

(4)

where the quasiparticle energy of the c-electron subsystem is given by

\[
E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}, \quad \text{and} \quad \epsilon_k = \epsilon_k - \mu, \quad \Delta_k^2 = T^2\phi_k^2(\rho_0^2)^2, \quad \Delta = \sqrt{(\Delta_0 - \mu)^2 + T^2|x_0|^2},
\]
β = 1/\k_B T. The c-electron dispersion is \( \epsilon_k = \tilde{\epsilon}_k - \epsilon_b = -2t [\cos(k_x a) + \cos(k_y a)] - 4t_2 \cos(k_x a) \cos(k_y a) - \epsilon_b \), with the nn and nnn hopping parameters \( t \) and \( t_2 \), respectively; \( \epsilon_b = \min \tilde{\epsilon}_k \). It should be noted that the energy gap in the c-band is due to nonzero Bose condensate amplitude (\(| \langle b \rangle | \neq 0 \)), and well defined Bogolyubov quasiparticles exist in the superconducting phase. The energy spectrum of the system is characterized by \( E_k \) and \( \Delta \). The superconducting order parameters: 

\[
\begin{align*}
x_0 &= \frac{1}{N} \sum_k \phi_k \langle c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger \rangle \quad \text{and} \quad \rho_0^c = \frac{1}{2N} \sum_i < b_i^\dagger + b_i > 
\end{align*}
\]

and the chemical potential \( \mu \) are given by

\[
\frac{\partial F}{\partial x_0} = 0, \quad \frac{\partial F}{\partial \rho_0^c} = 0, \quad \frac{\partial F}{\partial \mu} = 0. \tag{5}
\]

The superfluid density derived within the linear response method and BCS theory is of the form:

\[
\rho_s = \frac{1}{2N} \sum_k \left\{ \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 \frac{\partial f(E_k)}{\partial E_k} + \frac{1}{2} \frac{\partial^2 \epsilon_k}{\partial k_x^2} \left[ 1 - \frac{\tilde{\epsilon}_k}{E_k} \tanh \left( \frac{\beta E_k}{2} \right) \right] \right\}, \tag{6}
\]

where \( f(E_k) = 1/[\exp(\beta E_k) + 1] \) is the Fermi-Dirac distribution function. In the local limit: \( \lambda^{-2} = (16\pi e^2/\hbar^2 c^2)\rho_s \), where \( \lambda \) is the London penetration depth.

Let us also consider the pair propagator for c-electron subsystem

\[
G_2(\mathbf{q}, \omega) = \frac{1}{N} \langle \langle B_{\mathbf{q}} | B_{\mathbf{q}}^\dagger \rangle \rangle_\omega, \tag{7}
\]

where \( \langle \langle B_{\mathbf{q}} | B_{\mathbf{q}}^\dagger \rangle \rangle_\omega \) is the time Fourier transform of the Green’s function: 

\[-i\Theta(t-t') \langle [B_{\mathbf{q}}(t), B_{\mathbf{q}}^\dagger(t')] \rangle >. \]

In the normal state, using the equation of motion technique and Random Phase Approximation one gets:

\[
G_2(\mathbf{q}, \omega) = \frac{\chi(\mathbf{q}, \omega)}{1 - v_{eff}(\omega) \chi(\mathbf{q}, \omega)}, \tag{8}
\]

where

\[
\chi(\mathbf{q}, \omega) = \frac{1}{N} \sum_k \phi_k^2 \frac{1 - f(\epsilon_{k+q/2}) - f(\epsilon_{k-q/2})}{\omega - \epsilon_{k+q/2} - \epsilon_{k-q/2}}, \tag{9}
\]

\[
v_{eff}(\omega) = \frac{\nu^2}{\omega - 2(\Delta_0 - \mu) \tanh [\beta(\Delta_0 - \mu)]}, \tag{10}
\]

\( \chi(\mathbf{q}, \omega) \) is the pair susceptibility and \( v_{eff}(\omega) \)-the effective interaction mediated by LP’s. Introducing the generalized T-matrix \( \Gamma(\mathbf{q}, \omega) \) via the relation \( G_2 = \chi^\Gamma/v_{eff} \), one has
Γ(q, ω) = \frac{v_{\text{eff}}(\omega)}{1 - v_{\text{eff}}(\omega)\chi(q, \omega)}.

