Complex order parameter symmetry and thermal conductivity

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Abstract. – Thermal behaviour of superconductors with complex order parameter symmetry is studied within a weak coupling theory. It is shown numerically, that the thermal nature of the different components of complex order parameters are qualitatively different. Within the complex order parameter scenario, the recent experimental observations by Krishna et al., [Science 277, 83 (1997)] on magnetothermal conductivity and by J. Ma et al., [Science 267, 862 (1995)] on temperature dependent gap anisotropy for high temperature superconductors can have natural explanation.

An important challenge for current research is to reconcile various conflicting results on symmetry of the superconducting order parameter in high $T_c$ cuprates by direct determination of the coexistence of other components with $d_{x^2-y^2}$ symmetry. Apparently, the long standing controversy concerning s-wave versus d-wave pairing in cuprates is gradually turning in favor of the $d_{x^2-y^2}$. For example, the precise measurements of spontaneously generated half-integral flux quanta on bicrystal and tricrystal films [1] together with the corner SQUID experiments [2] suggest that the superconducting gap changes sign on the Fermi surface. Recent measurements on magnetic penetration depth [3], the nuclear spin relaxation rate [4], angle resolved photoemission data [5] indeed provide evidence for the existence of corresponding low energy excitation states. While there exists some experimental evidence for each of these effects [6, 7, 8] it is by no means conclusive and an active debate continues.

Sun et al. [9] found a nonvanishing tunneling current along the c axis between $YBa_2Cu_3O_{6+x}$ and the conventional superconductor Pb, which cannot exist in a pure tetragonal d-wave superconductor. It has been argued by a number of authors that such data can be explained by considering an admixture of s wave component due to orthorhombicity in such materials [10]. A self-consistent electronic structure calculation for a $d_{x^2-y^2}$ and a $d_{x^2+y^2} + id_{xy}$ vortex [11] reveals that the scanning tunneling spectroscopy data on vortices in $YBa_2Cu_3O_{7-\delta}$ [8]

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is inconsistent with simple $d_{x^2-y^2}$ symmetry, but consistent with $d_{x^2-y^2} + id_{xy}$. Based on such recent important experimental findings, it was suggested by Laughlin \[12\] that there should be a tendency for the high $T_c$ superconductors to develop a small $d_{xy}$ order parameter (OP) on top of the usual $d_{x^2-y^2}$. Direct evidences for such suggestion are provided by the recent outstanding experimental data on thermal conductivity by Krishna et al., \[13\] and theoretically, by Wheatly et al, and most recently by Ramakrishnan \[12\]. We summarize below their essential findings \[13\] as it is found in this work that the complex order parameter symmetry has natural explanation to this data.

A series of high resolution measurements on thermal conductivity ($\kappa$) in the $Bi_2Sr_2CaCuO_8$ by Krishna et al. \[13\] show that the $\kappa$ at low temperature becomes field-independent above a temperature dependent threshold field $H_k(T)$. Below $T_c$ (92 K) and in zero field a broad anomaly in $\kappa$ was observed that peaks near 65 K and an applied field ($H \parallel c$) suppresses the anomaly. This remarkable result indicates a phase transition separating a low-field state where the thermal conductivity decreases with increasing field and a high-field one where it is insensitive to applied magnetic field. The authors argue that this phase transition is not related to the vortex lattice because of the temperature dependence of the field $H_k(T)$ (which is roughly proportional to $T^2$) as well as its magnitude. Instead, they suggest a field-induced electronic transition leading to a sudden vanishing of the quasi-particle contribution to the heat current. Possible scenarios would be the induction of either $id_{xy}$ or $is$ component with $d_{x^2-y^2}$ symmetry with application of a weak field. Such proposition of complex order parameter symmetry in cuprate superconductors reminds us of another important data on angle resolve photoemission experiment (ARPES) by J. Ma et al., \[14\] in which a temperature dependent gap anisotropy in the oxygen-annealed $Bi_2Sr_2CaCuO_{8+x}$ compound was found. The measured gaps along both high symmetry directions (\(\Gamma-M\) i.e, Cu-O bond direction in real space and \(\Gamma-X\) i.e, diagonal to Cu-O bond) are non-zero at lower temperatures and their ratio is strongly temperature dependent. The experimental observation \[14\] is however, not reproduced by any other group. This observed feature cannot be explained within a simple $d$-wave scenario and has been taken as a signature of a two component order parameter, $d_{x^2-y^2}$ type close to $T_c$ and a mixture of both $s$ and $d$ otherwise \[13\]. While the conductivity data in cuprates \[13\] indicate a finite induction of $is$ (or $id_{xy}$) component with $d_{x^2-y^2}$ due to application of magnetic field, the ARPES data \[14\] indicates they are intrinsically so.

