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

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(March 24, 2022)

We study the phase transition from a $d_{x^2−y^2}$ to $d_{x^2−y^2} + d_{xy}$ superconductor using the tight-binding model of two-dimensional cuprates. As the temperature is lowered past the critical temperature $T_c$, first a $d_{x^2−y^2}$ superconducting phase is created. With further reduction of temperature, the $d_{x^2−y^2} + d_{xy}$ phase is created at temperature $T = T_c$. We study the temperature dependencies of the order parameter, specific heat and spin susceptibility in these mixed-angular-momentum states on square lattice and on a lattice with orthorhombic distortion. The above-mentioned phase transitions are identified by two jumps in specific heat at $T_c$ and $T_{c1}$.

PACS number(s): 74.20.Fg, 74.62.-c, 74.25.Bt

Inspite of many theoretical and experimental studies on high-$T_c$ cuprates the exact symmetry of the order parameter is still a subject of active research [1]. However, there is evidence that the cuprates have singlet $d$-wave Cooper pairs and the order parameter has $d_{x^2−y^2}$ symmetry in two dimensions [1]. Recent measurements [2] of penetration depth and superconducting specific heat at different temperatures $T$ and related theoretical analyses [2] also support this. However, several phase-sensitive measurements of the order parameter of the cuprates indicate a significant mixing of a distinct angular momentum component with a predominant $d_{x^2−y^2}$ state at temperatures below a second critical temperature $T_{c2}$. For temperatures between $T_{c2}$ and $T_c$ only the $d_{x^2−y^2}$ state survives. Below $T_{c1}$ the order parameter can have a mixed-symmetry state of type $d_{x^2−y^2} + \exp(i\theta)d_\chi$, where $\chi$ represents a state of different symmetry. The most probable possibilities for $\chi$ are the $s$ or $d_{xy}$ wave. The possibility of a mixed $(s−d)$-wave symmetry was first suggested theoretically by Ruckenstein et al. and Kotliar [3].

There are experimental evidences based on Josephson supercurrent for tunneling between a conventional $s$-wave superconductor (Pb) and twinned or untwinned single crystals of YBa$_2$Cu$_3$O$_{7−\delta}$ (YBCO) that YBCO has mixed $d_{x^2−y^2} \pm s$ or $d_{x^2−y^2} \pm is$ symmetry [3] at lower temperatures. Recently, the existence of these mixed-symmetry states has been explored to explain the nuclear magnetic resonance data in the superconductor YBCO and the Josephson critical current observed in YBCO-SNS and YBCO-Pb junctions [4].

Kouznetsov et al. [5] performed some $c$-axis Josephson tunneling experiments by depositing conventional superconductor (Pb) across a single twin boundary of a YBCO crystal. By measuring the critical current as a function of the angle and magnitude of a magnetic field applied in the plane of the junction they also found the evidence of a mixed-symmetry order parameter in YBCO involving $d_{x^2−y^2}$ and $s$ waves. By measuring the microwave complex conductivity in the superconducting state of high quality YBa$_2$Cu$_3$O$_{7−\delta}$ single crystals at 10 GHz using a high-Q Nb cavity Sridhar et al also suggested the existence of a multicomponent superconducting order parameter in YBCO [6].

A similar conclusion of the existence of mixed-symmetry states may also be obtained based on the results of angle-resolved photoemission spectroscopy experiment by Ma et al. in which a temperature dependent gap anisotropy in oxygen-annealed Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ was detected [7]. The measured gaps along directions $\Gamma−M$ and $\Gamma−X$ are non-zero at low temperatures and their ratio was strongly temperature dependent. Using Ginzburg-Landau theory, Betouras and Joynt [8] demonstrated that one way of explaining this behavior is to employ a mixed-symmetry state of the $d_{x^2−y^2} + s$-wave type. They also conclude that the actual symmetry of the order parameter should vary substantially from one compound to another and for different levels of doping. This also suggests the possible appearance of a $d_{x^2−y^2} + d_{xy}$ state under favorable conditions.

