Field Driven Pairing State Phase Transition in $d_{x^2−y^2} + i d_{xy}$-Wave Superconductors

Bo Lei$^1$, S. A. Aruna$^1$, and Qiang-Hua Wang$^{1,2}$

$^1$Physics Department and National Laboratory of Solid State Microstructures, Institute for Solid State Physics, Nanjing University, Nanjing 210093, China
$^2$Physics Department, University of California at Berkeley, CA 94720

Within the framework of the Ginzburg-Landau theory for $d_{x^2−y^2} + i d_{xy}$-wave superconductors, we discuss the pairing state phase transition in the absence of the Zeeman coupling between the Cooper pair orbital angular momentum and the magnetic field. We find that above a temperature $T_a$, the pairing state in a magnetic field is pure $d_{x^2−y^2}$-wave. However, below $T_a$, the pairing state is $d_{x^2−y^2} + i d_{xy}$-wave at low fields, and it becomes pure $d_{x^2−y^2}$-wave at higher fields. Between these pairing states there exists a field driven phase transition. The transition field increases with decreasing temperature. In the field-temperature phase diagram, the phase transition line is obtained theoretically by a combined use of a variational method and the Virial theorem. The analytical result is found to be in good agreement with numerical simulation results of the Ginzburg-Landau equations. The validity of the variational method is discussed. The difference to the case with the Zeeman coupling is discussed, which may be utilized to the detection of the Zeeman coupling.

74.60.Ec, 74.25.Dw, 74.20.De

The phase-sensitive experiment with a tricrystal superconducting ring magnetometry demonstrated that in high temperature superconductors, the dominant pairing channel is the $d_{x^2−y^2}$-wave one. However, it is not yet clear whether there were some sub-dominant pairing channels. It is even less clear what would be the symmetry of a sub-dominant pairing channel if it existed at all. Such questions arise from a number of experiments, e.g., the observation of surface-induced broken time-reversal-symmetry ($T$ hereafter) in YBCO tunnel junctions, the observation of fractional vortices trapped in a boundary junction, and the abnormal field dependence of the low temperature thermal conductivity $k_c$ in BSCCO superconductors. These unusual phenomena can not be adequately explained by the $d_{x^2−y^2}$-wave pairing channel alone. Some sub-dominant channels (such as $s$- or $d_{xy}$-wave ones) might have played a role in these phenomena. Thus it is interesting to study theoretically the properties of the superconductors in the presence of sub-dominant pairing channels.

As a model study, we consider the relevant singlet sub-dominant pairing channel to be the $d_{xy}$-channel, which has been hotly discussed recently in the context of the abnormal thermal conductivities in BSCCO superconductors. In this paper, using a Ginzburg-Landau (GL) theory for $d_{x^2−y^2} + i d_{xy}$-wave superconductors, we discuss the pairing state phase transition driven by the magnetic field. In the absence of the Zeeman coupling between the Cooper pair orbital angular momentum and the magnetic field (see below), we find that above a temperature $T_a$, the pairing state in a magnetic field is pure $d_{x^2−y^2}$-wave. However, below $T_a$, the pairing state is $d_{x^2−y^2} + i d_{xy}$-wave at low fields, and it becomes pure $d_{x^2−y^2}$-wave at higher fields. There exists a field driven phase transition between these pairing states. The transition field increases with decreasing temperature. In the field-temperature phase diagram, we are able to obtain the phase transition line using a variational method and the Virial theorem. The analytical result is in good agreement with that obtained from numerical simulation of the Ginzburg-Landau equations.

