Phase transition from a $d_{x^2-y^2}$ to $d_{x^2-y^2} + id_{xy}$ superconductor

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Abstract

The temperature dependencies of specific heat and spin susceptibility of a coupled $d_{x^2-y^2} + id_{xy}$ superconductor in the presence of a weak $d_{xy}$ component are investigated in the tight-binding model (1) on square lattice and (2) on a lattice with orthorhombic distortion. As the temperature is lowered past the critical temperature $T_c$, first a less ordered $d_{x^2-y^2}$ superconductor is created, which changes to a more ordered $d_{x^2-y^2} + id_{xy}$ superconductor at $T_{c1} (< T_c)$. This manifests in two second order phase transitions identified by two jumps in specific heat at $T_c$ and $T_{c1}$. The temperature dependencies of the superconducting observables exhibit a change from power-law to exponential behavior as temperature is lowered below $T_{c1}$ and confirm the new phase transition.

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The unconventional high-$T_c$ superconductors [1] with a high critical temperature $T_c$ have a complicated lattice structure with extended and/or mixed symmetry for the order parameter [2,3]. For many of these high-$T_c$ materials, the order parameter exhibits anisotropic behavior. The detailed nature of anisotropy was thought to be typical to that of an extended $s$-wave, a pure $d$-wave, or a mixed $(s + \exp(i\theta)d)$-wave type. Some high-$T_c$ materials have singlet $d$-wave Cooper pairs and the order parameter has $d_{x^2-y^2}$ symmetry in two dimensions [2,3], which has been supported by recent studies of temperature dependence of some superconducting observables [1,12]. In some cases there is the signature of an extended $s$- or $d$-wave symmetry. The possibility of a mixed angular-momentum-state symmetry was suggested sometime ago by Ruckenstein et al. and Kotliar [14,15]. There are experimental evidences based on Josephson supercurrent for tunneling between Pb and YBa$_2$Cu$_3$O$_7$ (YBCO) [16], and on photoemission studies on Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ [17] among others which are difficult to reconcile employing a pure $s$- or $d$-wave order parameter. These observations suggest that a mixed $[s + \exp(i\theta)d]$ symmetry is applicable in these cases [18,19].

More recently Krishana et al. [20] reported a phase transition in the high-$T_c$ superconductor Bi$_2$Sr$_2$CaCu$_2$O$_8$ induced by a magnetic field from a study of the thermal conductivity as a function of temperature and magnetic field. Laughlin [21] have suggested that the new superconducting phase is the time-reversal symmetry breaking $d_{x^2-y^2} + id_{xy}$ state. Similar conclusion has been reached by Ghosh [22] in a recent work from a study of the temperature dependence of thermal conductivity. This has led to the possibility of the transition to a $d_{x^2-y^2} + id_{xy}$ phase from a pure $d_{x^2-y^2}$ phase of Bi$_2$Sr$_2$CaCu$_2$O$_8$. From a study of vortex in a $d$-wave superconductor using a self-consistent Bogoliubov-de Gennes formalism, Franz and Tešanović [23] also predicted the possibility of the creation of a $d_{x^2-y^2} + id_{xy}$ superconducting state. Although, the creation of the mixed superconducting state $d_{x^2-y^2} + id_{xy}$ is speculative, Franz and Tešanović conclude that a dramatic change should be observed (in the observables of the superconductor) as the superconductor undergoes a phase transition from a $d_{x^2-y^2}$ state to a $d_{x^2-y^2} + id_{xy}$ state. In this work we study the effect of this
phase transition on superconducting specific heat and spin susceptibility in the absence of magnetic field. The general trend of observables under the $d_{x^2-y^2}$ to $d_{x^2-y^2} + id_{xy}$ wave phase transition of the superconductor, as studied here, is expected to be independent of the external magnetic field. We recall that there have been several studies on the formation of a mixed $(s + id)$-wave superconducting state from a pure $d$-wave state \[24–29\].

