Critical field in a superconductivity model with local pairs

Marcin Mierzejewski and Maciej M. Maška*

Department of Theoretical Physics, Institute of Physics, University of Silesia, 40-007 Katowice, Poland

We analyze the role of Zeeman and orbital pair breaking mechanisms in models which are appropriate for short coherence length superconductors. In particular, we investigate attractive Hubbard and pair hopping models. The orbital pair breaking mechanism dominates in the majority of models with $s$-wave and $d$-wave superconducting order parameters. On the other hand, the repulsive pair hopping interaction leads to a $\eta$ type of pairing that is stable against the orbital pair breaking. External magnetic field reduces this type of pairing predominantly due to the Zeeman coupling. According to recent experiments this mechanism is responsible for closing of the pseudogap. Moreover, the temperature dependence of the gap closing field in $\eta$ phase fits experimental data accurately. We discuss whether the preformed pairs in the $\eta$ phase could be responsible for the pseudogap phenomenon.

DOI: 10.1103/PhysRevB.69.054502

I. INTRODUCTION

For almost 20 years after the discovery of high-temperature superconductors (HTSC’s) the mechanism responsible for their unusual properties remains unclear. The complex phase diagram of HTSCs suggests that there may be no single mechanism that dominates over the entire doping range. In particular, the normal-state properties in underdoped and overdoped regimes are different. Highly overdoped compounds in the normal state exhibit some properties of Fermi liquid, whereas the superconducting state may be described within the weak-coupling BCS theory.\(^1\) On the other hand, in the underdoped regime the HTSC’s exhibit unconventional features. The most remarkable of them are the extremely short coherence length and a pseudogap that opens in the normal state. Presence of the pseudogap has been confirmed by means of various experimental techniques such as angle-resolved photoemission,\(^2,4\) intrinsic tunneling spectroscopy,\(^5,6\) nuclear-magnetic-resonance,\(^7,8\) infrared,\(^9\) and transport\(^10\) measurements. Although there is no complete theoretical description of the pseudogap, one usually considers this phase as a precursor of the superconductivity. According to such a hypothesis formation of Cooper pairs starts at temperature $T^\ast$,\(^10\) higher than the superconducting transition temperature $T_c$. At $T_c$, these preformed pairs undergo Bose-Einstein condensation.

Recent observations of a vortexlike Nernst signal above $T_c$ (Ref. 11) seem to confirm this hypothesis. This signal evolves smoothly into the analogous signal below the superconducting phase transition.\(^12\) The Meissner effect does not occur in the pseudogap phase due to strong phase fluctuations rather than due to vanishing of the superfluid density. Therefore, theoretical description of the suppression of the Meissner effect requires an approach beyond the mean-field level. Despite the absence of the Meissner effect above $T_c$, one can observe inhomogeneous magnetic domains that are recognized as precursors to the Meissner state.\(^13\) This can be interpreted in terms of phase fluctuations of the local order parameter.\(^14\)

The short coherence length indicates that the pairing takes place in the real space, leading to bosonlike objects. A few models are commonly used to describe systems with local pairs; namely, the attractive Hubbard (AH) model,\(^15\) fermion-boson,\(^16\) and purely bosonic models,\(^17\) as well as the Penson-Kolb (PK) model,\(^18\) i.e., the tight-binding model with local pair hopping. These models should be considered as the effective approaches which do not explain the microscopic origin of the pairing interaction.

Another unusual property of HTSC’s is related to their behavior in the external magnetic field. In particular, temperature dependence of the upper critical field $H_{c2}$ has a positive curvature\(^19,20\) contrary to classical superconductors, where a negative curvature is observed. Moreover, $H_{c2}$ does not saturate even at genuinely low temperature. Recent experiments\(^21\) show that also the pseudogap is destroyed by sufficiently high magnetic field $H_{pg}$. Although the temperature dependence of $H_{pg}$ has a negative curvature, it significantly differs from the predictions of the standard Helfand-Werthammer theory;\(^22\) namely, $H_{pg}(T)$ has a large slope at temperatures close to $T^\ast$ and saturates already at $T \approx 0.7T^\ast$. These features may help in verification of the preformed Cooper pairs hypothesis and, more generally, to choose the most appropriate model of HTSC’s.