In this note, we work out the phase diagram of a superconductor with complex order parameter symmetries such as $d_{x^2-y^2} + id_{xy}$ and $d_{x^2-y^2} + is$ (for our purpose) comprising the amplitudes of different components of order parameters as a function of the relative pairing strength in different channels. It is found that the appearence of $d_{xy}$ component hardly affects the $d_{x^2-y^2}$ component in the case of a $d_{x^2-y^2} + id_{xy}$ symmetry, whereas the occurence of $s$-component strongly suppresses the $d_{x^2-y^2}$ gap for $d_{x^2-y^2} + is$ symmetry. These effects have been substantiated by calculating the temperature dependence of different components (e.g, $\Delta_{xy}$, $\Delta_s$ and $\Delta_{d_{x^2-y^2}}$). Interestingly enough, the thermal growth of $d_{x^2-y^2}$ is locked at the onset of the $s$-wave component in $d_{x^2-y^2} + is$ symmetry whereas no such strong competition is found in case of $d_{x^2-y^2} + id_{xy}$ symmetry. These anomalous thermal behaviors are likely to have important impacts on different physical properties like the specific heat, Knight shift etc. Within this complex order parameter scenario, we calculate electronic thermal conductivity and the temperature dependent gap anisotropy ($\Delta_{\Gamma-M}/\Delta_{\Gamma-X}$ Vs. $T$). Resemblance of the calculated results with the observed data are remarkable.

Assuming the applicability of weak coupling theory to high $T_c$ cuprates, the superconducting gap equation may be written as

$$\Delta_k = \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E'_{k'}} \tanh \left( \frac{\beta E'_{k'}}{2} \right),$$

(1)
where the pairing potential $V_{kk'}$ for a two component order parameter with a separable form and the corresponding gap functions are obtained as,

$$V_{kk'} = \sum_{j=1}^{2} V_{j} f_{k}^{j} f_{k'}^{j} \quad \& \quad \Delta_{k} = \sum_{j=1}^{2} \Delta_{j} f_{k}^{j} \tag{2}$$

For a $d_{x^2-y^2} + id_{xy}$ symmetry, $V_{1} = V_{d_{x^2-y^2}}$, $V_{2} = V_{d_{xy}}$, $f_{k}^{1} = (\cos k_{x} - \cos k_{y})$, $f_{k}^{2} = 2 \sin k_{x} \sin k_{y}$ and the corresponding component gap functions are $\Delta_{1} = \Delta_{d_{x^2-y^2}}$ and $\Delta_{2} = i \Delta_{d_{xy}}$. Similarly, for a corresponding $d_{x^2-y^2} + is$ phase, $V_{2} = V_{s}$, $f_{k}^{2} = \text{constant}$ and $\Delta_{2} = i \Delta_{s}$. Substituting (2) in (1) and separating the real and imaginary parts, gap equations for different components may be written as,

$$\Delta_{j} = \sum_{k} V_{j} \frac{\Delta_{j} f_{k}^{j}}{2E_{k}} \tanh(\frac{\beta E_{k}}{2}) \tag{3}$$

where the quasiparticle energy spectrum of the superconducting state is given by $E_{k} = \sqrt{(\epsilon_{k} - \mu)^{2} + |\Delta_{k}|^{2}}$, $\epsilon_{k} = -2t(\cos k_{x} + \cos k_{y})$ being the normal state band energy. The coupled equations (3) are solved numerically selfconsistently together with a number conserving equation to fix chemical potential ($\mu$), for a given set of parameters. Then the self-consistent values of the order parameters are used to calculate thermal conductivity using the formula proposed by Bardeen et al. [16], long time ago.

