Superconductivity in a two-component model with local electron pairs

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Superconductivity in the two component model of coexisting local electron pairs (hard-core charged bosons) and itinerant fermions coupled via charge exchange mechanism is discussed. The cases of isotropic $s$-wave and anisotropic pairing of extended $s$-wave and $d_{x^2-y^2}$ symmetries are analyzed for a 2D square lattice within the BCS-mean field approximation and the Kosterlitz-Thouless theory. The phase diagrams and superconducting characteristics of this induced pairing model as a function of the position of the local pair (LP) level and the total carrier concentration are determined. The model exhibits several types of interesting crossovers between the BCS like behavior and that of LP’s. In addition, the Uemura plots are obtained for extended $s$ and $d_{x^2-y^2}$ pairing symmetries. Finally, we analyze the pairing fluctuation effects (in 3D) within a generalized $T$-matrix approach. Some of our results are discussed in connection with a two-component scenario of preformed pairs and unpaired electrons for high temperature superconductors.

I. INTRODUCTION

A mixture of interacting charged bosons (local electron pairs with $q = 2e$) and electrons can show features which are intermediate between those of local pair (bipolaronic) 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 [1–13]. A similar model has also been adopted for the description of a resonance $s$-wave superfluidity in Fermi atomic gases with a Feshbach resonance [14,15].
Recently, we have studied a generalization of this model to the case of anisotropic pairing [11–13]. Here, we briefly outline the study and present some further results concerning the phase diagrams and superconducting properties of such a system in the case of isotropic $s$-wave and anisotropic $d$-wave pairing, for a 2D square lattice (Sec.II-III), as well as for $s$-wave pairing for a 3D simple cubic (sc) lattice (Sec.IV).

II. THE MODEL

We consider the model of coexisting electron pairs (hard-core bosons ”b”) and itinerant ”c” electrons defined by the following effective Hamiltonian

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

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}\left(\sum_{k\sigma}\langle c_{k\sigma}^\dagger c_{k\sigma}\rangle + 2\sum_i\langle b_i^\dagger b_i\rangle\right) = n_c + 2n_B. n_c$ is the concentration of c-electrons, $n_B$ is the number of local pairs per site. $J_{ij}$ is the pair hopping integral. $\tilde{H}_C$ denotes Coulomb interaction terms. 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. We will consider 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 $b_q$:

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

$B_q^\dagger = \sum_k\phi_k c_{k+q/2,\uparrow}^\dagger c_{-k+q/2,\downarrow}^\dagger$ 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 constant (1) for on-site pairing ($s$), $\phi_k = \gamma_k = \cos(k_x) + \cos(k_y)$ for extended $s$-wave ($s^*$) and $\phi_k = \eta_k = \cos(k_x) - \cos(k_y)$ 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 superconducting state of the model is characterized by two order parameters: \( x_0 = \frac{1}{\mathcal{N}} \sum_k \phi_k \langle c_{k+}^\dagger c_{k-} \rangle \) and \( \rho_0 = \frac{1}{2\mathcal{N}} \sum_i \langle b_i^\dagger b_i \rangle \). In the BCS-mean-field approximation (MFA) the free energy of the system (for \( \tilde{H}_C = 0 \)) is evaluated to be:

\[
F/N = -\frac{2}{\beta \mathcal{N}} \sum_k \ln \left[ 2 \cosh(\beta \mathcal{E}_k/2) \right] - \frac{1}{\beta} \ln \left[ 2 \cosh(\beta \Delta) \right] + C, \tag{3}
\]

\[
C = -\epsilon_b + \Delta_0 + \mu(n_c + 2n_B) - 2\mu - 2I|x_0|\rho_0^x + J_0(\rho_0^x)^2, \tag{4}
\]

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

\[
\mathcal{E}_k = \sqrt{\bar{\epsilon}_k^2 + \bar{\Delta}_k^2}, \quad \bar{\epsilon}_k = \epsilon_k - \mu, \quad \bar{\Delta}_k = I^2 \phi_k^2 (\rho_0^x)^2, \quad \Delta = \sqrt{(\Delta_0 - \mu)^2 + (-I|x_0| + J_0\rho_0^x)^2}. \]

\[
J_0 = \sum_{i \neq j} J_{ij}. \quad \beta = 1/k_B T. \]

