Pairing in Planar Organic Superconductors

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Abstract. The nature of superconductivity in planar organics is still a controversial problem. We investigate theoretically d-wave and anisotropic s-wave pairing in $\kappa-(BEDT-TTF)_2X$ compounds. Assuming strong dimerization, we consider a single band model with elliptical Fermi surface to calculate density of states, specific heat and spin susceptibility as functions of temperature. The obtained results, compared with experiments, should help to resolve the question of pairing symmetry.

INTRODUCTION

Planar organic superconductors belong to the wide class of "exotic" superconductors, following the so called Uemura trend, T_c approximately proportional to λ_L^2, together with heavy fermions, borocarbide superconductors and high T_c cuprates.[1] Organic superconductors share many unconventional features with the later compounds,and in particular there are striking parallels between high T_c cuprates and $\kappa-(BEDT-TTF)_2X$ salts. These molecules, in the following abbreviated as $\kappa-(ET)_2X$, with layered structure, are very anisotropic quasi-2D superconductors with T_c up to about 10 K, depending on the pressure and the ion X, which can be I_3, $Cu[N(CN)_2]Br$ or $Cu(SCN)_2$.[2] Also, both in high T_c cuprates and $\kappa-(ET)_2X$ the superconducting state is located in the proximity of the antiferromagnetic phase. These are indications of possible spin-fluctuations mediated superconductivity, with nodes in the superconducting gap.[3] This argument has suggested that d-wave gap form, well established in cuprates, may occur in planar organics as well. However, in the later case the experimental data are controversial. Beside those indicating the d-wave pairing, there is much evidence for the s-wave, or generalized s-wave pairing.[1] An extensive review of experimental results in favor of d-wave pairing and gap nodes, and of those against this possibility, can be found in the review articles by Brandow,[1] and by Singleton and Mielke.[4]

In specific heat measurements, the evidence against gap nodes comes from the activated behavior found by the group of Wosnitza,[5] implying a BCS (strong coupling) temperature behavior and a fully gaped superconducting state. By contrast, an earlier measurement has shown a T^2 dependence of the electronic specific heat $C_s(T)$, implying the nodal structure of the gap.[6]

Similar dichotomy is found in many studies of the temperature dependence of the London penetration depth $\lambda_L(T)$, with power-law (nodes) behavior, and activated (nodeless) behavior.[1, 4]

This controversy could be resolved by assuming for example, an anisotropic s-wave pairing, with the nodes, which could be present in the in the carefully prepared samples.

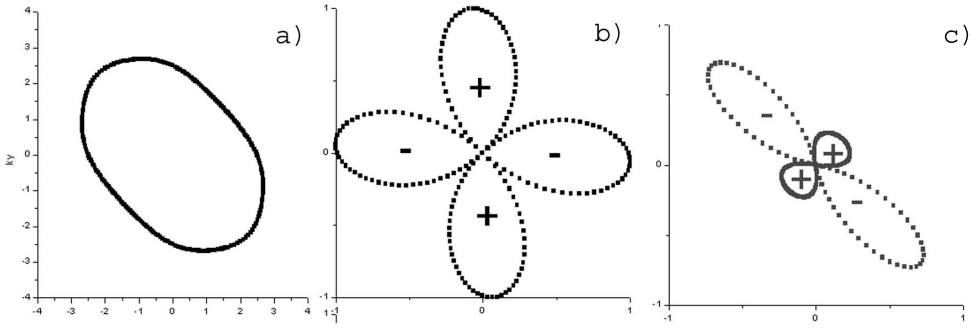

FIGURE 1. a) The shape of Fermi surface. Polar plot for pairing potentials: b) d-wave and c) anisotropic s^*-wave.

