Phase transition between \(d\)-wave and anisotropic \(s\)-wave gaps in high temperature oxides superconductors

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We study models for superconductivity with two interactions: \(V^>\) due to antiferromagnetic(AF) fluctuations and \(V^<\) due to phonons, in a weak coupling approach to the high temperature superconductivity. The nature of the two interactions are considerably different; \(V^>\) is positive and sharply peaked at \((\pm \pi, \pm \pi)\) while \(V^<\) is negative and peaked at \((0, 0)\) due to weak phonon screening. We numerically find (a) weak BCS attraction is enough to have high critical temperature if a van Hove anomaly is at work, (b) \(V^>\) (AF) is important to give \(d\)-wave superconductivity, (c) the gap order parameter \(\Delta(k)\) is constant \((s\)-wave) at extremely overdope region and it changes to anisotropic \(s\)-wave as doping is reduced, (d) there exists a first order phase transition between \(d\)-wave and anisotropic \(s\)-wave gaps. These results are qualitatively in agreement with preceding works; they should be modified in the strongly underdope region by the presence of antiferromagnetic fluctuations and ensuing AF pseudogap.

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One of the most significant works in recent condensed matter physics is undoubtedly the discovery of high \(T_c\) copper oxides [1]. It seems the high value of \(T_c\) can not be understood by the ‘classical’ BCS theory [2], a large amount of experimental and theoretical works have been performed. In fact, quite a few number of high \(T_c\) superconductors(HTSC) are found.

A phase diagram with doping and temperature is very rich, with the antiferromagnetic ordered phase, the superconductive phases – underdope and overdope –, a pseudogap region as well as a ‘normal’ metallic range. Electron doped compounds show a similar succession of AF, superconductive and normal metallic phases, with lower critical temperatures. It is notable that, in common with the classical BCS case, the superconductive state occurs through a condensation of cooper singlet pairing \((\mathbf{k} \uparrow, -\mathbf{k} \downarrow)\).

Currently there are many works that ignore phonon-mediated interactions and, in many cases, van Hove anomaly altogether. In these studies one considers mostly interaction due to AF fluctuations. The main justification for these approaches is that the energy scale for magnetic interaction is \(\approx 1000K\) which is somewhat larger than the Debye temperature of \(\approx 300K\). In fact, the solutions of the gap equation with only positive interaction due to AF fluctuations gives \(T_c \approx 100K\) [3,4] which is consistent with the experimental results. However it is not surprising since \(T_c\) varies a lot depending on the coupling constants.

On the other hand there are a number of works [5,6] which show enhancement of \(T_c\) due to a van Hove anomaly. In most of these investigations, the main purpose is to obtain high critical temperature which is consistent with the \(T_c\) observed at optimal doping. Therefore almost all the works except ref.[6] assume that a van Hove anomaly is on the Fermi surface at optimal doping. In this way the decrease of \(T_c\) from the optimal as doping is increased or decreased is natural. However, the systematic computation of doping dependence has not been done. A potentially serious problem of these approaches is that antiferromagnetic (AF) fluctuations which should be important in the underdoped region are not taken into account.

Recently, Friedel and Kohmoto [4] consider the case where the van Hove anomaly is at ‘Fermi level’ for undoped(half-filling). Besides phonon mediated interaction, one from AF fluctuations is considered. Indeed, it was shown the AF instabilities decrease faster with increasing doping than the effect of the van Hove anomaly on superconductivity [2]. They argue the followings: Phonon or electron mediated weak BCS attraction is enough to have high critical temperature if a van Hove anomaly is at work near enough to the Fermi level. This could apply to electron doped compounds and also to compounds with CuO\(_2\) planes overdope in holes, where \(T_c\) decreases with increasing doping. If phonons dominate, it should lead to an anisotropic but mainly \(s\) superconductive gap and probably also in electron doped compounds. A \(d\) gap should develop as observed in a number of cases if AF fluctuations are strong enough. In the underdope range, the observed decrease of \(T_c\) with hole doping can be related in all cases to the development of antiferromagnetic fluctuations which produces a magnetic pseudogap, thus lowering the density of states at the Fermi level. The observed mainly \(d\) superconductive gap then can be attributed to antiferromagnetic fluctuations.