First we study the temperature dependence of the order parameter of the mixed $d_{x^2-y^2} + id_{xy}$ state within the Bardeen-Cooper-Schrieffer (BCS) model \[30,31\]. The BCS model for a mixed $d_{x^2-y^2} + id_{xy}$ state becomes a coupled set of equations. The ratio of the strengths of the $d_{x^2-y^2}$- and $d_{xy}$-wave interactions should lie in a narrow region in order to have a coexisting $d_{x^2-y^2}$- and $d_{xy}$-wave phases in the case of $d_{x^2-y^2} + id_{xy}$ symmetry. As the $d_{x^2-y^2}$-wave ($d_{xy}$-wave) interaction becomes stronger, the $d_{xy}$-wave ($d_{x^2-y^2}$-wave) component of the order parameter quickly reduces and disappears and a pure $d_{x^2-y^2}$-wave ($d_{xy}$-wave) state emerges.

The order parameter of each of $d_{x^2-y^2}$ and $d_{xy}$ states has nodes on the Fermi surface and may change sign along the Fermi surface. The $s$-wave order parameter does not have this property. Because of this, many $d$-wave superconducting observables have power-law dependence on temperature, whereas the $s$-wave observables exhibit exponential dependence. We find that in the present coupled $d_{x^2-y^2} + id_{xy}$ state the order parameter does not exhibit nodes and change of sign along the Fermi surface and exhibits a typical $s$-wave like behavior. Consequently, the observables in the coupled $d_{x^2-y^2} + id_{xy}$ state does not exhibit typical $d$-wave power-law dependence on temperature, but rather a typical $s$-wave exponential dependence.

For a weaker $d_{xy}$-wave admixture, in the present study we establish in the two-dimensional tight-binding model (1) on square lattice and (2) on a lattice with orthorhombic distortion another second-order phase transition at $T = T_{c1} < T_c$, where the superconducting phase changes from a pure $d_{x^2-y^2}$-wave state for $T > T_{c1}$ to a mixed $d_{x^2-y^2} + id_{xy}$-wave state for $T < T_{c1}$. The specific heat exhibits two jumps at the transition points $T = T_{c1}$ and $T = T_c$. The temperature dependencies of the superconducting specific heat and spin...
susceptibility change drastically at $T = T_{c1}$ from power-law behavior for $T > T_{c1}$ to exponential behavior for $T < T_{c1}$. We find that the observables for the normal state are closer to those for a pure superconducting $d_{xy}$ state than to those for a pure superconducting $d_{x^2-y^2}$ state. Consequently, superconductivity in $d_{x^2-y^2}$ wave is more pronounced than in pure $d_{xy}$ wave. Hence as temperature decreases the system passes from the normal state to a “less” superconducting $d_{x^2-y^2}$-wave state at $T = T_c$ and then to a “more” superconducting state $d_{x^2-y^2} + i d_{xy}$ with dominating s-wave behavior at $T = T_{c1}$ signaling a second phase transition.

The profound change in the nature of the superconducting state at $T = T_{c1}$ becomes apparent from a study of the entropy. At a particular temperature the entropy for the normal state is larger than that for all superconducting states signaling an increase in order in the superconducting state. In the case of the present $d_{x^2-y^2} + i d_{xy}$ state we find that as the temperature is lowered past $T_{c1}$, the entropy of the superconducting $d_{x^2-y^2} + i d_{xy}$ state decreases very rapidly (not shown explicitly in this work) indicating the appearance of a more ordered superconducting phase and a second phase transition.