The GL free energy of a $d_{x^2−y^2} + i d_{xy}$-wave superconductor can be obtained from the modified Bardeen-Cooper-Shrieffer (BCS) gap equation, the Gor'kov theory or path integral formulation (in the weak coupling limit),

$$F = \int_{\Omega} \alpha_D |D|^2 + \alpha_D |D'|^2 + \Gamma[3|D|^4/8 + 3|D'|^2/8$$
$$+ |D|^2 |D'|^2/4 + (D^* D' + c.c.)^2/8]$$
$$+ K \left|\mathbf{II}D\right|^2 + \left|\mathbf{II}D'\right|^2 \right| + \int_{\Omega} (\nabla \times \mathbf{A})^2/8\pi,$$  \hspace{1cm} (1)

where $\Omega$ denotes integration over the $\alpha$-plane, $\mathbf{II} = -i\nabla - 2e\mathbf{A}/hc$ is the gauge invariant gradient and $\mathbf{B} = \nabla \times \mathbf{A}$ is the local induction (in the $z$-, or $c$-, direction). Here $D$ and $D'$ are order parameters in the $d_{x^2−y^2}$- and $d_{xy}$-channels, respectively. $\alpha_i = N(0)\ln T/T_i$ ($i = D, D'$), where $N(0)$ is the normal state density of states, and $T_i$ is the bare superconducting critical temperature in the $i$ channel. $K$ and $\Gamma$ are material-dependent parameters derivable from microscopic theories and are assumed to be temperature independent here for simplicity. We assume that $T_{D'} \ll T_D$, i.e., the dominant pairing channel is the $d_{x^2−y^2}$-wave channel, as this would be consistent with high temperature superconductors. In this paper, we do not consider the Zeeman coupling term $F_z \propto -iB(D^* D' - c.c.)$ in the free energy. On one hand, $F_z$ needs further identification by a strong coupling microscopic theory. On the other hand, the pairing states in a magnetic field in the absence of $F_z$ is interesting in its own right and should be compared to that in the...
the linearized GL equations, it was found that the upper critical field \( b_{c2} = B_{c2}/B_0 = 1 \) as long as \( \alpha \leq 1 \) (or \( T > 0K \)). Moreover, at the upper critical field the eigen solution to the linearized GL equations indicates that the order parameter \( d' \) vanishes identically, although it would be nonzero at the same temperature (\( < T_* \)) but at zero field. (iii) Combining both aspects we believe that there should be a field-driven pairing-state phase transition at \( T < T_* \) (or \( \alpha > \alpha_* \)), where at zero and low fields, the pairing state is the \( d_{x^2-y^2} \) wave, while at higher fields, it transforms to the pure \( d_{x^2-y^2} \)-wave. The mechanism is clear. Since the two order parameters are not coupled by mixed gradient terms, they are frustrated in the vortex state: while the coexistence of them lowers the homogeneous energy at \( \alpha > \alpha_* \), winding of both order parameters due to vortices increases the kinetic energy. The competing energies should drive a phase transition. Moreover, the transition field should increase with \( \alpha \) as the gaining of homogeneous energy increases relatively. On the other hand, at \( T > T_* \), the pairing state is always the pure \( d_{x^2-y^2} \)-wave at any fields below the upper critical field. This picture will be discussed in detail, in the proceeding section.

In our case, there are two order parameters. Even approximate solutions to the GL equations, such as for the conventional superconductors, \(^{13}\) are difficult to obtain. Thus we shall restrict ourselves to the variational treatment of the system. The basic idea is as follows. We employ a reference conventional system with one order parameter \( \psi \), and set \( d \) and \( d' \) to vary in space in the same manner as \( \psi \) does, but with different amplitudes which are to be optimized. Consequently, the behavior of the present system is then approximately given by these amplitudes.

For our purpose, let us recapitulate some known results for the reference system. The free energy is written as

\[
F = E_c \int \left\{ -|\psi|^2 + \frac{1}{2} (|\psi|^4 + |\psi|^2 + \kappa^2 b^2 \right\},
\]

where \( E_c = H_c^2 \xi^2 / 4\pi \) with \( H_c \) and \( \xi \) being the thermodynamic critical field and coherence length, respectively, in the absence of the \( d_{xy} \)-wave channel. All quantities under the integration symbol are now dimensionless: \( \alpha = \alpha_{D'} / \alpha_D = \ln(T/T_D) / \ln(T/T_D) \), \( d = D / D_0 \), \( d' = D'/D_0 \), \( r = R/\xi \), \( a = A / A_0 \), and \( b = B / B_0 \). Here \( D_0 = \sqrt{-4 \alpha_D / 3T} \) is the value of \( D \) in the absence of the order parameter \( D' \) and the magnetic field. \( \kappa \) (with \( \kappa \) is the corresponding upper critical field. Finally, \( \pi = -i \nabla - a \) now denotes dimensionless gauge invariant gradient (i.e., \( \pi = \Pi \xi \)).