More recently, Krishana et al. [9] reported a phase transition in the 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 applied field. Laughlin [10] provided a theoretical explanation of the observation by Krishana et al. [9] that for weak magnetic field a time-reversal symmetry breaking state of mixed symmetry is induced in 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 Tésanović [11] also predicted the possibility of a superconducting state of mixed symmetry. This mixed-symmetry state is likely to be a minor $s$ or $d_{xy}$ component superposed on a $d_{x^2−y^2}$ state for $T < T_{c1}$.

From different experimental observations it is now generally accepted that a time-reversal symmetry breaking state of type $d_{x^2−y^2} + i\chi$ is possible in the presence of an external field or magnetic impurity. This mixed-symmetry state is observed close to these impurities, surfaces/twin boundaries in the ab-plane or vortices. The nature of the mixed state varies from compound to compound. There are physical reasons for the appearance of these states. Either spin-orbit coupling with magnetic impurities or Andreev reflected bound states which...
create internal currents at the boundaries is responsible for these states \[14\]. However, orthorhombicity plays a crucial role in the generation of time-reversal symmetric mixed states. For example, it is established from a Ginzburg-Landau functional analysis \[15\] that the orthorhombicity has a consequence in the development of a \( d + s \) state instead of a time-reversal symmetry broken one. Moreover, from a theoretical point of view, time-reversal symmetric states of type \( d_{x^2−y^2} + \chi \) are expected to be allowed depending on the orthorhombic distortion.

There have been some studies \[16\] on the phase transition to a \( d_{x^2−y^2} + \exp(i\theta)\chi \) phase from a \( d_{x^2−y^2} \) phase with \( \theta = \pi/2 \) and \( \chi = d_{xy} \) or a \( s \) state. From theoretical considerations we find that there are two possibilities for the phase \( \theta \): 0 or \( \pi/2 \). For \( \theta = 0 \), we find numerically that there is no stable \( d_{x^2−y^2} + s \) phase. Here we study the phase transition to a \( d_{x^2−y^2} + d_{xy} \) phase from a \( d_{x^2−y^2} \) phase below \( T_{c1} \). In particular we study the temperature dependencies of the order parameter, specific heat, and spin susceptibility in the mixed-symmetry state.

There is no suitable microscopic theory for high-\( T_c \) superconductors and there is controversy about a proper description of the normal state and the pairing mechanism for such materials \[17\]. In the absence of a microscopic theory, a phenomenological tight-binding model in two dimensions with the proper lattice symmetry will be used \[17\]. This model has been successful in describing many properties of high-\( T_c \) materials.

We study the temperature dependencies of specific heat and susceptibility of a \( d_{x^2−y^2} + d_{xy} \)-wave superconductor with a weaker \( d_{xy} \) wave both on square lattice and on a lattice with orthorhombic distortion. The order parameter of a \( d_{x^2−y^2} + d_{xy} \)-wave superconductor has nodes on the Fermi surface and changes sign across it, and consequently, its superconducting observables also exhibit power-law dependencies on temperature. On the other hand, the order parameters for the mixed \( d_{x^2−y^2} + is \) and \( d_{x^2−y^2} + id_{xy} \)-wave states do not have a node on the Fermi surface and the corresponding observables have an exponential dependencies on temperature. In the present study on \( d_{x^2−y^2} + d_{xy} \)-wave states the specific heat exhibits two jumps at \( T = T_{c1} \) and \( T = T_{c} \), which clearly exhibits the phase transition at \( T_{c1} \).

In the present two-dimensional tight binding model the effective interaction \( V_{kq} \) for transition from a momentum \( q \) to \( k \) is taken to be separable, and is expanded in terms of some general basis functions \( \eta_i \) labelled by the index \( i \), as
\[
V_{kq} = -\sum \eta_i \eta_k \eta_q - \sum q \eta_{ik} \eta_{iq}.
\]
The functions \( \eta_i \) are associated with a one dimensional irreducible representation of the point group of square lattice \( C_{4v} \) and are appropriate generalizations of the circular harmonics incorporating the proper lattice symmetry. The effective interaction after including the two appropriate basis functions for singlet pairing is taken as
\[
V_{kq} = -V_1 \eta_1 \eta_k \eta_q - V_2 \eta_2 \eta_k \eta_q,
\]
where \( \eta_1 \equiv (\cos q_x - \beta \cos q_y) \) corresponds to \( d_{x^2−y^2} \) symmetry, \( \eta_2 \equiv \sin q_x \sin q_y \) corresponds to \( d_{xy} \) symmetry, and \( \beta = 1 \) corresponds to a square lattice, and \( \beta \neq 1 \) represents orthorhombic distortion. In this case the quasiparticle dispersion relation is given by \( \epsilon_k = -2t(\cos k_x + \beta \cos k_y - \gamma \cos k_x \cos k_y) \), where \( t \) and \( \beta t \) are the nearest-neighbour hopping integrals along the in-plane \( a \) and \( b \) axes, respectively, and \( \gamma t/2 \) is the second-nearest-neighbour hopping integral. The energy \( \epsilon_k \) is measured with respect to the Fermi surface.

