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1999 J. Phys.: Condens. Matter 11 L371

(http://iopscience.iop.org/0953-8984/11/30/103)

J. Phys.: Condens. Matter **11** (1999) L371–L377. Printed in the UK PII: S0953-8984(99)04073-4

LETTER TO THE EDITOR

Higher anisotropic d-wave symmetry in cuprate superconductors

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Received 7 May 1999

Abstract. We derive a pair potential from tight binding further neighbour attraction that leads to superconducting gap symmetry similar to that of the phenomenological spin fluctuation theory of high temperature superconductors (Monthoux *et al* 1991 *Phys. Rev. Lett.* **67** 3448). We show that higher anisotropic d-wave than the simplest d-wave symmetry is one of the important ingredients responsible for higher BCS characteristic ratio.

Pairing symmetry of the superconducting energy gap in high temperature superconductors still remains an open problem a decade since its discovery. Various experimental results which lead to conflicting conclusions resulted no concrete consensus to the theory of pairing mechanism for high T_c superconductors. However, there are strong evidences that the pairing state of the cuprate superconductors could be d-wave like; experimental observations that are sensitive to the phase [1] and nodes [2] of the gap, reported a sign reversal of the order parameter supporting d-wave pairing. On the other hand, a group of experiments on the same $YBa_2Cu_3O_7$ (YBCO) material indicate existence of a significant s-component [3]; had YBCO been a d-wave superconductor, it would be orthogonal to the s-wave state of Pb resulting in zero Josephson supercurrent (while in experiment a well defined c-axis current is seen) and there are strong evidences that the electron doped $Nd_{2-x}Ce_xCuO_4$ superconductors are s-wave type [4]. There are also indications, both from theories and experiments, that the high T_c materials may have a mixed pairing symmetry (e.g., d $\pm$ s or d + is/d_{xy} etc) in the presence of external magnetic field, magnetic impurity [5], interface effects etc [6]. In addition, there exist important clues that indicate pairing state even in the bulk of the cuprates and in the absence of magnetic field may also have a mixed pairing state, with a minor component coexisting with predominant d-wave (i.e., $\mathrm{d}+\mathrm{e}^{\mathrm{i}\theta}\alpha$ scenario, $\alpha = \mathrm{s}, \mathrm{d}_{xy}$) [7]. The angle resolved photoemission spectroscopy (ARPES) study by Kelley *et al* provides strong indication that the $Bi_2Sr_2CaCu_2O_{8+\delta}$ compound is d-wave like in the under- and optimally doped regime whereas *not* d-wave like in the slightly overdoped but high-T_c sample. Raman measurements confirmed the unexpected behaviour of gap symmetry (from predominant $d_{x^2-y^2}$ in under- or optimally doped to anisotropic s-wave type in overdoped) by overdoping $Bi_2Sr_2CaCu_2O_{8+\delta}$ and almost similar phenomena are also found in the other high-T_c material $Tl_2Ba_2CuO_{6+\delta}$ [8]. Now, observation of any s component will have stringent constraints to various potential theories of high T_c superconductors, namely, antiferromagnetic spin fluctuation theory [9], because, antiferromagnetic spin fluctuation theory leads to attraction in the d-wave channel and pair breaking in the s-wave channel (but in a model calculation via spin fluctuation in heavy fermion systems by Miyake *et al* [10] indicates possibility of anisotropic s-wave pairing as well). On the other hand, pairing mechanisms based on electron–phonon interactions, polarons etc would be compatible with pure d-wave, pure s-wave or an admixture of the two [11].