The important difference between the above GL free energy Eq.\(^2\) and that for a \( d + is \)-wave superconductor lies in the fact that in the former, we have no mixed gradient coupling between the two order parameters. \(^{10}\) Therefore, we can expect that the single vortex remains to be circularly symmetric. This should be contrasted to the four-fold and two-fold symmetric vortices in \( d + is \) wave superconductors. \(^{11}\) An even more subtle consequence of the absence of the mixed gradient is that there are three possible solutions, namely: the pure \( d \) solution, the pure \( d' \) solution, and the mixed-wave solution. The physical solution of the system corresponds to that with the lowest free energy. In this respect, it is not impossible that there would be a phase transition between these solutions in the field-temperature phase diagram. Indeed, this picture was conjectured recently from the behaviors of the superconductor at zero field and the upper critical field, \(^4\) which we summarize for completeness as follows.

(i) At zero field, it is easy to see that the two order parameters develop a relative phase difference of \( \pm \pi/2 \) in order to minimize the free energy. This \( d_{x^2-y^2} \pm id_{xy} \)-wave pairing state is \( T \)-breaking, which was recently argued to be relevant to the abnormal thermal conductivity in BSCCO superconductors. \(^{17}\) The amplitudes of the two order parameters are \( d^2 = 3(3 - \alpha) / 8 \) and \( d'^2 = 3(3\alpha - 1) / 8 \). Thus, \( d_{xy} \)-wave appears only when \( \alpha > 1 / 3 \), with a \( T \)-breaking transition point at \( \alpha_* = 1 / 3 \). According to the above definition of \( \alpha \), this amounts to a transition temperature \( T_* = \sqrt{T_D^3 / T_D} \). The zero-field \( T \)-breaking transition is a second-order phase transition, in that \( d' \) emerges continuously at \( T < T_* \). (ii)
\(d' = \pm i\nu \psi\), with two real and positive variational amplitudes \(\mu\) and \(\nu\). The \(d'\) order parameter adopts a residual relative phase to \(d\) in order to lower the free energy Eq.\(5\). Substitution of these ingredients into Eq.\(2\) yields a free energy in terms of \(\mu, \nu\), and \(e_i\) \((i = 2, 4, k)\). In dimensionless form, the free energy density is

\[
f = \mu^2 e_2 + \alpha \nu^2 e_2 + (\mu^4 + \nu^4)e_4 + 2\mu^2 \nu^2 e_1^2/3 + (\mu^2 + \nu^2)e_k + \kappa^2 b^2.
\]  

(5)

Minimizing \(f\) with respect to \(\mu\) and \(\nu\), we get:

\[
\mu^2 = 3[(\alpha - 3)e_2 - 2e_k]/(16e_4);
\]  

(6)

\[
\nu^2 = 3[(1 - 3\alpha)e_2 - 2e_k]/(16e_4).
\]  

(7)

At low and intermediate fields, the magnetization curve in the reference system in the limit \(\kappa \gg 1\) is: \(h = \frac{b + \ln(1/b)}{2\kappa^2}\) (in dimensionless form). In combination with Eq.\(4\), we have \(e_k = b\ln(1/b)\). On the other hand, in the present field regime, the distance between two vortices is much larger than the coherence length, hence we can assume \(e_2 \simeq -1\) and \(e_4 \simeq 1/2\). This approximation would certainly violate Eq.\(4\) up to the order of \(e_k < 1\), but suffices to yield an order of magnitude estimate of \(\mu\) and \(\nu\). Substituting the approximate \(e_i\)’s into Eqs.\(5\) and \(6\), we get \(\mu^2 \approx 3(3/2 - \alpha/2 - b\ln(1/b))/4\), and \(\nu^2 \approx 3(-1/2 + 3\alpha/2 - b\ln(1/b))/4\). We clearly see that \(\mu^2 > 0\) as long as \(\alpha \leq 1\) (i.e., \(d_{xy}\)-channel is subdominant). This means that the \(d_{x^2-y^2}\)-wave order parameter \(d\) is always present in the system. The \(d_{xy}\)-wave order parameter \(d'\) is present provided that \(\nu^2 > 0\). Thus the field-driven phase transition is determined by \(\nu^2 = 0\), or