$$\kappa = \sum_{k} \frac{(E_{k} v_{k} \cos \theta)^{2}}{TT} (- \frac{\partial f_{k}^{0}}{\partial E_{k}}) \tag{4}$$

where $v_{k} \cos \theta$ is the component of group velocity parallel to $-\nabla T$, $T$ is the relaxation rate and $f_{k}^{0}$ is the Fermi distribution function. It is important to consider the correct energy dependence of $T$ to include strong inelastic and impurity scatterings. Phase diagrams of a $d_{x^2-y^2} + id_{xy}$ and that of a $d_{x^2-y^2} + is$ superconductor evaluated at $T = 5$ K are presented in the figures 1(a) and 1(b) respectively. The phase diagram for $d_{x^2-y^2} + id_{xy}$ superconductors presented in Fig. 1(a) comprises the amplitudes of $\Delta_{d_{x^2-y^2}}$, $\Delta_{d_{xy}}$ as a function of the relative pairing strength between the two channels, $V_{d_{x^2-y^2}} / V_{d_{xy}}$. When the relative pairing strength is about 0.65 the $\Delta_{d_{xy}}$ starts developing and its appearance affects the $\Delta_{d_{x^2-y^2}}$ component only a little, only when $\Delta_{xy} \gg \Delta_{d_{x^2-y^2}}$. A similar phase diagram for the $d_{x^2-y^2} + is$ superconductors is presented in Fig. 1(b). It is clear from Fig. 1(b) that with the onset of the $s$ wave component, the $\Delta_{d_{x^2-y^2}}$ component is strongly suppressed resulting in a pure $s$-wave phase for $V_{d_{x^2-y^2}} / V_{s} < 0.39$. This is because of the peculiar momentum dependence of $\Delta_{d_{x^2-y^2}}(k)$ and $\Delta_{d_{xy}}(k)$; the regions of the Fermi surface where $\Delta_{d_{x^2-y^2}}(k)$ is maximum $\Delta_{d_{xy}}(k)$ is minimum and vice versa. This is however, the case for $\Delta_{d_{x^2-y^2}}(k)$ and an isotropic $\Delta_{s}$ symmetry. Note, while obtaining phase diagrams in figures 1(a) and 1(b), the stability conditions of different phases are also checked through free energy comparison.

The strong competition between the $d_{x^2-y^2}$ and $s$-wave components in the $d_{x^2-y^2} + is$ phase is more distinctly evident in Fig. 2(b). In Fig. 2(b) temperature dependence of different components of the complex order parameter $d + is$ is presented for various values of $V_{d_{x^2-y^2}} / V_{s}$ (such that both the order parameters coexist). The curves with left arrow sign correspond to thermal dependence of the the $s$-wave component and the rest that for the $d$-wave component. It is shown that with the onset of $s$-wave component the thermal growth of the $d$-wave component is arrested. This scenario is however absent in case of a $d + id$ superconductor (cf. Fig. 2(a)). In Fig. 2(a), with the decrease of the ratio $V_{d_{x^2-y^2}} / V_{d_{xy}}$ the
$d_{xy}$ component enhances substantially but the magnitude of $d_{x^2-y^2}$ component is reduced only marginally. To note, from figures 2(a) and 2(b) that the transition temperature ($T_c = 84$ K) is always determined by the $d_{x^2-y^2}$ component irrespective of $d + id$ or $d + i$ is symmetry of the OP. Or in other words, we have $d_{x^2-y^2}$ symmetry towards higher temperatures close to $T_c$ and an admixture of either $d + id$ or $d + i$ is otherwise. Furthermore, the only parameter that has been tuned through out is the ratio $V_{d_{x^2-y^2}}/V_{d_{xy}}$ and the other cut-off parameter $\Omega_c = 0.6$ (measured with respect to the hopping integral $t$) is kept fixed.

According to the proposal [13] (see also 12), application of the magnetic field induces either a $d_{xy}$ or a $id_{xy}$ component to the $d_{x^2-y^2}$ symmetry (i.e. stronger the field more the induction of complex component) and thereby the magnetothermal conductivity is suppressed at lower temperatures with magnetic field. In the complex order parameter scenario, we have a device to enhance the complex component (to the $d_{x^2-y^2}$ symmetry) by reducing the parameter $V_{d_{x^2-y^2}}/V_{d_{xy}}$ or $V_{d_{x^2-y^2}}/V_s$. Hence, an essentially similar physical effect can be brought in. As a word of caution, however, it is not known whether the magnetic field simply reduces the relative pairing strength in a complex order parameter symmetry. In figures 3(a) and 3(b) thermal conductivities of a pure superconductor with complex order parameter symmetries ($d + id$ or $d + i$) are presented for various values of the relative pairing strength between different channels. By pure superconductor we mean that the impurity bound states are neglected and only essentially anisotropic superconducting states which meet the case of resonance scattering is considered.