II. MODEL

In the present paper, we show that opening of the pseudogap and its dependence on the magnetic field can be described within a model with local pair hopping. Our starting point is the two-dimensional (2D) Penson-Kolb model with the Hamiltonian given by

$$
H = \sum_{i,j,\sigma,\tau} t_{ij} c_{i\sigma}^\dagger c_{j\tau} + \sum_{\sigma} \left( g \mu_B H_{z} \sigma - \mu_{B} c_{i\sigma}^\dagger c_{i\sigma} \right) - \frac{1}{2} J \sum_{\langle i,j \rangle} e^{i\Phi_{ij}} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger c_{j\downarrow} c_{i\uparrow},
$$

where $c_{i\sigma}^\dagger$ creates (annihilates) an electron with spin $\sigma$ at site $i$, $t_{ij}$ is the single electron hopping integral between sites $i$ and $j$, $\mu$ is the chemical potential, and $J$ is the nearest-neighbor pair hopping interactions. The external magnetic field perpendicular to the lattice, $H_{z}$, shifts the energy levels by $g \mu_B H_{z} \sigma$ ($g$ denotes gyromagnetic ratio and $\mu_B$ is Bohr
we assume coupling. For a nonzero single-electron hopping integral, the repulsive one (\( J \)) and modifies the hopping terms. The single-electron hopping integral acquires the Peierls factor

\[
\Phi_{ij} = \frac{e}{\hbar c} \int_{R_i}^{R_j} A \cdot dI,
\]

whereas the phase factor in the pair hopping term is twice larger.

The Penson-Kolb model can be derived from a general microscopic tight-binding Hamiltonian where the Coulomb repulsion may lead to the pair hopping interaction. In such a case \( J \) is negative (repulsive Penson-Kolb model). However, we assume \( J \) to be an effective parameter that can be negative as well as positive. It can be explained as a result of renormalization originating, e.g., from electron-phonon coupling. For a nonzero single-electron hopping integral, \( J \to -J \) is not a symmetry of the PK model. However, superconducting correlations occur in the Penson-Kolb model for attractive pair hopping interaction (\( J > 0 \)) as well as for the repulsive one (\( J < 0 \)), provided \( |J| \) is large enough. The latter case is usually referred to as \( \eta \)-type pairing when the total momentum of the paired electrons is \( \mathbf{Q} = (\pi, \pi) \) and the phase of superconducting order parameter alters from one site to the neighboring one. It has been shown that flux quantization and Meissner effect appear in this state. However, the presence of on-site Coulomb repulsion (Penson-Kolb-Hubbard model), provided that this interaction is not too strong.

**A. Density of states**

At the mean-field level, for \( J > 0 \) one obtains an isotropic superconducting gap, identical to the one obtained for the AH model. On the other hand, in the case of \( \eta \)-type pairing (\( J < 0 \)), the density of states is finite for arbitrary energy.
B. Response to magnetic field

In contradistinction to the AH model, the external magnetic field explicitly enters the term responsible for superconductivity, i.e., the pair hopping interaction. Therefore, the differences between AH and PK models may show up in the electromagnetic properties. 28 We investigate the temperature dependence of critical field $H_{c1}$. It is defined as the highest magnitude of the magnetic field, for which there exists a nonzero solution for the superconducting order parameter:

$$\Delta_1 = \langle c_{i}^\dagger c_{i}\rangle.$$  

(4)

We carry out calculations at the mean-field level neglecting phase fluctuations and short-range correlations. Such an analysis of the PK model becomes exact in the limit of infinite dimension. In the present case it is impossible to determine the phase coherence of the Cooper pairs, and the physical interpretation of the critical field is not unique. In the strongly overdoped regime of cuprates, where the pseudogap does not appear, it can correspond to the upper critical field. On the other hand, for underdoped systems, and within the precursor scenario of pseudogap, it can be interpreted as $H_{pg}$, i.e., the field at which the incoherent pairs appear. In the regime between $H_{c2}$ and $H_{pg}$, strong thermal and quantum fluctuations are present. 29 The role of phase fluctuations in the attractive PK model has been analyzed within the Kosterlitz-Thouless scenario. 28 In this approach the phase coherence sets in at temperature lower than the critical temperature obtained from the mean-field approximation. We refer to Ref. 28 for a thorough investigation of these temperatures carried out in the absence of diamagnetic pair breaking mechanism. The lower temperature is interpreted as a transition temperature between the pseudogap and superconducting phases.