\[
b\ln(1/b) = (3\alpha - 1)/2.
\]  

(8)

At high fields closer to the upper critical field, the vortices are densely distributed, hence the system can not be treated as above because the order parameters are drastically suppressed by the magnetic field. Fortunately, in this case we can resort to the high-field Abrikosov vortex lattice solution. In the reference system one has \(2e_4 = \beta_A e_2^2\), where \(\beta_A\) is the Abrikosov constant. We combine this with Eq.\(4\) to find \(e_2 = (\sqrt{1 - 4\beta_A e_4} - 1)/(2\beta_A)\). On the other hand, the dimensionless magnetization curve in high fields is \(h = (1 - b)/(2\kappa^2\beta_A)\), [2] substitution of which into Eq.\(4\) gives \(e_k = b(1 - b)/\beta_A\). Putting the above together, we have in the high field regime: \(\mu^2 = 3[(\alpha - 3)e_2 - 2e_k]/(8\beta_A e_4^2)\), and \(\nu^2 = 3[(1 - 3\alpha)e_2 - 2e_k]/(8\beta_A e_4^2)\), where both \(e_2\) and \(e_k\) can be expressed as functions of \(b\). Again the condition \(\nu^2 = 0\) determines the field-driven phase transition line:

\[
b = (1 + \sqrt{9\alpha^2 - 12\alpha + 4})/2.
\]  

(9)

The phase transition lines Eqs.\(8\) and \(9\) are the main results of this work. They are plotted in Fig.1 (solid lines). Note that we have skipped the unphysical portions of Eq.\(8\) at high fields and Eq.\(9\) at low fields. Also note that the dimensionless upper critical field is unity, but the physical upper critical field \(B_c\) depends on temperature.

On the other hand, \(\alpha\) depends on temperature also (see the definition above). The field regime between the two solid lines in Fig.1 can not be determined theoretically by our approach, in that the order parameters are already suppressed by the field so that the London approximation fails on one hand, but the Abrikosov solution is still not reliable enough on the other hand.

In order to check the accuracy of the variational method, we now obtain the transition line by numerical simulation of the GL equations derived from Eq.\(2\). The simulation is performed in a unit cell of the vortex lattice and the magnetic induction is treated as being uniform for simplicity. The latter assumption is suitable at not too low fields and at \(\kappa \gg 1\), which is relevant to high-\(T_c\) superconductors. The simulation method is well documented in the literature. [3] From our simulation result, it is verified that the local relative phase difference between the two order parameters is indeed \(\pm \pi/2\). This result provides a strong support to the validity of our analytical treatment. The maximum amplitude of the order parameter \(d'\) in the vortex solution, namely, \(|d'|_{\text{max}} = |D'|_{\text{max}}/D_0\), as a function of \(\alpha\) at various magnetic fields is plotted in Fig.2, where we can clearly see that at a fixed field, \(d'\) drops to zero at a specific value of \(\alpha\). This signals a field-driven phase transition from the \(d_{x^2-y^2} + id_{xy}\)-wave pairing state to the pure \(d_{x^2-y^2}\)-wave one (with vortices in the system). The transition value of \(\alpha\) decreases with decreasing magnetic field. The set of transition points are plotted in Fig.1 (squares). In the high field regime, the analytical result is in good agreement with the numerical result, whereas in the low field regime, the result is only in qualitative agreement. This is understandable from the fact that we have neglected the vortex core energy and have adopted a crude approximation for the spatial variation of the order parameters in our analytical treatment. In principle, the two order parameters have different coherence lengths. They determine the length scales for the spatial variations of the order parameters. Our approximation is equivalent to assign the same coherence length to both order parameters. The good agreement at high fields is also understandable from the view that in this case the vortices are strongly overlapped so that the length scale approximation is not essential. In numerical simulations we find some signs of abrupt drop of \(d'\) as a function of \(b\) or \(\alpha\) in the parameter space. This may points to a weakly first-order transition. However, our analytical result is clearly a second order phase transition within the specified approximation.