0953-8984/99/300371+07$30.00

Therefore, it is evident from the above discussion that the symmetry of the order parameter and the associated mechanism of pairing in high T_c cuprates are not at all clear, but is essential to have a first step development towards an understanding of the mystery of pairing mechanism. The spin fluctuation theory is one of the potential theories of high T_c superconductivity which can account for a number of anomalous properties observed in cuprates. It is a phenomenological theory with a few small parameters, like the phenomenological form of the spin susceptibility $\chi(Q)$, the magnetic coherence length ξ, the magnon frequency ω_{SF} extracted from nuclear magnetic resonance (NMR) experiment [12]. The approximate momentum distribution of the superconducting energy gap function obtained by the authors of [9] is,

$$\Delta_{SF}(k) = \Delta(0)(\cos k_x a - \cos k_y a)\sum_N(\cos k_x a + \cos k_y a)^N. \qquad (1)$$

This is not a *lowest order* d-wave symmetry as is usually considered in the literature. It was Lenck and Carbotte, who first pointed out this fact [13]. They obtained the superconducting gap function by using BCS theory with the phenomenological spin susceptibility as the pairing interaction by using the fast-Fourier-transform technique, without any prior assumption about the symmetry of the gap function. They concluded that the gap structure although it has nodal lines along $k_x = k_y$ cannot have the simple form of $\cos k_x a - \cos k_y a$ with a the lattice parameter. In a weak coupling theory language, in order to get a gap symmetry as $\Delta_{SF}(k)$ one needs a pair potential which also has the same symmetry. We show in a tight binding picture by considering higher neighbours attraction that such potential is derivable up to the third order term in equation (1). After obtaining the pair potential we calculate the explicit structure of gap function thus obtained and found to be similar to that of Lenck and Carbotte. We also point out that such higher anisotropic d-wave symmetry is key to understand the larger $2\Delta(k)_{max}/k_B T_c$ BCS ratio.

In the spirit of the tight binding description assuming that the overlap of orbitals in different unit cells is small, compared to the diagonal overlap values, the matrix element $V(k, k')$ may be written as,

$$V(\vec{q}) = \sum_{\vec{\delta}} V_{\vec{\delta}} e^{i\vec{q}\vec{R}_\delta} = V_o^r + 2\sum_{n=1}^{3} V_n(\cos q_x na + \cos q_y na) \qquad (2)$$

where $\vec{R}_\delta = \pm na$ locates nearest neighbours and further neighbours; since we shall only be interested in the d-wave channel (i.e., in a square lattice we are not considering second, fifth etc neighbour matrix elements as it gives rise to d_{xy}, s_{xy} channels). Thus we get, from the requirement of singlet pairing symmetry i.e., $\Delta(k) = \Delta(-k)$,

$$V(k, k') = V_o^r + \sum_n V_n f_k^n f_{k'}^n + \sum_n V_n g_k^n g_{k'}^n \qquad (3)$$

where f_k^n (g_k^n) $= \cos k_x na \mp \cos k_y na$, V_o^r is the on-site term (the label r stands for repulsion, but could be attractive as well giving rise to isotropic s wave pairing) and the third term in equation (3) responsible for extended s-wave pairing will be omitted from further discussion.

In deriving equations (2), (3) we have taken into account attractions only along the x and y axis neighbours. However, such attractive interaction between the fourth neighbours also gives rise to an unconventional d-wave pairing channel, the pair potential for the fourth neighbour interaction that leads to singlet d-wave pairing may be obtained as,

$$\begin{aligned} V(k, k') = {} & 2V_4(\cos k_x - \cos k_y)(1 + 2\cos k_x \cos k_y)(k \to k') \\ & +2V_4(\cos k_x - \cos k_y)(2\sin k_x \sin k_y)(k \to k') \end{aligned} \qquad (4)$$

where V_4 indicates strength of fourth neighbour attraction.

Thus considering only the d-wave channel one gets the anisotropic pair potential as,

$$V(k,k') = V_1 f_k f_{k'} + 4V_3 f_k f_{k'} g_k g_{k'} + 2V_4 f_k f_{k'}[(1+d_{k_{xy}})(1+d_{k'_{xy}}) + s_{k_{xy}} s_{k'_{xy}}]$$
$$+16V_6 f_k f_{k'} \left(g_k^2 - \frac{s_{k_{xy}}}{2} - \frac{3}{4}\right)\left(g_{k'}^2 - \frac{s_{k'_{xy}}}{2} - \frac{3}{4}\right)$$
$$\approx V f_k f_{k'}(1 + g_k g_{k'} + g_k^2 g_{k'}^2) \qquad (5)$$