For the sake of simplicity we define

$$\Delta_i = \frac{1}{2} \sum_j' e^{2i\Phi_{ij}} \Delta_j,$$  

(5)

where the prime denotes that the summation is carried out over the nearest neighbors of site $i$. Then, the mean-field Hamiltonian takes on the following form:

$$H = \sum_{i,j,\sigma} t_{ij} e^{i\Phi_{ij}} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\sigma} (g \mu_B H z \sigma - \mu) c_{i\sigma}^\dagger c_{i\sigma} - J \sum_i (c_{i}^\dagger c_{i}^\dagger \Delta_i + H.c.).$$  

(6)

At the mean-field level, the only difference between PK and AH models is the presence of $\Delta_i$, in Eq. (6) instead of $\Delta_1$. Therefore, in order to calculate the critical field one can follow an approach that has previously been developed for the lattice gas with on-site attraction. 30 Then, one ends up with the lattice version of the Gor’kov equations:

$$\Delta_i = \frac{J}{2\sqrt{N}} \sum_{j,\omega_n} \sum_{p_x, p_y, k_x} \chi(p_x, p_y, k_x, -p_y) \times [2 \cos(2\pi x) g(p_x, p_y, x) g(k_x, -p_y, x)$$

$$+ g(p_x, p_y, x+1) g(k_x, -p_y, x+1) + g(p_x, p_y, x-1)$$

$$\times g(k_x, -p_y, x-1) g(p_x, p_y, x') g(k_x, -p_y, x'),$$

(7)

$$G(i,j,\omega_n)$$ denotes the one-electron Green’s function in the presence of a uniform and static magnetic field. $\omega_n$ denotes the fermionic Matsubara frequency. Using Eq. (5) one can eliminate $\Delta_i$ from the Gor’kov equations. Then, $H_{crit}(T)$ can be calculated from

$$\Delta_i = \frac{J}{2\beta} \sum_{j,\omega_n} e^{2i\Phi_{ij}} \Delta_j G(i, i, \omega_n) G(i, j, -\omega_n)$$  

(8)

or

$$\Delta_i = \frac{-J}{2\beta} \sum_{j,\omega_n} (-1)^{j+l} e^{2i\Phi_{ij}} \Delta_j G(i, i, \omega_n) G(i, j, -\omega_n).$$  

(9)

Equations (8) and (9) are equivalent since $(-1)^{j+l} = -1$, for the neighboring sites $j$ and $l$. However, it is more convenient to use the first (second) of them for attractive (repulsive) pair hopping interaction.

In the following we consider only nearest-neighbor one-particle hopping integral $t$ and we use the Landau gauge $A = H_z(0, x, 0)$. The Harper equation

$$g(p_x, p_y, x+1) + 2 \cos(h x - p_y a) g(p_x, p_y, x)$$

$$+ g(p_x, p_y, x-1)$$

$$= -t^{-1} E(p_x, p_y) g(p_x, p_y, x),$$  

(10)

determines eigenvalues $E(p_x, p_y)$ of the one-particle hopping term. The corresponding eigenstates are enumerated by $p_x, p_y$, and are of the form

$$U_{xy}(p_x, p_y) = e^{i p_y a} g(p_x, p_y, x).$$  

(11)

In the above expression $x, y$ are integers which enumerate lattice sites in $\hat{x}$ and $\hat{y}$ directions, whereas $h/(2 \pi)$ is a ratio of the flux through a lattice cell to one flux quantum. We refer to Ref. 30 for the details.