The essential feature of the BCS theory is the pairing picture. This has been well established in the ‘classical’ superconductors. Also there is almost no sign of breakdown of this picture in HTSC. However, in order to obtain the so called ‘BCS formula’, one needs
the approximations: (a) The pairing interaction is weak, (b) The density of states is not too fast varying near the Fermi surface, (c) The pairing interaction is constant within the cutoffs ±k_BT_D near the Fermi surface and zero otherwise. These approximations lead to the BCS formula: 
\[ T_c \approx 1.13k_BT_D\exp\left\{-1/N(0)V\right\}, \]
\[ \Delta(T = 0)/k_BT_c \approx 1.75, \]
the universal specific heat jump at \( T_c \), the isotope effect with exponent \( \alpha = 1/2 \) etc.

We assume (a) throughout this work, but (b) is certainly not appropriate as shown below. There is a large enhancement of the density of states close to the van Hove anomalies. The approximation (c) is oversimplified and will be replaced by weakly screened phonon mediated interaction, by AF repulsive interaction, and in addition by both. Therefore we expect that the BCS formula can be violated in experiments, even if the BCS theory with a singlet pairing is correct.

In order to examine the above ideas, we consider a model on the square lattice with specific interactions between electrons and solve the gap equation for general values of hole doping. The effects of pseudogap are not taken into account nor the correction due to the small couplings between CuO_2 planes and the ensuing fluctuations of superconductivity near \( T_c \). Then \( T_c \) keeps rising while doping decreases. This contrasts with the behavior of HTSC whose \( T_c \) decreases and eventually vanishes in underdope region.

The high \( T_c \) oxides have a square lattice of Cu atoms and O atoms in between the Cu atoms (here we neglect the orthorombic distortion which exists for some HTSC). We take an effective tight-binding picture to consider the Cu sites only, then with effective transfer \( t \), we have the following results.

For undoped compounds, the Fermi level is then a square. Doping by electrons and by holes produce almost square Fermi surfaces with nearly symmetric deviations from the undoped square surface. This fundamental symmetry between electron and hole dopings fits well the general symmetry of the phase diagram observed for electron and for hole doped compounds.

As a result of this geometry the Fermi level sits also near a strong peak in the density of states, which diverges logarithmic at \( (\pm \pi, 0) \), \( (0, \pm \pi) \) for the undoped compounds. This van Hove anomaly is characteristic of the (quasi) two-dimensional compounds, where it is much stronger than in more isotropic 3d compounds.

The kinetic part of the square lattice model with only nearest-neighbor hopping can be written \( \varepsilon(k) \approx -2t(\cos k_x + \cos k_y) \) where the transfer \( t \) is typically 0.25eV and energy will be measured in units of \( t \) from now on. In this energy dispersion, there are two saddle points which lead to the van Hove singularities at \( (\pm \pi, 0) \) and \( (0, \pm \pi) \). The gap equation is

\[ \Delta(k) = -\frac{1}{2} \sum_{k'} V_{kk'} \Delta(k') \tanh\left(\frac{E_{k'}}{2k_BT}\right) \frac{1}{E_{k'}}, \]

where \( \Delta(k) \) is the gap order parameter, \( V_{kk'} \) is the interaction between electrons, and \( E_k = \sqrt{\left[\varepsilon(k) - \mu\right]^2 + \Delta(k)^2} \) where \( \mu \) is the chemical potential.

- **BCS isotropic interaction** \( V_{kk'} = \text{const.}(= -3t < 0) \). In the overdope range one can reasonably neglect the effects of AF fluctuations in the ‘normal’ metallic range. A high critical temperature \( T_c \) can then be obtained in the mean field BCS approximation.