For the 2D square lattice the \( c \)-electron dispersion is

\[
\epsilon_k = \bar{\epsilon}_k - \epsilon_b = -2t \left[ \cos(k_x) + \cos(k_y) \right] - 4t_2 \cos(k_x) \cos(k_y) - \epsilon_b, \]

with the nn and nnn hopping parameters \( t \) and \( t_2 \), respectively, \( \epsilon_b = \min \bar{\epsilon}_k \). 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 Bogoliubov quasiparticles can exist in the superconducting phase. The order parameters and the chemical potential are given by

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

The superfluid stiffness derived within the linear response method and BCS theory, for the case \( J_{ij} = 0 \), is of the form:

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

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

The mean-field transition temperature \( (T_c)^{MFA} \), at which the gap amplitude vanishes, yields an estimation of the \( c \)-electron pair formation temperature \([12,13]\) and is given by

\[
1 = \left[ J_0 + \frac{I^2}{N} \sum_k \phi_k^2 \frac{\tanh \left( \beta \epsilon_k / (\Delta_0 - \mu) / 2 \right)}{2\epsilon_k} \right] \tanh \left[ \frac{\beta \epsilon_k (\Delta_0 - \mu)}{2(\Delta_0 - \mu)} \right]. \tag{7}
\]

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 Kosterlitz-Thouless (KT) theory for 2D superfluids \([16]\), 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 (in-plane) superfluid density $\rho_s$ at $T_c$ [16]:

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

(8)

where $\rho_s(T)$ is given by Eq.(6) and $x_0(T), \rho_0(T), \mu(T)$ are given by Eqs.(5). Thus, the critical temperature denoted further by $T_c^{KT}$ is determined from the set of four self-consistent equations. In the weak coupling limit ($|I_0|/2D \ll 1, J_0 = 0, D$-the half-bandwidth, $I = -|I_0|), T_c^{KT}/T_c^{MFA} \rightarrow 1$ if $|I_0|/2D \rightarrow 0$.

III. RESULTS FOR 2D ELECTRON SPECTRUM

A comprehensive analysis of the phase diagrams and superfluid properties of the model Eq.(1) for different pairing symmetries including $s$, the extended $s$ ($s^*$) and $d_{x^2-y^2}$-wave symmetries was performed in Refs. [11–13]. Below we will discuss these results including some additional ones. (The term $H_C$ will not be considered).

In the absence of interactions, depending on the relative concentration of "c" electrons and LP’s we distinguish three essentially different physical situations. For $n \leq 2$ it will be:

(i) $\Delta_0 < 0$ such that at $T = 0K$ all the available electrons form local pairs ($2n_B \gg n_c$) (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+b" or Mixed regime, $0 < 2n_B, n_c < 2$) (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 and pairs of "c" electrons. In this process "c" electrons become "polarized" into Cooper pairs and local pairs increase their mobility by decaying into "c" electron pairs. In 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 concerns 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 can move via a mechanism of virtual excitations into empty c-electrons states. Such a mechanism gives rise to the long range hopping of LP’s (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 (bipolaronic) superconductor [1,6,17]. 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 s-wave pairing symmetry plotted as a function of the position of the LP level $\Delta_0$ at fixed $n$ are shown in Fig.1. In Fig.2, we show the transition temperatures for the $d_{x^2-y^2}$-symmetry.

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, 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].

A closer inspection 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 $\mu \approx \Delta_0$ [12,13]. 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 calculated the binding energies of c- electron pairs and found that $T_c^{MFA}$ essentially scales with the half of their binding energy for $\Delta_0 < 0$. The superconducting transition temperature is here always much lower than the c-pair formation temperature ($T_c^{MFA}$) and decreases rapidly with $|\Delta_0/D|$. In such a case, the superconducting state can be formed by two types of coexisting bosons: preformed c- electron pairs and LP’s [12,15].