Detailed theory of thermal conductivity for unconventional (pure) superconductors are discussed by many authors [17]. It is worth mentioning that both the $d + id$ and $d + i$ symmetries are parity and time reversal symmetry violating states. Also both the symmetries correspond to a fully gapped situation similar to an isotropic $s$ wave superconductor. A large suppression in the normalized thermal conductivity ($\frac{\kappa(T)}{\kappa_0(T)}$) at lower temperatures with lowering of $V_{d_{x^2-y^2}}/V_{d_{xy}}$ or $V_{d_{x^2-y^2}}/V_s$ is seen in Fig.s 3(a, b). Apart from a low temperature anomaly, a broad maxima is found around $T = 61$ K below $T_c = 84$ K in both the cases (cf Fig. 3(a) and Fig. 3(b)). Also there is only a very little change in the conductivity at lower temperatures, when the ratio $V_{d_{x^2-y^2}}/V_{d_{xy}}$ or $V_{d_{x^2-y^2}}/V_s$ is lower enough (for example cf. Fig 3(a) for $V_{d_{x^2-y^2}}/V_{d_{xy}} = 0.446$ and 0.435). For higher values of $V_{d_{x^2-y^2}}/V_{d_{xy}} = 0.555$ or $V_{d_{x^2-y^2}}/V_s = 0.455$ the low temperature anomaly is worth noticing. The $id_{xy}$ or component being small (for those values of $V_{d_{x^2-y^2}}/V_{d_{xy}} = 0.555$ or $V_{d_{x^2-y^2}}/V_s = 0.455$) exists only up to very lower temperatures (cf. Figs. 2(a) and 2(b) also) and hence it corresponds to a situation of a pure $d$-wave with nodes at higher temperatures to that of a fully gapped $d + id$ or $d + i$ is superconductor at lower temperatures. This results in power law falling of thermal conductivity at higher temperatures to a sudden exponential fall of the same at lower temperatures and hence explains the lower temperature anomaly. However, such temperature dependence changes from power law to exponential even at higher temperatures as the complex component is or $id$ becomes substantial. These results are in complete agreement with the experimental findings [13]. There is another extra cusp like feature seen in case of $d + i$ superconductors (e.g. $V_{d_{x^2-y^2}}/V_s = 0.455$) at around $T = 14$ K. This is reflection to the arresting of the growth of $d$ wave component with the appearence of $s$ component seen in Fig. 2(b). However, our figures 3(a, b) does not show suppression of the broad peak at around 61 K with field which is seen in experiment. This is because the applied field in the experiment is temperature dependent (roughly proportional to $T^2$). Therefore, it turns out that the suppression in the broad peak may be associated with the temperature field coupled with the magnetic field in [13]. So in order to see the net effect of a pure magnetic field in thermal conductivity, it would be suggestive to repeat the same experiment [13] with magnetic field which is independent of...
temperature. Finally, the temperature dependent gap anisotropy i.e, the ratio $\Delta_{\Gamma-M}/\Delta_{\Gamma-X}$ as a function of temperature is plotted in the inset Fig. 1(a) for a superconducting gap function with $d_{x^2-y^2} + id_{xy}$ symmetry. It is seen that the temperature dependent gap anisotropy could be as high as 7 for $V_{d_{x^2-y^2}}/V_{d_{xy}} = 0.446$ (at a temperature where the $d_{xy}$ component becomes vanishingly small). Note, in the $d_{x^2-y^2} + id_{xy}$ scenario, the $\Delta_{\Gamma-M} \propto \Delta_{d_{x^2-y^2}}$ and $\Delta_{\Gamma-X} \propto \Delta_{d_{xy}} (\Gamma - M \equiv (0, \pi) \text{ and } \Gamma - X \equiv (\pi/2, \pi/2))$ and therefore, the inset Fig. 1(a) can be qualitatively estimated from Fig. 2(a). In inset Fig. 1(a), the large value of the gap ratio can be obtained only when the $d_{xy}$ component is comparable to the $d_{x^2-y^2}$ component. Similar feature is also true in case of $d_{x^2-y^2} + is$ superconductors (not shown in figure) \[3\].

While the inset Fig. 1(a) would naturally account the experimental observation by Ma et al. \[4\], according to Laughlin’s conjecture \[12\] the $d_{xy}$ component cannot be too large.

In summary, motivated by recent experimental data concerning superconducting pairing symmetry in high temperature superconductors we illustrated in this letter some interesting features of the complex order parameter symmetry. Taking examples of $d+id$ and $d+is$, it is shown that the different components of a complex OP interfer with each other very differently. Thermal conductivity is calculated in the complex order parameter phase and found to be in agreement with experimental observations based on coupled effect of temperature and magnetic field. The present work neither resolves pairing mechanism nor establishes pairing symmetry in cuprates but, with reference to recent experimental results \[3\], the results presented in this work may have some important bearings to high-$T_c$ cuprate superconductors.