where we assumed $2V_1 = 4V_3 = 4V_4 = 16V_6$ =V (say) and considered only the appropriate contributing terms in V_4 and V_6 that lead to the gap structure in equation (1) (in deducing the second result of equation (5)). In equation (5) V_1, V_3, V_4, V_6 represents strength of attraction between the first, third, fourth, sixth neighbours respectively and the momentum form factors are $d_{k_{xy}} = 2\sin k_x \sin k_y$, $s_{k_{xy}} = 2\cos k_x \cos k_y$, $f_k = \cos k_x - \sin k_x$, $g_k = \cos k_x + \cos k_x$, with $f_k^2 = (f_k)^2$ and $g_k^2 = (g_k)^2$. The actual approximations involved to get the second result of the above equation are,

$$2V_4 f_k f_{k'}[(1+d_{k_{xy}})(1+d_{k'_{xy}}) + s_{k_{xy}} s_{k'_{xy}}] \sim \tfrac{V}{2} f_k f_{k'}$$
$$V_6 f_k f_{k'}(4g_k^2 - 2s_{k_{xy}} - 3)(4g_{k'}^2 - 2s_{k'_{xy}} - 3) \sim 16V_6 f_k f_{k'} g_k^2 g_{k'}^2. \qquad (6)$$

This approximation is considered just to retain the form of the gap structure (1), however, the full form of the potential, the first result of equation (5) will also be explicitly used. It turns out that the full potential leads to results very close to that obtained in the spin fluctuation theory whereas the form in equation (1) is just an artifact of the approximations used in [9].

We shall show now that the pair-potential in the second result of equation (5) can produce the gap symmetry of the spin fluctuation theory given in equation (1) up to the third order term i.e., $\Delta(k) = \Delta(0) f_k(1 + g_k + g_k^2)$. (Note, in a weak coupling BCS theory one would tend to think of a potential, $V(k,k') = V F_k F_{k'}$, where $F_k = f_k(1 + g_k + g_k^2)$ should be essential to produce the above gap symmetry.) Supposing the pair-potential in the second result of (5) does produce the gap symmetry in (1) up to the third order term, we insert the pair potential (the second result of equation (5)) and the corresponding gap function into the BCS gap equation, $\Delta(k) = \sum'_k (E_{k'})^{-1} V_{k,k'} \Delta(k') \tanh(\beta E_{k'}/2)$. Then comparing the k-dependence from both sides of the gap equation one gets the required gap equation that produces the approximated spin fluctuation (ASF) gap symmetry is obtained as,

$$\Delta(0) = \sum_{k'} (V/3) F_{k'}^2 \frac{\Delta(0)}{2E_{k'}} \tanh\left(\frac{\beta E_{k'}}{2}\right). \qquad (7)$$

This is exactly the gap equation one would find using the pair potential $V(k,k') = V F_k F_{k'}$ which certainly produces the required gap symmetry $\Delta(k) = \Delta(0) f_k(1+g_k+g_k^2)$ (the pair vertex in (7) is only renormalized to $V/3$). The symbols in equation (7) have their usual meanings with the superconducting quasiparticle energy given by, $E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta^2(k)}$, μ is the chemical potential which controls the band filling with the help of a number conserving equation. The temperature dependence of the chemical potential is taken care of in the self-consistent numerical solutions of the gap equation. We use the band dispersion ϵ_k obtained from the angle resolved photoemission experiment by Norman *et al* [14] for the Bi-based cuprates. The dispersion gives experimentally measured hopping amplitudes up to fifth neighbours which is plausible in the present calculation since further neighbours attractive pairing interaction is considered.