At a finite \( T \), one has the following BCS equations
\[
\Delta_k = -\sum \eta_i \eta_k \frac{\Delta_1}{2E_q} \tanh \frac{E_q}{2k_B T},
\]
with
\[
E_q = (|\epsilon_q - E_F|^2 + |\Delta_q|^2)^{1/2},
\]
where \( E_F \) is the Fermi temperature and \( k_B \) the Boltzmann’s constant. The order parameter has the following anisotropic form:
\[
\Delta_q = \Delta_1 \eta_1 + C \Delta_2 \eta_2.
\]
where \( C \) is a complex number of unit modulus \( |C|^2 = 1 \). If we substitute Eqs. (0.1) and (0.3) into the BCS equation (0.2), one can separate the resultant equation in its real and imaginary parts. The resultant equations only have solution for real \( \Delta_1 \) and \( \Delta_2 \), when the complex parameter \( C \) is either purely real or purely imaginary.

The solution for purely imaginary \( C \), e.g., \( C = i \) have been extensively studied in relation to mixed \( d_{x^2−y^2} + is \) and \( d_{x^2−y^2} + id_{xy} \) states \[17\]. Here we consider the solution for \( C = 1 \), for \( d_{x^2−y^2} + d_{xy} \) state. Using the form (0.3) of \( \Delta_q \) with \( C = 1 \) and potential (0.1), Eq. (0.2) becomes the following coupled set of BCS equations
\[
\Delta_1 = V_1 \sum \eta_1 \eta_k \eta_q \eta_1 \eta_1 + \Delta_2 \eta_2 \eta_2 \frac{1}{2E_q} \tanh \frac{E_q}{2k_B T},
\]
\[
\Delta_2 = V_2 \sum \eta_2 \eta_k \eta_q \eta_1 \eta_1 + \Delta_2 \eta_2 \eta_2 \frac{1}{2E_q} \tanh \frac{E_q}{2k_B T},
\]
where both the interactions \( V_1 \) and \( V_2 \) are assumed to be energy-independent constants for \( |\epsilon_q - E_F| < k_B T_D \) and zero for \( |\epsilon_q - E_F| > k_B T_D \), where \( k_B T_D \) is a purely mathematical cutoff introduced to eliminate the ultraviolet divergence in the BCS equation and should be compared with the physically motivated Debye cutoff in the case of the conventional superconductors.

We solved the coupled set of equations (0.4) and (0.5) numerically 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 cut off \( k_B T_D = 0.02586 \text{ eV} \) \( (T_D = 300 \text{ K}) \) in both cases. The parameters for these two cases are the following: (1) Square lattice \(- (a) t = 0.2586 \text{ eV}, \beta = 1, \gamma = 0, V_2 = 8.5t, \) and \( V_1 = 0.73t, T_c = 71 \text{ K}, T_{c1} = 28 \text{ K}; (b) t = 0.2586 \text{ eV}, \beta = 1, \gamma = 0, V_2 = 9.0t, \) and \( V_1 = 0.73t, T_c = 71 \text{ K}, T_{c1} = 55 \text{ K}; (2) Orthorhombic distortion \(- (a) t = 0.2586 \text{ eV}, \)
\( \beta = 0.95, \) and \( \gamma = 0, \) \( V_2 = 8.35t, \) and \( V_1 = 0.97t, \) \( T_c = 70 \) K, \( T_{c1} = 30 \) K; (b) \( t = 0.2586 \) eV, \( \beta = 0.95, \) and \( \gamma = 0, \) \( V_2 = 8.7t, \) and \( V_1 = 0.97t, \) \( T_c = 70 \) K, \( T_{c1} = 50 \) K. For a very weak \( d_{x^2-y^2}\)-wave \( (d_{xy}\text{-wave}) \) coupling the only possible solution corresponds to \( \Delta_1 = 0 \) \( (\Delta_2 = 0). \) We have studied the solution only when a coupling is allowed between Eqs. (0.4) and (0.5).