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REFERENCES

[1] Tsuei C. C., et al., Phys. Rev. Lett., 73 (1994) 593; Kirtley J. R., et al., Nature (London), 373 (1995) 225.
[2] Wollman D. A., et al., Phys. Rev. Lett., 71 (1993) 2134; Mathai A., et al., Phys. Rev. Lett., 74 (1995) 4523.
[3] Hardy W. N., et al., Phys. Rev. Lett., 70 (1993) 3999; Bonn D. A., et al., ibid. 68 (1992) 2300; Zhang K., et al., ibid 73 (1994) 2484.
[4] Martindale J. A., et al., Phys. Rev. Lett., 68 (1992) 762.
[5] Shen Z.-X., et al., Phys. Rev. Lett., 70 (1993) 1553; Ding H., et al., ibid 74 (1995) 2784.
[6] Moler K. A., et al., Phys. Rev. Lett., 74 (1995) 1202
[7] Maggio-Aprile I., et al., Phys. Rev. Lett., 75 (1995) 2754.
[8] Sun A. G., et al., Phys. Rev. Lett., 72 (1994) 2267; Sun A. G., et al., Phys. Rev.B, 54 (1996) 6734.
[9] Sigrist M., et al., Phys. Rev. B, 53 (1996) 2385; Walker M. B., Phys. Rev. B, 53 (1996) 5835; Sigrist M., et al., Z. Phys. B, 68 (1987) 9; Li Q. P., et al., Phys. Rev. B, 48 (1993) 437; Beal-Monod M. T., et al., Phys. Rev. B, 53 (1996) 5775.
[10] Franz M. and Tesanovic Z., cond-mat/9710258 (1997).
[11] Laughlin R. B., cond-mat/9709195 (1997); Wheatley J., et al., Solid State Comm., 88 (1993) 593; Ramakrishnan T. V., cond-mat/9803069 (1998).
[12] Krishna K., et al., Science, 277 (1997) 83.
[13] Ma, J. et al., Science, 267 (1995) 862.
[14] Mitra M., Ghosh Haranath and Behera S. N., Euro. Jr. Phys. B, 267 (1998) 371.
[15] Bardeen J., et al., Phys. Rev., 113 (1959) 982.
[16] Hirschfeld H., et al., Solid State Commun., 58 (1986) 111; Arfi B. and Pethick C. J., Phys. Rev. B, 38 (1988) 2312; Barash Yu. S. and Svidzinsky, Phys. Rev. B, 53 (1996) 15254.
Figure Captions

Fig 1. Phase diagram of superconductors with complex order parameter symmetries (a) $d_{x^2-y^2}+id_{xy}$ and (b) $d_{x^2-y^2}+is$. The notations $V_{d_{x^2-y^2}}$, $V_{d_{xy}}$, $V_s$ refer to pairing strengths in the respective channels. The inset Fig. 1(a) represents temperature dependent gap anisotropy in the $d_{x^2-y^2}+id_{xy}$ scenario.

Fig 2. Thermal variations of different components of the superconducting gap amplitudes in the complex order parameter (a) $d_{x^2-y^2}+id_{xy}$ and (b) $d_{x^2-y^2}+is$ symmetry for various values of $V_{d_{x^2-y^2}}/V_{d_{xy}}$ and $V_{d_{x^2-y^2}}/V_s$ respectively. Strong interference between different gap components in $d_{x^2-y^2}+is$ symmetry is worth noticing in contrast to that in $d_{x^2-y^2}+id_{xy}$ phase.

Fig. 3 Normalised thermal conductivity (in arbitrary units) as a function of temperature is shown in case of (a) $d_{x^2-y^2}+id_{xy}$ and (b) $d_{x^2-y^2}+is$ pairing symmetry. (The notations $\kappa_{s,n}$ refer to thermal conductivity in the superconducting and normal state respectively). Loss of quasi-particle current with the enhancement of the complex component is seen at lower temperatures.
\[
\Delta_{d_{x-y}}^{2} - \Delta_{s} \quad \text{and} \quad \Delta_{d_{x-y}}^{2} + i\Delta_{d_{xy}}
\]

(a)

(b)
\( V_{d_x^2 - y}^{2/N_{d_{xy}}} \)