Before closing, let us comment on the difference of our system to that with a Zeeman coupling. In the latter case, it was shown that a \(d_{x^2-y^2} + id_{xy}\) pairing state is always induced by vortices. [3] In other words, there
is no further pairing state phase transition in intermediate magnetic fields. Moreover, Balatsky [16] recently argued that the Zeeman coupling enhances superconductivity near the upper critical field. These distinct differences to the case discussed above can be utilized for the detection of the Zeeman coupling.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China and the National Centre for Research and Development of Superconductivity of China. QHW was also supported by the Berkeley Scholars Program financed by the Hutchison Whampoa Company, Hong Kong.

[1] C. C. Tsuei, J. R. Kirtley, M. Rupp, J. Z. Sun, A. Gupta, M. B. Ketchenm, C. A. Wang, and Z. F. Ren, J. H. Wang, and M. Bhushan, Science 271, 329 (1996)
[2] M. Covington, et al, Phys. Rev. Lett. 79, 277 (1997); M. Fogelström, D. Rainer, and J. A. Sauls, ibid 79, 281 (1997).
[3] J. R. Kirtley, et al, Phys. Rev. B 51, 12057 (1995). M. Sgrist, D. B. Bailey, and R. B. Laughlin, Phys. Rev. Lett. 74, 3249 (1995) for a theoretical interpretation.
[4] K. Krishana, et al, Science 277, 83 (1997).
[5] H. Aubin, K. Behnia, S. Ooi, and T. Tamegai, Phys. Rev. Lett. 82, 624 (1999).
[6] R. B. Laughin, Phys. Rev. Lett. 80, 5188 (1998).
[7] Qiang-Hua Wang, Z. D. Wang and Q. Li, Phys. Rev. B 60, 15364(1999)
[8] T. Koyama, and M. Tachiki, Phys. Rev. B 53, 2662(1996).
[9] Qiang-Hua Wang, and Z. D. Wang, cond-mat/9909399.
[10] Yong Ren, Ji-Hai Xu, and C. S. Ting, Phys. Rev. B 53, 2249 (1996).
[11] Q. Li, Z. D. Wang and Qiang-Hua Wang, Phys. Rev. B 59, 613 (1999)
[12] M. Tinkham, “Introduction to Superconductivity”, McGraw-Hill 1996.
[13] M. M. Doria, J. E. Gubernatis, and D. Rainer, Phys. Rev. B 39, 9573 (1989).
[14] The Virial theorem in full dimension reads: $\frac{1}{2} HB = E_k + 2E_f$ where $H$ is the applied magnetic field, $B$ is the average induction field, $E_k$ is the kinetic energy of the superfluid, and finally, $E_f$ is the magnetic energy in the GL free energy. [13]
[15] Q. Wang and Z. D. Wang, Phys. Rev. B 54, 15645 (1996); Z. D. Wang and Q.-H. Wang, ibid. 55, 11756 (1997).
[16] A. V. Balatsky, Phys. Rev. B 61, 6940 (2000); cond-mat/9903272.
[17] Mei-Rong Li, P. J. Hirshfeld, and P. Wöfle, cond-mat/0003160.

FIG. 1. Solid lines: analytical phase transition line; Squares: transition points extracted from numerical simulations. The error bars indicate the increment of the field in the field-scanning.
FIG. 2. The maximum of $|d'|$, i.e., $|D'|_{\max}/D_0$ as a function of $\alpha$ at various fields. The arrows indicate the estimated positions at which $d'$ drops to zero.