Following the same principle as deriving equation (7) we get the gap equation for the higher anisotropic d-wave (HAD) symmetry $\Delta(k) = \Delta(0)[f_1(k) + f_3(k) + f_{4a}(k) + f_{4b}(k) + f_6(k)]$ using the full potential i.e., the first result of the equation (5) as,

$$\Delta(0) = \sum_{k'} (V/5) \tilde{F}_{k'}^2 \frac{\Delta(0)}{2E_{k'}} \tanh\left(\frac{\beta E_{k'}}{2}\right) \qquad (8)$$

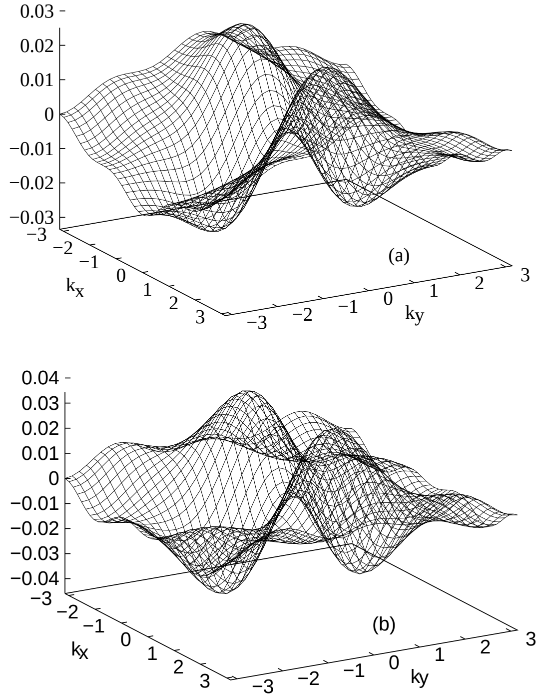

Figure 1. Momentum dependence of the superconducting energy gap function which has symmetry of that of the approximate spin fluctuation (ASF) theory (up to third order in (1)). The required attractive potential is derived within the approximation (6) (a). Note the strong resemblance of this gap structure with that obtained by Lenck and Carbotte (cf. figure 1 of [13]). This higher anisotropic d-wave gap function yields a $2\Delta(k)_{max}/k_BT_c = 6$ where the $\Delta(k)_{max}$ is not at $(k_x, k_y) = (0, \pm\pi)$ but around $(0, \pm 1.57)$. (b) Momentum dependence of the superconducting energy gap function when the attractive potential is derived exactly without the approximation (6) leading to higher anisotropic d-wave (HAD) symmetry. Contrast, the deviation in the gap structure due to the approximation (6) in (a). These gap structures (a, b) are indeed consistent with that obtained by Lenck and Carbotte (cf. [13]). The exact HAD symmetry gap structure (b) although it has similar structure to ASF symmetry, the gap becomes more sharply peaked in different k directions. Unlike the simplest d-wave its maximum occurs around $(0, \pm 1.41)$ which yields a $2\Delta(k)_{max}/k_BT_c = 8.15$, the value very much consistent with the original spin fluctuation model [9]. The parameter V is adjusted such that both the gap functions have the same bulk $T_c = 84$ K at the band-filling $\rho = 0.8$. Undoubtedly, these gap structures are quite different from the *lowest order* usual d-wave symmetry usually considered in the literature.

where $\tilde{F}_k = f_1(k) + f_3(k) + f_{4a}(k) + f_{4b}(k) + f_6(k)$ with $f_1(k) = (1/\sqrt{2}) f_k$, $f_3(k) = f_k g_k$, $f_{4a}(k) = (1/\sqrt{2}) f_k (1 + s_{k_{xy}})$, $f_{4b}(k) = (1/\sqrt{2}) f_k d_{k_{xy}})$, $f_6(k) = f_k (g_k^2 - s_{k_{xy}}/2 - 3/4)$. Now, we present our numerical results in figures 1 and 2, for a fixed cut-off frequency $\Omega_c = 500$ K. The bulk T_c in all the figures is fixed at $T = 84$ K for the band filling $\rho = 0.8$, which required a change in V in the superconducting gap equations (7) (8) and the same for the usual d-wave. In figures 1(a), (b) we present the k-anisotropy of the gap function in the first Brillouin zone for k_x, k_y, which clearly produces d-wave like solution i.e., nodal lines along $k_x = k_y$ directions as well as change in the sign of the gap function. However, the overall anisotropy is very different from the simplest *lowest order* d-wave ($\Delta(k) = \Delta(0)(\cos k_x a - \cos k_y a)$) form—but rather a *higher anisotropic d-wave*. Figure 1(a) represents momentum anisotropy for the ASF model