We base the present study on the two-dimensional tight binding model which we describe below. This model is sufficiently general for considering mixed angular momentum states, with or without orthorhombic distortion, employing nearest and second-nearest-neighbor hopping integrals. The effective interaction in this case can be written as

$$V_{kq} = -V_1 (\cos k_x - \beta \cos k_y)(\cos q_x - \beta \cos q_y)$$

$$- V_2 (\sin k_x \sin k_y)(\sin q_x \sin q_y).$$

Here $V_1$ and $V_2$ are the couplings of effective $d_{x^2-y^2}$- and $d_{xy}$-wave interactions, respectively. As we shall consider Cooper pairing and subsequent BCS condensation in both these waves the constants $V_1$ and $V_2$ will be taken to be positive corresponding to attractive interactions. In this case the quasiparticle dispersion relation is given by

$$\epsilon_k = -2t[\cos k_x + \beta \cos k_y - \gamma \cos k_x \cos k_y],$$

(2)
where $t$ and $\beta t$ are the nearest-neighbor hopping integrals along the in-plane $a$ and $b$ axes, respectively, and $\gamma t/2$ is the second-nearest-neighbor hopping integral.

We consider the weak-coupling BCS model in two dimensions with $d_{x^2-y^2}+id_{xy}$ symmetry. At a finite $T$, one has the following BCS equation

$$\Delta_k = -\sum_q V_{kq} \frac{\Delta_q}{2E_q} \tanh \frac{E_q}{2k_BT}$$

with $E_q = [(\epsilon_q - E_F)^2 + |\Delta_q|^2]^{1/2}$, where $E_F$ is the Fermi energy and $k_B$ the Boltzmann constant. The order parameter $\Delta_q$ has the following anisotropic form: $\Delta_q \equiv \Delta_1 (\cos q_x - \beta \cos q_y) + i \Delta_2 \sin q_x \sin q_y$. Using the above form of $\Delta_q$ and potential (1), Eq. (3) becomes the following coupled set of BCS equations

$$\Delta_1 = V_1 \sum_q \frac{\Delta_1 (\cos q_x - \beta \cos q_y)^2}{2E_q} \tanh \frac{E_q}{2k_BT}$$

$$\Delta_2 = V_2 \sum_q \frac{\Delta_2 (\sin q_x \sin q_y)^2}{2E_q} \tanh \frac{E_q}{2k_BT}$$

where the coupling is introduced through $E_q$. In Eqs. (4) and (5) both the interactions $V_1$ and $V_2$ are assumed to be energy-independent constants for $|\epsilon_q - E_F| < k_BT_D$ and zero for $|\epsilon_q - E_F| > k_BT_D$, where $k_BT_D$ is the usual Debye cutoff.

The specific heat is given by

$$C(T) = -\frac{2}{T} \sum_q \frac{\partial f_q}{\partial E_q} \left( E_q^2 - \frac{1}{2} T \frac{d||\Delta_q||^2}{dT} \right)$$

where $f_q = 1/(1 + \exp(E_q/k_BT))$. The spin susceptibility $\chi$ is defined by

$$\chi(T) = \frac{2\mu_N^2}{T} \sum_q f_q (1 - f_q)$$

where $\mu_N$ is the nuclear magneton.

We solved the coupled set of equations (4) and (5) numerically by the method of iteration and calculated the gaps $\Delta_1$ and $\Delta_2$ at various temperatures for $T < T_c$. We have performed calculations (1) on a perfect square lattice and (2) in the presence of an orthorhombic distortion with Debye cut off $k_BT_D = 0.02586$ eV ($T_D = 300$ K) in both cases. The parameters
for these two cases are the following: (1) Square lattice – (a) $t = 0.2586$ eV, $\beta = 1, \gamma = 0, V_1 = 0.73t$, and $V_2 = 6.8t, T_c = 71$ K, $T_{c1} = 28$ K; (b) $t = 0.2586$ eV, $\beta = 1, \gamma = 0, V_1 = 0.73t$, and $V_2 = 7.9t, T_c = 71$ K, $T_{c1} = 47$ K; (2) Orthorhombic distortion – (a) $t = 0.2586$ eV, $\beta = 0.95, and \gamma = 0, V_1 = 0.97t$, and $V_2 = 6.5t, T_c = 70$ K, $T_{c1} = 25$ K; (b) $t = 0.2586$ eV, $\beta = 0.95, and \gamma = 0, V_1 = 0.97t$, and $V_2 = 8.0t, T_c = 70$ K, $T_{c1} = 52$ K. For a very weak $d_{x^2-y^2}$-wave ($d_{xy}$-wave) coupling the only possible solution corresponds to $\Delta_2 = 0$ ($\Delta_1 = 0$).