The one-electron Green’s function can be expressed with the help of eigenvalues and eigenstates of the normal-state Hamiltonian. Then, the summation over Matsubara frequencies in Eqs. (8) and (9) can be explicitly carried out. In the Landau gauge, the presence of magnetic field does not change the plane-wave behavior in $\hat{y}$ direction [see Eq. (11)]. Therefore, the superconducting order parameter depends only on $x$ and pairing of electrons takes place for the same $\hat{y}$ components of momenta as in the absence of magnetic field, i.e., $(p_x, -p_y)$ for $J > 0$ and $(p_x, \pi - p_y)$ for $J < 0$. Taking these features into account, one can rewrite the Gor’kov equations for the attractive,
conditions. We have carried out calculations for $150 \times 150$ cluster with periodic boundary conditions (bc) along the $\hat{y}$ axis. As the Landau gauge breaks the translation invariance along $\hat{x}$ axis, we have used fixed bc in this direction. As our previous calculations suggest such a size of cluster is sufficient to obtain convergent results.\(^{30}\) The calculations are carried out at the mean-field level and, therefore, we restrict ourselves only to model parameters for which the critical temperature $k_B T_{\text{crit}}$ is much less than the Fermi energy.

Figure 3 shows the temperature dependence of $H_{\text{crit}}$ obtained for attractive and for repulsive pairing interactions. These results are compared with $H_{\text{crit}}(T)$ calculated from the 2D AH model\(^{30}\) with $U = -t$. We have adjusted the strength of the pair hopping interaction to obtain the same critical temperature in the absence of magnetic field. For $J > 0$, $H_{\text{crit}}(T)$ in PK model is very close to that of AH model. It means that in the case of $s$-wave pairing the Peierls factor in the pair hopping term leads only to a small decrease of superconducting correlations. The differences between the attractive PK and AH models show up for stronger pairing. However, this requires investigation beyond the mean-field level. In the absence of magnetic field, the transition temperature in the PK model increases monotonically with $J$, whereas in the AH model $T_c$ has a maximum for some finite $U$ (cf. Fig. in Ref. 28). On the other hand, the temperature dependence of $H_{\text{crit}}$ in the $\eta$ state differs qualitatively from the $s$-wave case; namely, $H_{\text{crit}}(T)$ has a very large slope for a weak magnetic field and saturates already at relatively high temperature. Such a behavior of the critical field resembles $H_{\text{pg}}(T)$ that has recently been observed in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$.\(^{21}\) At the end of this section, we compare our results with the experimental data.

Within the Helfand-Werthammer theory, the temperature dependence of critical field is predominantly determined by the diamagnetic pair breaking mechanism. The Zeeman coupling becomes important only for sufficiently strong magnetic field. This feature holds also in the case of the lattice gas.\(^{31}\) In order to investigate the role of the Zeeman and orbital couplings in the PK model, we have repeated our calculations in the absence of the Zeeman term. The resulting $H_{\text{crit}}(T)$ is shown in Fig. 4.

In contradistinction to the $s$-wave superconductivity, the diamagnetic pair breaking is of minor importance in the case of $\eta$-pairing. This feature is responsible for extremely high values of $H_{\text{crit}}$ in the absence of Zeeman term (see Fig. 4). Experimental investigations\(^{21}\) show that the pseudogap closing field scales linearly with $T^\delta$. In Ref. 21 the value of the scaling factor has been interpreted in favor of the Zeeman
coupling as a mechanism that closes the pseudogap. This pair breaking mechanism dominates also in the case of \( \eta \) pairing.

In order to explain the different role of Zeeman coupling for \( \eta \) and \( s \)-wave pairings one can recall the argumentation presented in Ref. 32; namely, this difference can be understood on the basis of the densities of states in these phases. In the regime of a weak magnetic field and low temperature \( (\mu_B H, k_BT \ll |\Delta|) \) \( s \)-wave state is essentially unaffected by the Zeeman coupling (at zero temperature the gap function and the ground state are completely unaffected). Due to a finite gap, the occupation of quasiparticle states at the Fermi level remains small. On the other hand, the density of states in the \( \eta \) phase is always finite, provided the pairing potential is not too strong. Therefore, for arbitrary weak magnetic field there are electrons with energetically favorable spin polarization. Similar argumentation also holds for the different response of \( s \) and \( d_{x^2-y^2} \) superconductors to the Zeeman magnetic field.\(^{32}\) The \( d_{x^2-y^2} \)-wave gap vanishes at four nodal points on the Fermi surface only. Therefore, the difference in the sensitivity to the Zeeman field between \( s \) and \( \eta \) phases is much bigger than between \( s \) and \( d_{x^2-y^2} \) phases.