Comparing $T_c$ vs $\Delta_0$ plots for various pairing symmetries 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 $n_c$. 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 $n_c$ (compare Fig.5) [12].

The region between $T_c^{MFA}$ and $T_c^{KT}$, where the system can exhibit a pseudogap, expands with increasing intersubsystem coupling $|I_0|$. As we have found [13], except for $|I_0|/D \ll 1$ the coupling dependences of $T_c^{MFA}$ and $T_c^{KT}$ are qualitatively different. $T_c^{MFA}$ is an increasing function of $|I_0|$ for all the pairing symmetries. On the other hand, $T_c^{KT}$ $vs$ $|I_0|$ increases first, goes through a round maximum and then decreases (similarly as it is observed in the attractive Hubbard model). 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 $T_c^{KT}$ are close to the upper bound for the phase ordering temperature which is given by $\pi \rho_s(0)/2$.

Concerning the evolution of superconducting properties with increasing $n$ at fixed $\Delta_0$ one finds three possible types of density driven changeovers [12,8]: (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 the $c$-band, the system remains in the LP regime for any $n \leq 2$.

Let us also comment on the effects of a weak interlayer coupling on the calculated transition temperatures [9,18]. In the KT theory the 2D correlation length behaves as follows for $T > T_c^{KT}$: $\xi(T) = a \exp \left(b/\sqrt{T/T_c^{KT} - 1}\right)$, where $b \approx 1.5$ and $a$ is the size of the vortex core. If $U_c$ is the coupling energy per unit length between the planes and $U_c \ll T_c^{KT}$, then the actual $T_c$ can be estimated by calculating the energy needed to destroy phase coherence between two regions of size $\sim \xi^2$ in different planes i.e. $T_c \sim cU_c (\xi(T_c)/a)^2$, where $c$ is the interplanar distance. The resulting equations for $T_c$ can be solved asymptotically

$$T_c = T_c^{KT} \left(1 + \frac{4b^2}{\ln^2(T_c^{KT}/cU_c)}\right), \quad (9)$$

therefore $T_c$ is only weakly dependent on the interplanar distance $c$ and is close to $T_c^{KT}$, if $U_c \ll T_c^{KT}$. In the presence of the interplanar coupling there is no discontinuous jump in $\rho_s$ but a crossover from 2D like to 3D like (XY) behavior occurs.
IV. SUPERFLUID TRANSITION FROM THE PSEUDOGAP STATE

Let us now consider the pseudogap behavior and present the recent evaluation of the superconducting transition temperature from a pseudogap state by going beyond the BCS-MFA. In our analysis we have applied a generalized $T$-matrix approach adapted to a two-component boson-fermion model [21]. Our approach is an extension of the pairing fluctuation theory of the BCS-Bose-Einstein crossover [19,20] developed previously for a one-component fermion systems with attractive interaction. The numerical results presented in Fig.3. are for a 3D sc lattice assuming the tight-binding dispersion for fermions and bosons of the following form: $\epsilon_k = D(1 - \tilde{\gamma}_k)$, $D = zt$; $J_q = J_0 \tilde{\gamma}_q$, $J_0 = zJ$, $\tilde{\gamma}_k = [\cos(k_x) + \cos(k_y) + \cos(k_z)] / 3$, $z = 6$.

The results are shown for both cases with and without the direct hopping of LP’s $J_{ij}$. The calculated $T_c$’s are much lower as compared to BCS-MFA results (these are given by Eq.(7)), and if $J = 0$, $T_c$ is strongly depressed as soon as the LP level is close to the bottom of the electronic band. In the pseudogap region the electronic spectrum is gapped, and the pseudogap parameter at $T_c$ for $\Delta_0 > 0$ essentially measures a mean square amplitude of the pairing field (of the “c” electrons). The values of pseudogap parameter at $T_c$ are comparable to the zero temperature gap values in the fermionic spectrum, except for the c-regime.