(11)

An instability of the normal phase occurs at \Gamma^{-1}(0, 0) = 0 (the Thouless criterion), and \( T_c \) is given by

\[ 1 = \frac{I^2}{2(\Delta_0 - \mu)} \tanh \left[ \beta_c^{\text{MFA}}(\Delta_0 - \mu) \right] \frac{1}{N} \sum_k \frac{\vartheta_k^2 \tanh \left( \frac{\beta_c^{\text{MFA}} \epsilon_k}{2\tilde{\epsilon}_k} \right)}{2\tilde{\epsilon}_k}, \]

(12)

in full agreement with the MFA expression which one obtains from Eqs. (5), if \( x_0 \to 0, \rho_0^s \to 0 \).

The MFA transition temperature \( T_c^{\text{MFA}} \) at which the gap amplitude vanishes yields an estimation of the \( c \)-electron pair formation temperature [1]. Due to the fluctuation effects the superconducting phase transition will occur at a critical temperature lower than that given by the BCS-MFA theory. In 2D, \( T_c \) can be derived within the KT theory for superfluid [11], which describes the transition in terms of vortex-antivortex pair unbinding. We evaluate \( T_c \) using the KT relation for the universal jump of the superfluid density \( \rho_s \) at \( T_c \) [11,12] :

\[ \frac{2}{\pi} k_B T_c = \rho_s(T_c), \]

(13)

where \( \rho_s(T) \) is given by Eq. (6) and \( x_0(T), \rho_0^s(T), \mu(T) \) are given by Eqs. (5). Hence, the critical temperature denoted further by \( T_c^{\text{KT}} \) is determined from the set of four self-consistent equations.

2 Results and discussion

We have performed a comprehensive analysis of the phase diagrams and superfluid properties of the model (1) for different pairing symmetries [10]. Below we will discuss these results including the supplementary ones. In Fig. 1 we show the ground state diagrams as a function of \( n \) and \( \Delta_0/D \), plotted for \( |I_0| = 0 \) (\( I = -|I_0| \)) and two fixed values of \( t_2/t \). A weak intersubsystem coupling \( |I_0| \) will not change much characteristic lines of the diagrams, while increasing \( |I_0| \) expands the range of the LP+E regime [13]. Depending on the relative concentration of "\( c \)" and "\( d \)" electrons we distinguish three essentially different physical situations (in the absence of interactions). For \( n \leq 2 \) it will be:

(i) \( \Delta_0 < 0 \) such that at \( T = 0K \) all the available electrons form local pairs (of
"d" electrons) (the "local pair" regime, $2n_B \gg n_c$) (LP); (ii) $\Delta_0 > 0$ such that the "c" electron band is filled up to the Fermi level $\mu = \Delta_0$ and the remaining electrons are in the form of local pairs (the c+d regime or Mixed, $0 < 2n_B, n_c < 2$) (LP+E); (iii) $\Delta_0 > 0$ such that the Fermi level $\mu < \Delta_0$ and consequently at $T = 0K$ all the available electrons occupy the "c" electron states (the c-regime or"BCS", $n_c \gg 2n_B$) (E).

For $|I_0| \neq 0$, in the case (ii) superconductivity is due to the interchange between local pairs of "d" electrons and pairs of "c" electrons. In this process "c" electrons become "polarized" into Cooper pairs and "d" electron pairs increase their mobility by decaying into "c" electron pairs. To this intermediate case neither the standard BCS picture nor the picture of local pairs applies and superconductivity has a "mixed" character. The system shows features which are intermediate between the BCS and preformed local pair regime. This regards the energy gap in the single-electron excitation spectrum ($E_g(0)$), the $k_B T_c/E_g(0)$ ratio, the critical fields, the Ginzburg ratio $\kappa$, the width of the critical regime as well as the normal state properties. In case (i) the local pairs of "d" electrons can move via a mechanism of virtual excitations into empty c-electrons states. Such a mechanism gives rise to the long range hopping of pairs of "d" electrons (in analogy to the RKKY interaction for s-d mechanism in the magnetic equivalent). The superconducting properties are analogous to those of a pure local pair superconductor [1,6]. In case (iii), on the contrary, we find a situation which is similar to the BCS case: pairs of "c" electrons with opposite momenta and spins are exchanged via virtual transitions into local pair states.