Since the diamagnetic pair breaking mechanism is ineffective in the \( \eta \)-pairing state, we restrict further discussion to the Zeeman mechanism only. This allows us to avoid problems connected with the numerical solution of the Harper equation. In such a case, one can easily evaluate the free energy below the transition temperature and discuss details of the phase transition.

In Fig. 5 we show that our results fit very well the pseudogap closing field reported in Ref. 21. The second-order phase transition separates the \( \eta \)-paired state and normal state for a weak magnetic field. In this regime \( H_{\text{crit}} \) has been calculated from a self-consistent BCS-like equation. Below \( T/T_{\text{crit}}(0) \approx 0.6 \) the phase transition is of the first order, and the phase boundary has been determined by a comparison of the free energy in the normal and paired state. It is worth mentioning that the experimental results concerning \( H_{\text{pg}} > 60 \) T have been obtained from extrapolation of the lower-field data.\(^{21}\)

\( H_{\text{crit}} \) obtained in the AH model also fits the experimental data, provided the diamagnetic pair breaking is switched off.\(^{33}\) In such a case, all the considered models give rise to a similar temperature dependence of \( H_{\text{crit}} \). The dotted line in Fig. 5 represents results for \( s \)-wave pairing. \( H_{\text{crit}}(T) \) for \( d \)-wave pairing is almost the same. Note that difference between both pairing symmetries becomes important in the presence of diamagnetic pair breaking.\(^{30}\) One can see that various models may reproduce \( H_{\text{pg}}(T) \), provided this pair breaking is switched off. However, neglecting this mechanism is justified in the case of \( \eta \) pairing only. In the case of \( s \)- or \( d \)-wave pairing the diamagnetic pair breaking dominates and, therefore, one should find an additional mechanism (or a specific regime) that makes the diamagnetic pair breaking ineffective. Otherwise AH and attractive PK models lead to \( H_{\text{crit}}(T) \) that significantly differs from \( H_{\text{pg}}(T) \), as can be inferred from Figs. 3 and 5.

Most of the results presented in this section have been obtained for the half-filled band. The inset in Fig. 6 shows the mean-field transition temperature \( T_{\text{crit}} \) as a function of the occupation number \( n \). The inset illustrates the jump of the order parameter at the phase transition. We have used the same model parameters as for the \( \eta \) pairing in Fig. 3. The dotted line shows \( H_{\text{crit}}(T) \) calculated for the AH model without the diamagnetic pair breaking. Here, for \( T/T_{\text{crit}} < 0.6 \) the transition is of the first order.
in strongly overdoped regime. In Fig. 6 we show $H_{\text{crit}}$ calculated away for half filling. As is visible, for small doping the temperature dependence of $H_{\text{crit}}$ is qualitatively the same. Comparison of $H_{\text{crit}}$ calculated in the presence and absence of the diamagnetic pair breaking shows that this mechanism is ineffective for this doping (see solid lines). However, for doping close to $n_c$ this pair breaking becomes important (see dashed lines).