The critical temperature is plotted in Fig. 1 for weak coupling region where \( N|V| \leq 0.3 \) where \( N \) is DOS near the bottom of the band. At the bottom of the band \( T_c \approx 10K \) which is quite reasonable for weak coupling BCS theory. It has an exact particle-hole duality. In the extremely overdope region, the BCS prediction is well satisfied because DOS is not so fast varying within the cutoffs. This is no longer true for lower dopings where DOS is larger and changes rapidly. The enhancement of \( T_c \) is considerable there, about 150K at undoped. The gap is s-wave since the interaction is constant. This result shows that weak BCS interaction is enough to have high \( T_c \).

We stress that this enhancement of \( T_c \) is only induced by the DOS effect. The coupling does not play any role. It seems that it is not totally unrealistic to expect extremely high \( T_c \) like room temperature. However, there exist AF effects near undoped in the all known high \( T_c \) superconductors. It is likely to suppresses \( T_c \).

![Critical temperature plot](image)

**FIG. 1.** Critical temperature \( T^\mu_c \) vs chemical potential for BCS attractive interaction \( V_{kk'} = -3t < 0 \).

- **Weakly screened phonon-mediated interaction** \( V^<_{kk'} \).

Let us consider the interaction

\[ V^<_{kk'} = -\frac{|g_q|^2}{|q|^2 + |q_0|^2}, \]

where \( q = k - k' \), \( g_q \) is the electron-phonon coupling and \( 2\pi/k_0 \) is the screening length. This type of phonon contribution is used in ref.[8-9]. We take a large screening radius about 30 lattice spacing because of poor 2d
screening. The sign of $V_{k,k'}^<$ is always negative.

Critical temperature is displayed in Fig. 2. The gap $\Delta(k)$ now has an extended $s$-wave symmetry near half-filling. The new feature is that the gap not only depends on the angle of $k$ but also on the absolute value $|k|$ considerably being maximum at Fermi level. See Fig. 2(a),(b), and (c). Possibility of this phenomena has not been considered seriously in the past. In most of the previous works on superconductivity, $\Delta(k)$ is computed for $k$ at the Fermi level.

A notable feature is that $T_c$ does not decrease by doping very much. In this region it is very hard to have pure HTSC samples. Thus it is likely that our results do not apply. For extremely doped region we have also high $T_c$ superconductivity. This behavior will be discussed elsewhere [1].

**FIG. 2.** Critical temperature $T_c$ of weakly screened phonon-mediated interaction ($V_{k,k'}^< = -|q_0|^2/(q_0^2 + q_0^2)$), and polar plot of gaps at $T = 0$ for (a) $\mu = -3.6$ (extended isotropic $s$-gap), (b) $\mu = -2.0$ (slightly anisotropic $s$-gap), and (c) $\mu = -0.2$ (anisotropic $s$-gap). The distance from origin is the amplitude of gap for a given angle $\theta = \tan^{-1}(k_y/k_x)$. (d) (1)$\Delta(0)_{\text{max}}/k_BT_c$, and (2)$\Delta(0)_{\text{ave}}/k_BT_c$ vs $\mu$.

--AF fluctuation mediated interaction $V^>$. There are a number of attempts to obtain high $T_c$ within the weak coupling BCS theory only from repulsive interactions which are originated from AF fluctuations [3,4]. Here we take the form of interaction by Monthoue et al. [3] This interaction has peaks at $(\pm \pi, \pm \pi)$. We, however, take much weaker coupling about 1/10 compared with one used by Monthoue et al. [3] (The peak value of their interaction is about 80eV). We obtain relatively low $T_c$ ($T_c \sim 30K$ at undoped) and it vanishes at doping $c \sim 0.1$. The result obtained by using the coupling of ref.[4] is also confirmed.