The generic phase diagrams for different pairing symmetries plotted as a function of the position of the LP level $\Delta_0$ at fixed $n$ are shown in Fig.2a-c. In all the cases one observes a drop in the superfluid stiffness (and in the KT transition temperature) when the bosonic level reaches the bottom of the c-electron band and the system approaches the LP limit. In the opposite, BCS like limit, $T_c^{KT}$ approaches asymptotically $T_c^{MFA}$, with a narrow fluctuation regime. Between the KT and MFA temperatures, the phase fluctuation effects are important. In this regime a pseudogap in the c-electron spectrum will develop and the normal state of LP and itinerant fermions can exhibit non-Fermi liquid properties [5].

The analysis of the Mixed-LP crossover indicates that when the LP level is lowered and reaches the bottom of the fermionic band an effective attraction between fermions becomes strong, since it varies as $I^2/(2\Delta_0 - 2\mu)$ and $\mu \approx \Delta_0$ (Eq. 10). In this regime the density of c electrons is low and formation of bound c-electron pairs occurs. It gives rise to an energy gap in the single-electron spectrum independently of the pairing symmetry. We evaluated the binding energies of c- electron pairs and found that $T_c^{MFA}$ scales with the half of their
binding energy for $\Delta_0 \leq 0$. The superconducting transition temperature is here always much lower than the $c$-pair formation temperature ($T^MFA_c$) and rapidly decreases with $|\Delta_0/D|$. In such a case, the superconducting state can be formed by two types of coexisting (composite) bosons: preformed $c$-electron pairs and LP’s [10,14].

Comparing $T_c$ vs $\Delta_0$ plots for various pairings one finds that in the case of nn hopping only, the $d$ and $s$ -wave pairings are favorable for higher concentration of $c$-electrons, while the $s^*$-wave can be stable at low $n_c$. This is clearly seen from Fig.3, where the plots of $T^MFA_c$ vs $\Delta_0$ for $s, s^*$ and $d$-pairings are given for $n = 1, |I_0|/D = 0.25$, and from Fig.4 which shows variation of $n_c$ and $n_B$ with $\Delta_0/D$ for the same values of $n$ and $\Delta_0/D$ for $d$-wave pairing (for $s$ and $s^*$-wave symmetries the plots of $n_c$ and $n_B$ are very similar).

A strongly nonmonotonous behavior of $T_c$ vs $\Delta_0$ for $s^*$-wave pairing and $n > 1$ (cf. Fig.2b) reflects the fact that this type of pairing in a single band model is realized for low electron (or hole densities), if $t_2 = 0$ [1]. In general, with increasing $n_c$ ($\Delta_0/D$) one can have a sequence of transitions: $s^* \rightarrow d$ (or $s$) $\rightarrow s^*$ (if $1 < n \leq 2$), or the transitions: $s^* \rightarrow d$ (or $s$) (if $n \leq 1$).

The nnn hopping $t_2$ (with opposite sign to $t$) can strongly enhance $T_c$ for $d$-wave symmetry, moreover it favors the $d$ and $s$-wave pairings for lower values of $n_c$ [10].

The region between $T^MFA_c$ and $T^KT_c$, where the system can exhibit a pseudogap, expands with increasing intersubsystem coupling $|I_0|$. It is seen from Fig.5 that, except for $|I_0|/D \ll 1$ the coupling dependences of $T^MFA_c$ and $T^KT_c$ are qualitatively different. $T^MFA_c$ is an increasing function of $|I_0|$ for all the pairing symmetries. On the other hand, $T^KT_c$ vs $|I_0|$ increases first, goes through a round maximum and then decreases (similarly as it is observed in the attractive Hubbard model[12]). The position of the maximum corresponds to the intermediate values of $|I_0|/D$ and it depends on the pairing symmetry as well as the values of $\Delta_0/D$ and $n$. For large $|I_0|$, the $T^KT_c$ are close to the upper bound for the phase ordering temperature which is given by $\pi \rho_s(0)/2$.