As superconductivity does not occur in exactly two-dimensional systems, one assumes the existence of a weak interplane coupling. When the electrons are not confined to planes the fractal structure of the Hofstadter butterfly is disturbed. The electron movement along the magnetic field is not affected by the field. As a result, the Hofstadter subbands broaden and some of them may overlap. A similar broadening may be induced by disorder. For a strong magnetic field there are only few subbands in the spectrum. Then, a relatively large interplane hopping integral is needed to close gaps between subbands. On the other hand, for realistic values of the magnetic field there is a huge number of very narrow subbands and much weaker interplane coupling may close the gaps. However, this broadening of the Hofstadter subbands does not lead to a substantial modification of our results due to the fact that the energy spectrum enters the Gor’kov equations through the Cooper pairs’ susceptibility. Although, the Cooper pairs’ susceptibility is strongly peaked at the Fermi level, the eigenstates with energies of the order of $k_BT$ (with respect to the Fermi level) give a comparable contribution to the gap equation. Since the number of subbands within the energy range $k_BT$ is already very large, the influence of a weak interplane coupling may be negligible. The importance of the interplane coupling increases at genuinely low temperatures (i.e., for high magnetic field) when only few subbands are located within $k_BT$ range. However, the present approach is not applicable in this regime. The above argumentation may not hold in the case of coherent interlayer tunneling of Cooper pairs. In multilayer HTSC’s this mechanism may amplify superconductivity and enhance the superconducting transition temperature. The onset of the Cooper pair tunneling by the Josephson mechanism at $T_c$ may lead to the decrease of the out-of-plane kinetic energy. However, this mechanism should not affect $T^*$, which is related to the occurrence of incoherent Cooper pairs.

III. SUMMARY

Summarizing, we have investigated the PK model with attractive as well as repulsive pair hopping interaction. We have shown that the repulsive pair hopping term may lead to the occurrence of local minimum in the density of states which is characteristic for the pseudogap phase of underdoped cuprates. It originates from the splitting of the quasi-

particle peaks. Despite the on-site pairing the magnitude of the splitting is a direction-dependent quantity, provided $t' \neq 0$. Anisotropy of the pseudogap is observed in angle-resolved photoemission spectroscopy experiments. We have also calculated the temperature dependence of $H_{\text{crit}}$, defined as the highest magnetic field for which there exists a nonzero solution for the order parameter. We have found that in the case of $\eta$-type pairing, $H_{\text{crit}}(T)$ reproduces experimental data for the pseudogap closing field. These features do not occur for attractive pair hopping interaction. In this case, the gap structure as well as $H_{\text{crit}}(T)$ are similar to those obtained for AH model.

Our approach to the critical field accounts for both Zeeman and diamagnetic pair breaking mechanisms. In the case of $s$-wave pairing inclusion of the Zeeman coupling does not lead to any essential changes in $H_{\text{crit}}(T)$. On the other hand, Zeeman term is of crucial importance for $\eta$ pairing, whereas the diamagnetic pair breaking is ineffective. The experimentally observed $H_{\text{pg}}(T)$ is interpreted in favor of the Zeeman coupling as the pseudogap closing mechanism. If this interpretation is correct, $H_{\text{pg}}$ should be isotropic, i.e., independent of the orientation of magnetic field with respect to CuO$_2$ layers. This can be verified in future experiments (e.g., with magnetic field applied parallel to the CuO$_2$ planes when the orbital effects are absent).

In the absence of diamagnetic pair breaking various models reproduce $H_{\text{pg}}(T)$ properly. In order to choose the most appropriate one, it should be verified which of them allow for neglecting the diamagnetic pair breaking without additional assumptions. The PK model with $J<0$ is unique in a sense that the gap is closed predominantly due to the Zeeman interaction. As we have previously shown, other models appropriate for short coherence superconductors have ground states (with $s$-wave or $d$-wave symmetry) that are almost insensitive to the Zeeman interaction.

Collecting the features of $\eta$-paired state, the presence of the pseudogap, its anisotropy, Zeeman origin of $H_{\text{crit}}$, the presence of flux quantization, and the Meissner effect (consistent with the preformed Cooper pairs scenario), may lead to a tempting hypothesis that the pair hopping can be responsible for the pseudogap in HTSC’s. However, in order to avoid the problem of interpretation of the critical field, it should be verified beyond the mean-field level discussed in this paper.

ACKNOWLEDGMENTS

We acknowledge a fruitful discussion with S. Robaszkiewicz. This work was supported in part by the Polish State Committee for Scientific Research, Grant No. 2 P03B 050 23.

---

*Electronic address: maciek@phys.us.edu.pl