This contrasts with attractive interaction which always give superconductivity at low temperature for all doping. The gap is always $d$-wave for this type of repulsive interaction [10]. Also we do not obtain a gap which breaks the square symmetry like the one studied by ref.[12] even in low temperatures.

--The two types of interaction $V^> + V^<$. Finally we take both interactions into account. The two interactions do not cancel directly since $V^>$ has peaks at $(\pm \pi, \pm \pi)$ and $V^<$ at $(0,0)$. In any event, the peak of $V_{k,k'}^>$ is fixed at $(\pm \pi, \pm \pi)$ and the effect of the interaction near Fermi level strongly depends on doping. On the other hand $V_{k,k'}^<$ does not so much depend on doping. Thus the relative strength of the two interactions changes with doping.

The results are shown in Fig. 3. In case both $s$ and $d$ gap can comprise the (mixed) solution of gap equation for a given point $(\mu, T)$ in phase space, the gap function is chosen as the one which has the lower free energy. A notable feature is that, although $V^>$ is not more effective for superconductivity, it is very effective for $d$ wave gap. We find a first order transition line between $d$ and anisotropic $s$-wave gap. The latent heat is also displayed in Fig.3(d). There are experimental results which show a nodeless HTSC [13,14].

**FIG. 3.** Critical temperatures $T_c$ and the first order phase transition line (dotted line) for the interaction $V^> + V^<$, and polar plot of gaps at $T = 0$ for (a) $\mu = -3.6$ (extended isotropic $s$-gap), (b) $\mu = -1.0$ (anisotropic $s$-gap), and (c) $\mu = -0.2$ (d-gap). (d) is the latent heat across the first order transition line. (e) (1)$\Delta(0)_{\text{max}}/k_BT_c$, and (2)$\Delta(0)_{\text{ave}}/k_BT_c$ vs $\mu$.

The quantity $|\Delta(0)|_{\text{max}}/k_BT_c$ takes the usual BCS value about 1.75 for isotropic region (See Fig.3(e1)). In the anisotropic region it is larger and about 2.5 which is not surprising because the gap is anisotropic and even has nodes in $d$-wave cases. This ratio with $|\Delta(0)|_{\text{ave}}$ averaged over $k$ is also plotted in Fig.3(e2).

Our model has the particle-hole symmetry, thus we expect that the electron-doped compounds have similar gap structure. Mostly $s$-gap reported may be anisotropic and there may be a region of $d$-wave pairing in underdope region [15].

We also find a novel scaling relation: Namely, the absolute value of average gap function $|\Delta(T)|$ as a function of $T$ for different chemical potentials can be collapsed into
a universal curve by

\[ 1 - \frac{|\Delta(T)|}{|\Delta(0)|} = f(t/t_{\text{char}}) \tag{3} \]

where \( t = 1 - T/T_c \) is the reduced temperature and \( t_{\text{char}} \) is the characteristic reduced temperature for the decay of \( 1 - |\Delta(T)|/|\Delta(0)| \) as \( t \) increases for different chemical potentials, and \( f \) is a universal scaling function. Figure 4 shows a good scaling collapse of the rescaled gap functions in terms of \( t/t_{\text{char}} \) for different chemical potentials. We observe that \( |\Delta(T)| \) decreases as \( T \) increases by one fashion for \( \mu \) below \(-1.4\) and by the other fashion for \( \mu \) above \(-1.4\) (See fig.4(a)). In fact Fig.4(b) shows that there are two different scaling functions for \( \mu \) below and above \(-1.4\) at which \( T_c \) becomes minimum. This universal scaling does not apply for the region of first order phase transition.

To conclude, the presence of totally different types of interactions can be expected to lead to rich physics.

We find that the phonon-mediated interaction is enough to have high temperature superconductivity. The role of AF fluctuation is to have the d-wave gap. More importantly it gives the AF pseudogap which we do not take into account by technical difficulties. Probably the most important prediction is the existence of the first order phase transition between d and anisotropic s gaps which may be tested in experiments with clean samples in the overdope region.

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