With the direct LP hopping $J_0/D = 0.1$, which corresponds to $m_B = 10m_F$, the hard-core bosons can undergo a superfluid transition even without the intersubsystem coupling $|I_0|$. As we see from Fig.3 in the presence of the boson-fermion coupling $|I_0|$ the transition temperature is enhanced in the mixed regime.

In the self-consistent $T$-matrix approach the (amplitude) fluctuations of the order parameter are included at the Gaussian level. Nevertheless, it is interesting to observe that the phase diagram for $J_0 = 0$ shown in Fig.3 displays similar regimes as that of Fig.1 determined in Sec.III from BCS and KT theories.

V. FINAL REMARKS

In conclusion, we summarize the important features of the model considered [11–13,5].

1. Well defined Bogoliubov quasiparticles can exist in the superconducting ground state.
However, above $T_c$ (in a mixed regime) local pairs coexist with itinerant fermions and the normal state properties deviate from Fermi liquid behavior.

2. In the mixed regime, $T_{c}^{MFA} < T < T_{c}^{KT}$, the system will exhibit a pseudogap in the $c$-electron spectrum, which will evolve into a real gap as one moves to the LP regime. For $\Delta_0 < 0$, LP’s coexist with preformed $c$-electron pairs, which have the binding energy $E_b^c/2 \propto T_{c}^{MFA}$.

3. For $d$-wave pairing, the superfluid density exhibits linear in $T$ behavior at low $T$ due to the presence of nodal quasiparticles.

4. The Uemura-type plots i.e., the $T_c$ vs zero-temperature phase stiffness $\rho_s(0)$, are obtained for $d$, $s^*$ and $s$-wave symmetry in the KT scenario [12]. The reason for Uemura scaling $T_c \sim \rho_s(0)$ is the separation of the energy scales for the pairing and for the phase coherence. [11,12].

5. The calculated $T_c$’s in a 3D model beyond the BCS-MFA show crucial effects of pair fluctuations in the mixed and LP regimes.

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 remain 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 for all the pairing symmetries and can deviate strongly from BCS predictions (particularly in the d-wave case for which it is always enhanced) [12]. This feature is also found in several exotic superconductors. The Uemura plots 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 [11,12].
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FIG. 1. Phase diagrams of the induced pairing model as a function of $\Delta_0/D$ at fixed $n$ derived for $s$-wave symmetry. $J_0 = 0$ and $t_2 = 0$. $|I_0|/D = 0.25$, $D=4t$. The dashed lines show the BCS-MFA transition temperature (upper for $n = 1$ and lower for $n = 0.5$), while the lines with circles and triangles show the KT transition temperatures calculated for $n = 1$ and $n = 0.5$, respectively. LPN–normal state of predominantly LP’s, EM–electronic metal, LPS+ES–superconducting (SC) state, PG – pseudogap region. A weak interplanar coupling stabilizes the SC state.
FIG. 2. MFA and KT transition temperatures as a function of $\Delta_0/D$ at fixed $n = 1$ derived for $d_{x^2-y^2}$ - pairing symmetry. The dashed and dot-dashed lines show the BCS-MFA transition temperatures for $t_2 = 0$ and for $t_2/t = -0.45$, respectively. The line with diamonds shows the corresponding KT transition temperature calculated for $t_2 = 0$ and the line with circles for $t_2/t = -0.45$. $|J_0|/D = 0.25$, $J_0 = 0$. 
FIG. 3. Phase diagrams of the hard-core boson-fermion model as a function of $\Delta_0/D$ for $s$-wave pairing and sc lattice. $n = 0.5, |J_0|/D = 0.5, D = 6t$. The transition temperatures derived with a $T$-matrix approach are for two values of $J$, which are shown by the solid line ($J_0/D = 0.1$) and the line with symbols ($J_0 = 0$), respectively. The dashed lines indicate BCS-MFA transition temperatures (upper for $J_0/D = 0.1$, lower for $J_0 = 0$). LPN–normal state of predominantly LP’s, EM–electronic metal, LPS+ES–superconducting (SC) state, PG – pseudogap region.