In Figs. 1 and 2 we plot the temperature dependencies of different $\Delta$’s for the following two sets of $d_{x^2-y^2} + id_{xy}$-wave corresponding to models 1 and 2 above (full line – models 1(a) and 2(a); dashed line – models 1(b) and 2(b)), respectively. In both cases the temperature dependence of the $\Delta$’s are very similar. In the coupled $d_{x^2-y^2} + id_{xy}$-wave as temperature is lowered past $T_c$, the parameter $\Delta_1$ increases up to $T = T_{c1}$. With further reduction of temperature, the parameter $\Delta_2$ becomes nonzero and begins to increase and eventually both $\Delta_1$ and $\Delta_2$ first increases and then saturates as temperature tends to zero. Recently, the temperature dependencies of the order parameter of the $d_{x^2-y^2} + is$-wave superconducting state has been studied, where at $T = T_{c1}$, the transition from $d_{x^2-y^2}$ to $d_{x^2-y^2} + is$ state takes place. In that case, below $T = T_{c1}$ the $d_{x^2-y^2}$-wave component of the order parameter is suppressed, as the $s$-wave component becomes nonzero. No such suppression of the $d_{x^2-y^2}$-wave takes place in this case as the $d_{xy}$ component appears.

Now we study the temperature dependence of specific heat in some detail. The different superconducting and normal specific heats are plotted in Figs. 3 and 4 for square lattice [models 1(a) and 1(b)] and orthorhombic distortion [models 2(a) and 2(b)], respectively. In both cases the specific heat exhibits two jumps – one at $T_c$ and another at $T_{c1}$. From Eq. (6) and Figs. 1 and 2 we see that the temperature derivative of $|\Delta_1|^2$ has discontinuities at $T_c$ and $T_{c1}$ due to the vanishing of $\Delta_1$ and $\Delta_2$, respectively, responsible for the two jumps in specific heat. For a pure $d_{x^2-y^2}$ wave we find that the specific heat exhibits a power-law dependence on temperature. However, the exponent of this dependence varies with
temperature. For small \( T \) the exponent is approximately 2.5, and for large \( T \) \( (T \to T_c) \) it is nearly 2. In the \( d_{x^2-y^2} + id_{xy} \) model, for \( T_c > T > T_{c1} \) the specific heat exhibits \( d_{x^2-y^2} \)-wave power-law behavior; for \( T < T_{c1} \) the specific heat exhibits an \( s \)-wave like exponential behavior. For the \( d \)-wave model \( d_{x^2-y^2}, C_s(T_c)/C_n(T_c) \) is a function of \( T_c \) and \( \beta \). In Figs. 3 and 4 this ratio, for \( T_c = 70 \text{ K}, \) is approximately 3 (2.5) for \( \beta = 1 \) (0.95). In a continuum \( d \)-wave calculation this ratio was 2 in the absence of a van Hove singularity [12,13]. We also calculated the specific heat for the pure \( d_{xy} \) case. For square lattice with \( V_1 = 9.0 \) we obtain \( T_c = 67 \text{ K} \) and \( C_s(T_c)/C_n(T_c) = 1.82 \) and \( C_s(T)/C_n(T_c) \sim (T/T_c)^{1.4} \) for the whole temperature range. For orthorhombic distortion \( \beta = 0.95 \), with \( V_1 = 9.0 \) we obtain \( T_c = 69 \text{ K} \) and \( C_s(T_c)/C_n(T_c) = 1.94 \) and \( C_s(T)/C_n(T_c) \sim (T/T_c)^{1.5} \) for the whole temperature range. This power-law behavior with temperature in both the \( d \) waves is destroyed in the coupled \( d_{x^2-y^2} + id_{xy} \) wave and for \( T < T_{c1} \), we find an \( s \)-wave-like exponential behavior in both cases. In both the uncoupled \( d \) waves the order parameter \( \Delta \) has nodes on the Fermi surface and changes sign and this property is destroyed in the coupled \( d_{x^2-y^2} + id_{xy} \) wave, where the order parameter has a typical \( s \) wave behavior.