As for the evolution of superconducting properties with increasing $n$ one finds three possible types of density driven changeovers [10,13]: (i) for $2 \geq \Delta_0/D \geq 0$, ”BCS” $\rightarrow$ Mixed $\rightarrow$ ”BCS”; (ii) for $\Delta_0/D > 2$: ”BCS” $\rightarrow$ ”LP” and (iii) for $\Delta_0/D < 0$: ”LP” $\rightarrow$ ”BCS”. Only if the LP level is deeply located below the bottom of $c$-band, the system remains in the LP regime for any $n \leq 2$.

Some of our findings can be qualitatively related to experimental results for the cuprate HTS where a pseudogap exists. It has been suggested by ARPES experiments, that for underdoped cuprates the Fermi surface in the pseudogap phase is truncated around the corners due to the formation of preformed (bosonic) pairs with charge $2e$, whereas the ”electrons” on the diagonals re-
main unpaired [7a]. In the present two component model such a situation is obtained when LP’s and c-electrons coexist in the mixed regime. The linear $T$-dependence of the superfluid density has been observed experimentally in copper oxides and also in several organic superconductors. This points to an order parameter of $d_{x^2-y^2}$-wave symmetry and existence of nodal quasiparticles. In the present model the gap ratio is nonuniversal and can deviate strongly from BCS predictions (particularly in the d-wave case for which it is always enhanced) [10]. This feature is also found for several exotic superconductors. The Uemura plots i.e., the $T_c$ vs zero-temperature phase stiffness $\rho_s(0)$ (and the scaling $T_c \sim \rho_s(0)$) reported for cuprates and organic superconductors can be reproduced within the model for extended $s$- and $d$-wave order parameter symmetry ([9], Figs.11,13 in Ref.[10]).

Finally, we point out that to relate more quantitatively the present two-component scenario to the phase diagram of cuprates one has to consider doping dependences of the model parameters.

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Fig. 1. Ground state diagram of the model (1) as a function of $n = n_c + 2n_B$ versus $\Delta_0/D$ ($D = zt = 4t$) for $|I_0| = 0$, plotted for a square lattice with $t_2 = 0$ (thick solid lines), rectangular DOS (dashed lines) and with $t_2/t = -0.45$ (thin lines). LP - nonmetallic state of LP’s ($2n_B = n, n_c = 0$ for $n < 2$, $2n_B = 2 - n, n_c = 2$ for $n > 2$), E - metallic state of $c$-electrons ($n_c = n, 2n_B = 0$ for $n < 2, n_c = 2 - n, 2n_B = 2$ for $n > 2$), LP+E - mixed regime ($0 < n_c, 2n_B < 2$).
Fig. 2. Phase diagrams of the induced pairing model as a function of $\Delta_0/D$ derived for (a) $s$-wave, (b)- extended $s$-wave, (c) $d$-wave symmetry ($t_2 = 0$). In all the figures the dashed line shows the BCS-MFA transition temperature, while the line with diamonds the KT transition temperature calculated for $n = 1.5, |I_0|/D = 0.25$. LPN–normal state of predominantly LP’s, EM–electronic metal, LPS+ES–superconducting (SC) state, PG – pseudogap region.
Fig. 3. $T_c^{MFA}$ as a function $\Delta_0/D$ for different pairing symmetries plotted for $n = 1, |I_0|/D = 0.25, t_2 = 0$. Solid lines are the results for the $d = 2$ square lattice, while the dashed ones - for the quasi 2D case with $t_\perp/t = 0.1$
Fig. 4. (a) Variation of $n_c$ (concentration of $c$-electrons), $n_B$ (concentration of LP’s) and superconducting order parameters $\rho_0^x, x_0$ at $T = 0$ as a function of $\Delta_0 / D$, for $n = 1, |I_0| / D = 0.25, t_2 = 0$. $d$-wave pairing. (b) The corresponding plots of $n_c, n_B$ and $\mu / D$ at $T_c^{MF_A}$. 
Fig. 5. Temperatures $T_c^{MFA}$ and $T_c^{KT}$ as a function of $|I_0|/D$ for various types of pairing for a 2D lattice ($t_2 = 0$). The lines with full symbols and thick solid line denote the KT transition temperatures. The line with empty squares is $T_c^{MFA}$ for $d$-wave pairing ($\Delta_0/D = 1, n = 2$), while the line with open circles is $T_c^{MFA}$ for $s^*$-wave pairing ($\Delta_0/D = 0.5, n = 1$).