In Figs. 1 and 2 we plot the temperature dependencies of different \( \Delta \)'s for the following two sets of \( d_{x^2-y^2} + d_{xy}\) wave corresponding to models 1 and 2, respectively. In all cases, with the lowering of temperature passed \( T_c, \) the parameter \( \Delta_1 \) increases up to \( T = T_{c1}. \) As \( T \) is lowered further, \( \Delta_2 \) becomes nonzero at \( T = T_{c1} \) and begins to increase. As temperature is lowered, both \( \Delta_1 \) and \( \Delta_2 \) first increase and then attain a constant value at zero temperature.

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 Figs. 1 and 2 we see that the temperature derivative of \( |\Delta_q|^2 \) 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 (see, definition in Ref. [4]). 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. For the mixed \( d_{x^2-y^2} + d_{xy}\)-wave model, for \( T_c > T > T_{c1} \) the specific heat exhibits \( d\)-wave power-law behavior. For \( d\)-wave models \( C_s(T_c)/C_n(T_c) \) is a function of \( T_c \) and \( \beta. \) In
Figs. 2 and 3 this ratio for the $d_{x^2-y^2}$-wave case, for $T_c = 70$ K, is approximately $3 (2.44$ for $\beta = 1$ (0.95). For the $d_{xy}$-wave case, for $T_c = 70$ K, this ratio is approximately $1.81 (1.9$ for $\beta = 1 (0.95)$. In a continuum calculation this ratio was 2 in the absence of a van Hove singularity.

For comparison. In Figs. 5 and 6, we show the results for pure $d_{x^2-y^2}$ wave (solid line), pure $d_{xy}$ wave (dashed line), model 1(a) (dotted line), and model 1(b) (dashed-double-dotted line).

Next we exhibit the temperature dependence of spin susceptibility (defined in Ref. [4]) in Figs. 5 and 6 where we also plot the results for pure $d_{x^2-y^2}$ and $d_{xy}$ waves for comparison. In Figs. 5 and 6, we show the results for models 1 and 2 on square lattice and with orthorhombic distortion, respectively. For pure $d_{x^2-y^2}$ and $d_{xy}$ waves we obtain power-law dependencies on temperature. The exponent for this power-law scaling was independent of critical temperature $T_c$ but varied 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 $d_{x^2-y^2} + d_{xy}$ wave these exponents are nearly identical to the pure $d_{x^2-y^2}$ wave case. Hence, by studying the temperature dependency of spin susceptibility, it will be impossible to detect the phase transition at $T = T_c$ from a $d_{x^2-y^2}$ wave to a $d_{x^2-y^2} + d_{xy}$ wave, at least within the present tight-binding model.

In conclusion, we have studied the $d_{x^2-y^2} + d_{xy}$-wave superconductivity employing the two-dimensional tight binding BCS model on square lattice and also on a lattice with orthorhombic distortion and confirmed a second second-order phase transition at $T = T_c$ in the presence of a weaker $d_{xy}$ wave. This phase transition is marked by a jump in the specific heat at $T = T_c$. We have kept the $s$- and $d$-wave couplings in such a domain that a coupled $d_{x^2-y^2} + d_{xy}$-wave solution is allowed. The $d_{x^2-y^2} + d_{xy}$-wave state is similar to a $d_{x^2-y^2}$-wave-type state with nodes on the Fermi surface in the order parameter. Consequently, we find power-law temperature dependencies of specific heat and spin susceptibility in the $d_{x^2-y^2} + d_{xy}$ wave. The exponents of these power laws for the mixed $d_{x^2-y^2} + d_{xy}$ wave are very close to those for the pure $d_{x^2-y^2}$ wave.

The work was supported by the CNPq and FAPESP.

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