In Fig. 5 we study the jump \( \Delta C \) in the specific heat at \( T_c \) for pure \( s \)- and \( d \)-wave superconductors as a function of \( T_c \), where we plot the ratio \( \Delta C/C_n(T_c) \) versus \( T_c \). For a BCS superconductor in the continuum \( \Delta C/C_n(T_c) = 1.43 \) (1.0) for \( s \)-wave \( (d \)-wave) independent of \( T_c \) [12,13,31]. Because of the presence of the van Hove singularity in the present model this ratio increases with \( T_c \) as can be seen in Fig. 5. For a fixed \( T_c \), the ratio \( \Delta C/C_n(T_c) \) is larger for square lattice \( (\beta = 1) \) than that for a lattice with orthorhombic distortion \( (\beta = 0.95) \) for both \( s \) and \( d_{x^2-y^2} \) waves. However, for a \( d_{xy} \)-wave superconductor \( \Delta C/C_n(T_c) \) is smaller for square lattice \( (\beta = 1) \) than that for a lattice with orthorhombic distortion \( (\beta = 0.95) \). The jump in \( d_{xy} \) wave is smaller than that for \( s \) and \( d_{x^2-y^2} \) waves. At \( T_c = 100 \text{ K}, \) in the \( s \)-wave \( (d_{x^2-y^2} \)-wave) square lattice case this ratio could be as high as 3.63 (2.92), whereas for \( d_{xy} \) wave this ratio at 100 K is 1.15 (1.25) for square lattice (orthorhombic distortion).

Next we study the temperature dependencies of spin susceptibility for square lattice and
in the presence of orthorhombic distortion which we exhibit in Figs. 6 and 7, respectively. There we plot the results for pure $d_{x^2-y^2}$, $d_{xy}$, and $s$ waves for comparison, in addition to those for models 1(a), 1(b), 2(a) and 2(b). In all cases reported in these figures $T_c \approx 70$ K. For pure $d$-wave cases we obtain power-law dependencies on temperature. The exponent for this power-law scaling is independent of critical temperature $T_c$ but vary from a square lattice to that with an orthorhombic distortion. For $d_{x^2-y^2}$ wave, the exponent for square lattice (orthorhombic distortion, $\beta = 0.95$) is 2.6 (2.4). For $d_{xy}$ wave, the exponent for square lattice (orthorhombic distortion, $\beta = 0.95$) is 1.1 (1.6). For the mixed $d_{x^2-y^2} + id_{xy}$ wave, $d_{x^2-y^2}$-wave power-law behavior is obtained for $T_c > T > T_{c1}$. For $T < T_{c1}$, one has a typical $s$-wave behavior.