It can be easily removed by unintentional perturbations,by which the order parameter could be renormalized so that the nodes are removed.[1, 7]

In the present paper we consider two types of pairing as candidates for $\kappa-(ET)_2X$, standard d-wave[8] and anisotropic s-wave pairing.[1]

FORMULATION

Within a given conducting layer, the unit cell of $\kappa-(ET)_2X$ consists of four ET molecules, arranged in two dimers.[9] When the dimerization is strong, the four band model can be reduced to single band model. This model was used by Tanuma et al.[10] in a study of magnetotunneling specroscopy in $\kappa-(ET)_2$, as suitable to discuss the results for a given pairing symmetry. In the single band model, the dispersion relation is given by[10]

$$\xi_k = -2t(cosk_x a + cosk_y a) - 2t'(cosk_x a + cosk_y a) - \mu \tag{1}$$

with t, t' and μ chosen so to reproduce the Fermi surface observed experimentally by Shubnikov-de Haas measurements.[11] In the following, we use the above approximation to calculate the density of states (DOS) on the Fermi surface $N(E)$, electronic spesific heat $C_s(T)$,and the spin susceptibility $\chi_s(T)$. For d-wave pairing, we use the standard form

$$\Delta_k = 2\Delta_0(cosk_x a - cosk_y a) \tag{2}$$

and for the anisotropic s-wave (s^*-wave) pairing

$$\Delta_k = 2\Delta_0(cosk_x a + cosk_y a). \tag{3}$$

The Fermi surface and the polar plots of the used pairing potentials are represented in Fig. 1.

For 2D case, the density of states is obtained by averaging over the Fermi surface,

$$N(E) = < N(\varphi) Re \frac{E}{\sqrt{E^2 - |\Delta_k|^2}} >, \tag{4}$$

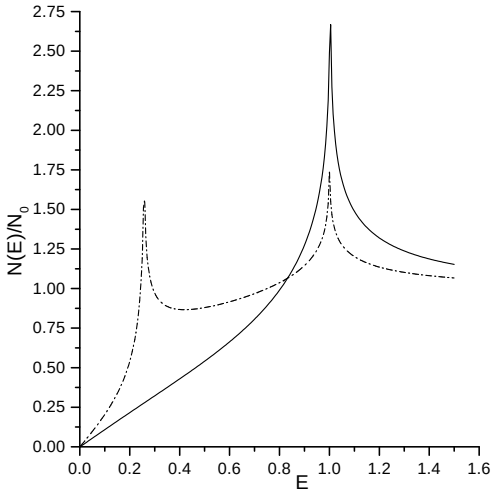

FIGURE 2. DOS for pairing potentials: d-wave - full line; anisotropic s^*-wave - dashed line.

where $<>=\frac{1}{2\pi}\int_0^{2\pi} d\varphi...$ and $N(\varphi)=\frac{1}{2\pi}k(\varphi)\frac{dk}{d\xi_k}$, $k(\varphi)$ describing the elliptical Fermi surface ($\hbar = k_b = 1$). Note that $N_0 =< N(\varphi) >$ is the density of states at the Fermi level in the normal state. The results for DOS, with above pairing potentials, are presented in Fig. 2. Whereas DOS for d-wave case has the standard form, the curve $N(E)$ for s^*-wave has two maxima.

Using $N(E)$ we may calculate the electronic specific heat, reduced to that in the normal state,[7]

$$\frac{C_s}{C_n}=\frac{3}{2\pi^2T^3}\int_0^\infty dE\frac{N(E)E^2}{\cosh^2(\frac{E}{2T})}+\frac{6}{\pi^2}\int_0^\infty dE\frac{\partial N(E)}{\partial E}\left[ln(1+e^{\frac{E}{T}})-\frac{E/T}{1+e^{-E/T}}\right] \quad (5)$$

where $C_n=\gamma_n T$ is the specific heat in the normal state, and $\gamma_n=\frac{2}{3}N_0\pi^2$. The results for d-wave, Eq. 2 and s^*-wave, Eq. 3, are presented in Fig. 3. Since in both cases there are nodes in the gap, see Fig. 1, the specific heat temperature dependencies are power laws at low T, although with different exponents. For comparison, the specific heat for isotropic s-wave , exponentially vanishing at low T, is plotted as well.