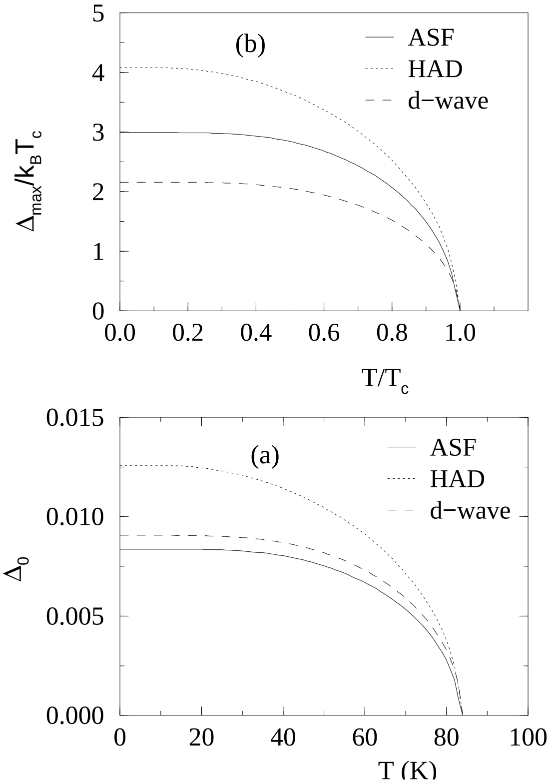

Figure 2. (a) Variation of the gap amplitude ($\Delta(0)$ in eV, see equations (1), (7), (8)) as a function of temperature in Kelvin. Note, the amplitude $\Delta(0)$ for the usual d-wave and the ASF (under approximation (6)) is almost the same whereas the HAD (without the approximation (6)) is quite different. The gap opens up very fast below T_c in the HAD case. (b) The BCS characteristic ratio $\Delta(k)_{max}/k_BT_c$ as a function of T/T_c in different models. The solid curve represents the result for the derived approximated spin fluctuation (ASF) symmetry within the approximation (6); the maximum of the gap opens up at a faster rate than the d-wave below T_c. The dotted line corresponds to the HAD symmetry when no approximation (6) is included; this maximum gap has the fastest growth with lowering in temperature below T_c. The dashed curve corresponds to a usual *lowest order* d-wave. Therefore, the special momentum anisotropic form in the spin fluctuation theory (Monthoux *et al* 1991 *Phys. Rev. Lett.* **67** 3448) is one of the crucial ingredients for such a high BCS characteristic ratio. (All the curves in the figure correspond to $T_c = 84$ K at the band filling $\rho = 0.8$.)

using gap equation (7) whereas the figure 1(b) represents the HAD symmetry using the gap equation (8). The HAD symmetry gap has sharper k-anisotropy than the ASF model although there exists overall similarity between the two, namely, the positions of maximum gap are very close. Since the calculation of Lenck and Carbotte [13] does not assume any form of the superconducting gap function and also does not include the retardation effect as in the original spin fluctuation model [9], we can therefore certainly rely on comparing our results with those of Lenck and Carbotte. A close comparison of our results with those of [13] will conclusively demonstrate that the pair potential derived with distant neighbours attraction in the d-wave channel in the present model *does* produce the gap symmetry of the spin fluctuation theory [9]. The present calculation thus may indicate that the phenomenological spin fluctuation theory includes longer range interaction which might be derivable from a generalized interaction (2).

In figure 1, the gap function shows more than one maximum (minimum) at the edges of the Brillouin zone, very similar to that obtained in [13]. The maximum (minimum) is also displaced from the usual position $((0, \pm\pi), (\pm\pi, 0))$ in the simplest d-wave (cf. figure 1 and the caption). Remarkably, this gap symmetry also produces a high value of $2\Delta(k)_{max}/k_BT_c = 6$ the same as that obtained in [13] (cf. figure 2(b)). In figure 1(b) where we present the same as in figure 1(a) but without the approximation (6) the BCS characteristic ratio $2\Delta(k)_{max}/k_BT_c = 8.15$. These are values close to typical of what is known for high-T_c systems [9]. Note, however, there may exist some differences between the two (work [13] and this one) in details because the band dispersions used in the two calculations are different which does affect pairing symmetry.