In conclusion, we have studied the $(d_{x^2-y^2} + id_{xy})$-wave superconductivity employing a two-dimensional tight binding BCS model on square lattice and also for orthorhombic distortion. We have kept the potential couplings in such a domain that a coupled $(d_{x^2-y^2} + id_{xy})$-wave solution is allowed. For a weaker $d_{xy}$ admixture, as temperature is lowered past the first critical temperature $T_c$, a weaker (less ordered) superconducting phase is created in $d_{x^2-y^2}$ wave, which changes to a stronger (more ordered) superconducting phase in $(d_{x^2-y^2} + id_{xy})$ wave at $T_{c1}$. The $d_{x^2-y^2} + id_{xy}$-wave state is similar to an $s$-wave-type state with no node in the order parameter. The phase transition at $T_{c1}$ from a $d_{x^2-y^2}$ wave to a $d_{x^2-y^2} + id_{xy}$ wave is marked by power-law (exponential) temperature dependencies of specific heat and spin susceptibility for $T > T_{c1}$ ($< T_{c1}$). Similar behavior has been observed for a $d_{x^2-y^2} + is$-wave state \[24\]. As the mixed state is $s$-wave like in both cases, from the present study it would not be possible to identify the proper symmetry of the order parameter $-d_{x^2-y^2} + id_{xy}$ opposed to $d_{x^2-y^2} + is$ and further phase sensitive tests of pairing symmetry in cuprate superconductors is needed.

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Figure Captions:

1. The order parameters $\Delta_1, \Delta_2$ in Kelvin at different temperatures for $d_{x^2-y^2} + id_{xy}$-wave models 1(a) (full line) and 1(b) (dashed line) for square lattice.

2. The order parameters $\Delta_1, \Delta_2$ in Kelvin at different temperatures for $d_{x^2-y^2} + id_{xy}$-wave models 2(a) (full line) and 2(b) (dashed line) in presence of orthorhombic distortion ($\beta = 0.95$).

3. Specific heat ratio $C(T)/C_n(T_c)$ versus $T/T_c$ for models 1(a) and 1(b) for square lattice: 1(a) (full line), 1(b) (dashed line), $d_{xy}$ (dotted line), normal (dashed-dotted line). In all cases $T_c \approx 70$ K.

4. Specific heat ratio $C(T)/C_n(T_c)$ versus $T/T_c$ for models 2(a) and 2(b) for orthorhombic distortion: 2(a) (full line), 2(b) (dashed line), $d_{xy}$ (dotted line), normal (dashed-dotted line). In all cases $T_c \approx 70$ K.

5. Specific heat jump for different $T_c$ for pure $s$ and $d$ waves: $s$ wave (solid line, square lattice), $s$ wave (dashed line, orthorhombic distortion), $d_{x^2-y^2}$ wave (dashed-dotted line, square lattice), $d_{x^2-y^2}$ wave (dashed-double-dotted line, orthorhombic distortion), $d_{xy}$ wave (dotted line, square lattice), $d_{xy}$ wave (dashed-triple-dotted line, orthorhombic distortion).

6. Susceptibility ratio $\chi(T)/\chi(T_c)$ for square lattice versus $T/T_c$: pure $d_{x^2-y^2}$ wave (solid line), pure $d_{xy}$ wave (dashed line), pure $s$ wave (dashed-dotted line), model 1(a) (dotted line), model 1(b) (dashed-double-dotted line). In all cases $T_c \approx 70$ K.

7. Susceptibility ratio $\chi(T)/\chi(T_c)$ in presence of orthorhombic distortion versus $T/T_c$: pure $d_{x^2-y^2}$ wave (solid line), pure $d_{xy}$ wave (dashed line), pure $s$ wave (dashed-dotted line), model 2(a) (dotted line), model 2(b) (dashed-double-dotted line). In all cases $T_c \approx 70$ K.
Figure 1
Figure 3

\[ \frac{C(T)}{C_n(T_c)} \]

vs

\[ \frac{T}{T_c} \]
Figure 4

The figure shows the graph of the function \( \frac{C(T)}{C_n(T_c)} \) against \( \frac{T}{T_c} \), where \( C(T) \) is the specific heat capacity of a material and \( C_n(T_c) \) is the specific heat capacity at the transition temperature. The graph includes several curves, with one labeled "normal."
Figure 5
Figure 6