Next, using the density of states we obtain the spin susceptibility, normalized to that in the normal state,[12]

$$\frac{\chi_s}{\chi_n}=\frac{1}{2T}\int_0^\infty E\frac{N(E)}{N_0}\frac{1}{cosh^2(\frac{E}{2T})} \quad (6)$$

The results for d-wave and s^*-wave, presented in Fig. 4, show both striking differences as compared to the isotropic s-wave.

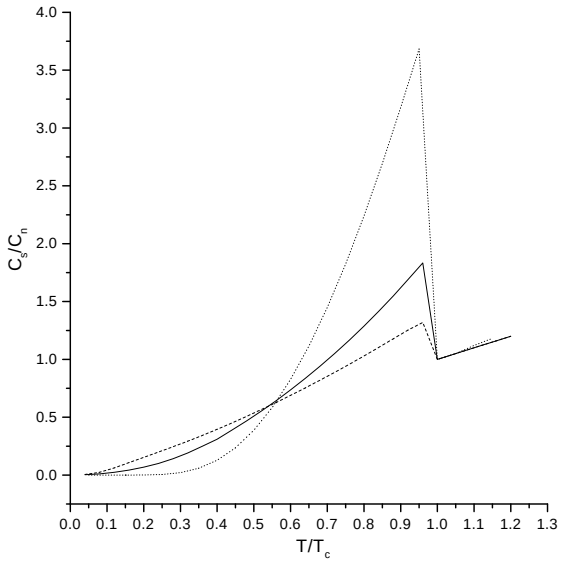

FIGURE 3. Specific heat for pairing potentials: d-wave - full line; anisotropic s^*-wave - dashed line, and s-wave - dotted line.

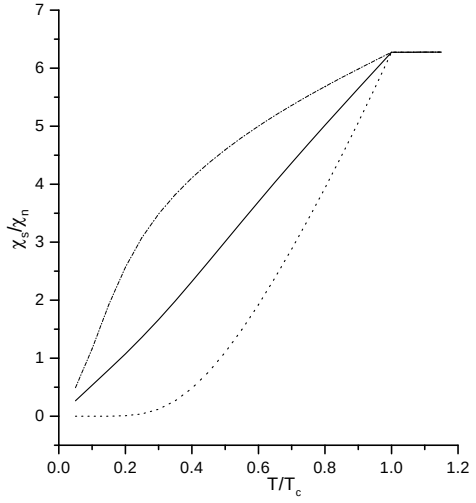

FIGURE 4. Spin susceptibility for pairing potentials: d-wave - full line; anisotropic s^*-wave - dashed line, and s-wave - dotted line.

DISCUSSION

Our main assumption about pairing in $\kappa-(ET)_2X$ is that the gap has anisotropic s-wave symmetry[1], and that it can be renormalized, e. g. by the cooling rate dependent disorder in some samples.[4] We discuss below the differences between our results for

$d_{x^2-y^2}$ and s^*-wave pairing, expecting that the later form will be seen in experiments in favor of gap nodes. First, the presence of two maxima in the density of states $N(E)$ found in the s^*-wave case should be manifested in the tunnelling experiments. So far, $\frac{dI}{dV}$ curves obtained by tunnelling spectroscopy were fitted, with a relative success, to a simple d-wave model.[13] The temperature dependence of the specific heat $C_s(T)$ in both considered cases is obviously different from the exponential behavior at low temperature for the isotropic s-wave. At low T, the exponent of the power law T^n, found in both cases, is smaller in the s^*-wave case. A pronounced difference between $d_{x^2-y^2}$ and s^*-wave pairing is found in the temperature dependence of the spin susceptibility $\xi_s(T)$. Whereas in the d-wave case this is a slightly concave, nearly liner curve, for s^*-wave it is convex, completely opposite to that for the isotropic s-wave.

In conclusion, we have shown that in above calculations one finds a net difference between the two considered types of pairing. Although we assume, following Brandow,[1] that the pairing in $\kappa-(ET)_2$ is of a generalized s-wave type, only a detailed comparison with experiment would show if this is the case, or if perhaps the pairing is of a more complicated type, like generalized d_{xy},[8, 10] or of a combined $s+d$ symmetry.[14]

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