Having discussed in detail the difference in the k-anisotropy of the (higher anisotropic d-wave) HAD symmetry with that of the usual d-wave and that such symmetries *do* reproduce the gap structure of the spin fluctuation theory, we now show explicitly in figures 2(a), (b) that due to strong anisotropy such gaps have different thermal behaviour in comparison to the usual d-wave which is principal cause for high value of $2\Delta(k)_{max}/k_BT_c$. In figure 2(a) the amplitudes of higher anisotropic d-wave symmetries (with and without approximation (6)) and that of the simple d-wave are displayed as a function of temperature (T)—all of them have $T_c = 84$ K at a band-filling $\rho = 0.8$. In figure 2(b) we pick up the temperature dependencies of the maximum gap of the three d-wave symmetries the same as in figure 2(a) and display the $\Delta(k)_{max}/k_BT_c$ as a function of the reduced temperature T/T_c. The gap opens up below T_c at the fastest rate for the HAD symmetry and at the slowest rate for the usual d-wave as the temperature is lowered.

Finally, to summarize, we have derived a pair potential from further neighbours attraction in the tight binding scenario which produces gap symmetry of the phenomenological spin fluctuation theory. This study may particularly be justified from the fact that in models of spin fluctuation mediated d-wave superconductivity an increase in the antiferromagnetic correlation length occurs with underdoping. Such an effect has also been realized very recently from angle resolved photoemission (ARPES) experiment by a well known group [16]. One of their principal observations is as the doping decreases the maximum gap increases, but the slope of the gap near the nodes decreases. This feature although consistent with d-wave symmetry cannot be fit by the simplest d-wave form of the gap but to a more generalized $B(\cos k_x - \cos k_y) + (1 - B)(\cos 2k_x - \cos 2k_y)$ where B is a fitting parameter. (Needless to say, in the present work consideration of only the first two terms of the first result in equation (5) i.e., first and third neighbour interactions exactly reproduces this symmetry). This led them to suggest the importance of longer range interaction in the theory of d-wave superconductivity as one approaches the insulator. It is worth pointing out that such ARPES experiments in the underdoped regime measure the pseudo-gap rather than the truly superconducting gap. In the present calculation, a close look to the dispersion used in equations (7), (8) will indicate that the Fermi surface (FS) is open in a certain direction i.e., the FS is gapped due to a pseudo-gap. However, if the pseudo-gap could be ascribed to fluctuation effects of the order parameter, then its value could be estimated by the mean-field BCS equation, while the truly superconducting transition can be estimated only by calculations that include fluctuation effects. We thus created an example that there exists in nature a pair potential (as we derive from real space) analogous to the spin fluctuation theory which is one of the leading potential theories in high temperature superconductors, despite the fact that the principal philosophy of the spin fluctuation is different. We thus emphasized, the importance of inclusion of further neighbour attraction in the usual d-wave theories as is also realized in the most recent experiment [16]. The Cu–O systems being in a complicated circuit, the effect of Coulomb repulsion may not be adequately treated with only on-site repulsion and therefore, effective attractive potential may be achieved only after considering more distant neighbour terms. With this calculation we also emphasized the role of gap anisotropy in BCS gap ratio which may be further improved adopting a strong coupling approach [15]. The higher anisotropic d-wave symmetry as obtained in this work will certainly be consistent with experimental studies in cuprates because of its similarity with d-wave but will have the advantage of avoiding Coulomb repulsion. We believe, this work along with [9, 12, 13, 16] will provide new insight to the usual d-wave theories of superconductivity.

The author thanks Sreekantha Sil for stimulating communications and useful comments via electronic mail on the subject. This work was partly supported by the Brazilian Funding Agency FAPERJ, project No E-26/150.925/96-BOLSA.

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